

## Supporting information for:

### Dendrimers with both Polar and Apolar Nanocontainer Characteristics

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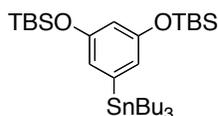
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#### Experimental Section:

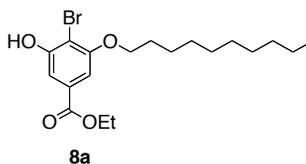
<sup>1</sup>H-NMR spectra were recorded on a 400 MHz or 300 MHz NMR spectrometer using the residual proton resonance of the solvent as the internal standard. Chemical shifts are reported in parts per million (ppm). When peak multiplicities are given, the following abbreviations are used: s, singlet; d, doublet; t, triplet; q, quartet; quin, quintet; d of d, doublet of a doublet; m, multiplet; br, broad. <sup>13</sup>C-NMR spectra were proton decoupled and recorded on a 100 MHz or 75 MHz NMR spectrometer using the carbon signal of the deuterated solvent as the internal standard. MALDI-ToF, EI and FAB mass spectra were obtained at the Coordinated Instrumentation Facility at University of Massachusetts. Flash chromatography was performed with 37-75 μm silica gel. Analytical thin layer chromatography was performed on silica plates with F-254 indicator and the visualization was accomplished by UV lamp or using an iodine chamber. THF was distilled over Na/Ph<sub>2</sub>CO ketyl. Dichloromethane was distilled over CaH<sub>2</sub>. All other chemicals were obtained from commercial sources and used as received, unless otherwise mentioned. 1-Bromo-3,5-bis-(*tert*-butoxy-dimethyl-silyloxy)-benzene and Ethyl-4-bromo-3,5-dihydroxybenzoate were synthesized previously in our laboratories (please see reference number 5 in the main text.)

#### Synthesis of compound (7):

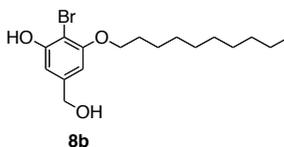


7

To a solution of 1-bromo-3,5-bis-(*tert*-butoxy-dimethyl-silyloxy)-benzene (4.2 g, 10 mmol) in anhydrous THF (60 mL) was added *n*-BuLi (8.12 mL of 1.6 M hexane solution, 13 mmol) under argon atmosphere at -78 °C and stirred for 30 min at that temperature. The Bu<sub>3</sub>SnCl (4.0 mL, 14.8 mmol) was added and stirred at -78 to 20 °C for 12 h. The reaction was quenched with water and extracted with diethyl ether. The solvent was removed under reduced pressure to afford the crude reaction mixture, which was purified by column chromatography (SiO<sub>2</sub>, hexanes) to afford 5.60 g (90%) of product as viscous oil.

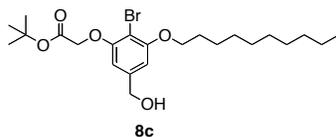
**Synthesis of compound (8a):**

Ethyl-4-bromo-3,5-dihydroxybenzoate (26.1 g, 100 mmol), potassium carbonate (13.8 g, 100 mmol), 18-Crown-6 (1.3 g, 5 mmol) and decyl iodide (17 mL, 80 mmol) were taken in 500 mL of acetone and refluxed for 10 h under argon atmosphere. The reaction mixture was allowed to cool and solvent was evaporated to dryness. The residue was partitioned between water and dichloromethane. The organic layer was separated, the aqueous layer extracted with dichloromethane. The combined organic layer was washed with brine and dried with anhydrous Na<sub>2</sub>SO<sub>4</sub> and evaporated to dryness. The residue was purified by silica gel column by eluting with CH<sub>2</sub>Cl<sub>2</sub>/hexane (80:20) to afford 16.0 g (39%) of **8a** as a colorless solid. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.34 (d, *J* = 1.2 Hz, 1H), 7.12 (d, *J* = 1.6 Hz, 1H), 6.20 (s, 1H), 4.37 (q, *J* = 7.2 Hz, 2H), 4.06 (t, *J* = 6.4 Hz, 2H), 1.87-1.80 (quin, 2H), 1.52-1.27 (m, 17H), 0.88 (t, *J* = 6.8 Hz, 3H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  166.0, 155.9, 153.3, 130.7, 109.3, 105.5, 105.1, 69.4, 61.3, 31.8, 29.49, 29.26, 29.23, 28.92, 25.8, 22.6, 14.19, 14.05; GC/MS (*m/z*, r.i): 402 (M<sup>+</sup>, 4), 261 (97), 259 (100), 231 (25), 216 (21), 187 (10), 160 (2), 110 (4), 79 (6), 71 (7), 55 (46).

**Synthesis of compound (8b):**

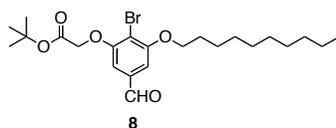
The ester **8a** (16.0 g, 39.2 mmol) was taken in dry THF (100 mL) and cooled to 0 °C. To this 2.0 M solution of (CH<sub>3</sub>)<sub>2</sub>S.BH<sub>3</sub> (118 mL, 235.0 mmol) was added under argon atmosphere dropwise for 30 min. The reaction mixture was allowed to stir at room temperature and further refluxed for 36 h. The reaction mixture was slowly added to a cold solution of 2N HCl and extracted with ethyl acetate. The organic layer was washed with brine solution and concentrated under reduced pressure to afford the crude mixture, which was purified by column chromatography (SiO<sub>2</sub>, 5% EtOAc in dichloromethane) to afford 12.6 g (87%) of product **8b**. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  6.65 (s, 1H), 6.51 (s, 1H), 5.66 (s, 1H), 4.62 (s, 2H), 4.02 (t, *J* = 6.4 Hz, 2H), 1.86-1.79 (quin, 2H), 1.52-1.27 (m, 14H), 0.88 (t, *J* = 6.6 Hz, 3H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  156.1, 153.4, 141.8, 106.3, 103.0, 99.0, 69.2, 64.7, 31.8, 29.52, 29.29, 29.04, 25.9, 22.6, 14.0; EI/MS (*m/z*, r.i): 360 (M+2, 22), 358 (M<sup>+</sup>, 22), 217 (100), 140 (5), 110 (5), 83 (4), 57 (8).

### Synthesis of compound (8c):



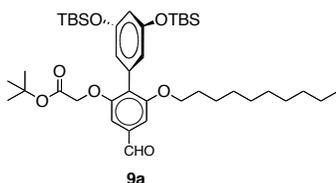
Compound **8b** (10.7 g, 29.2 mmol) was dissolved in acetonitrile (175 mL). To this solution were added,  $K_2CO_3$  (5.4 g, 39 mmol), NaI (4.8 g, 32 mmol) and 18-Crown-6 (0.5 g, 1.92 mmol) followed by *tert*-butyl bromoacetate (4.72 mL, 32 mmol). The reaction mixture was refluxed for 36 h. It was then cooled to room temperature and solvent was evaporated to dryness. The residue was partitioned between water and  $CH_2Cl_2$ . The organic layer was separated, and the aqueous layer was extracted with  $CH_2Cl_2$ . The combined organic layer was dried over  $Na_2SO_4$  and evaporated to dryness. The crude product was purified by silica gel chromatography by elution with EtOAc/hexane (25:75) to afford 11.9 g of compound **8c** (87% yield).  $^1H$ -NMR (400 MHz,  $CDCl_3$ )  $\delta$  6.58 (s, 1H), 6.43 (s, 1H), 4.61 (s, 2H), 4.59 (s, 2H), 4.01 (t,  $J = 6.4$  Hz, 2H), 1.86-1.79 (quin, 2H), 1.48 (s, 9H), 1.46-1.25 (m, 14H), 0.88 (t,  $J = 6.8$  Hz, 3H);  $^{13}C$ -NMR (100 MHz,  $CDCl_3$ )  $\delta$  167.4, 156.8, 155.6, 141.4, 104.7, 103.7, 100.8, 82.4, 69.3, 66.5, 64.9, 31.8, 29.50, 29.28, 29.06, 27.9, 25.9, 22.6, 14.07; EI/MS ( $m/z$ , r.i): 474 ( $M+2$ , 45), 472 ( $M^+$ , 45), 337 (68), 275 (68), 231 (23), 179 (10), 83 (12), 57 (100).

### Synthesis of compound (8):



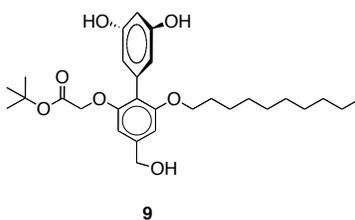
To a stirred solution of compound **8c** (11.8 g, 25.2 mmol) in dichloromethane (150 mL) was added pyridinium chlorochromate (6.54 g, 30.3 mmol). It was stirred at room temperature for 4 h. The reaction mixture was filtered over alumina and the filtrate was evaporated and purified by silica gel chromatography (8% EtOAc in hexanes) to afford 10.7 g of compound **8** (90%).  $^1H$ -NMR (400 MHz,  $CDCl_3$ )  $\delta$  9.87 (s, 1H), 7.05 (d,  $J = 1.6$  Hz, 1H), 6.90 (d,  $J = 1.6$  Hz, 1H), 4.67 (s, 2H), 4.10 (t,  $J = 6.4$  Hz, 2H), 1.9-1.82 (quin, 2H), 1.48 (s, 9H), 0.88 (t,  $J = 6.8$  Hz, 3H);  $^{13}C$ -NMR (100 MHz,  $CDCl_3$ )  $\delta$  190.7, 166.8, 157.4, 156.1, 135.9, 109.6, 106.7, 105.5, 82.7, 69.6, 66.4, 31.8, 29.45, 29.23, 29.19, 28.8, 27.9, 25.8, 22.5, 14.0; EI/MS ( $m/z$ , r.i): 472 ( $M+2$ , 5), 470 ( $M^+$ , 5), 370 (4), 335 (53), 229 (8), 149 (6), 97 (15), 57 (100).

### Synthesis of compound (9a):



Compound **7** (1.27 g, 2.0 mmol) and bromo aldehyde **8** (0.87 g, 1.85 mmol) were dissolved in deoxygenated DMF (4 mL) under argon atmosphere. To this 2 mol% Pd(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub> (0.014 g, 0.02 mmol) was added and the reaction mixture heated at 120-130 °C for 2 days. It was then cooled to room temperature and residue was partitioned between water and CH<sub>2</sub>Cl<sub>2</sub>. The organic layer was separated, and the aqueous layer was extracted with CH<sub>2</sub>Cl<sub>2</sub>. The combined organic layer was dried over Na<sub>2</sub>SO<sub>4</sub> and evaporated to dryness. The crude product was purified by silica gel chromatography by elution with EtOAc/hexane (5:95) to afford 0.78 g of compound **9a** (59% yield). <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  9.90 (s, 1H), 7.13 (s, 1H), 6.96 (s, 1H), 6.50 (d, *J* = 2.0 Hz, 2H), 6.32 (t, *J* = 2.2 Hz, 1H), 4.47 (s, 2H), 3.94 (t, *J* = 6.6 Hz, 2H), 1.68-1.61 (m, 2H), 1.43 (s, 9H), 1.40-1.20 (m, 14H), 0.98 (s, 18H), 0.87 (t, *J* = 6.8 Hz, 3H), 0.18 (s, 12H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  191.5, 167.6, 157.8, 156.4, 155.6, 136.3, 134.2, 126.7, 115.8, 111.3, 107.1, 82.3, 69.06, 65.94, 31.8, 29.55, 29.47, 29.30, 29.25, 28.98, 27.97, 25.79, 25.69, 22.66, 18.19, 14.09, -4.44; FAB/MS (*m/z*, r.i): 729 (M<sup>+</sup>, 45), 673 (85), 560 (20), 446 (15), 74 (100).

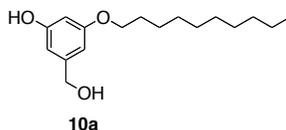
### Synthesis of compound (9):



The biaryl aldehyde **9a** (0.73 g, 1.0 mmol) was dissolved in anhydrous CH<sub>2</sub>Cl<sub>2</sub> (15 mL) under argon atmosphere. To this Tetrabutylammonium borohydride (0.25 g, 1.0 mmol) was added and stirred at room temperature for 12 h. The reaction mixture was quenched with water and extracted with dichloromethane. The organic layer was washed with brine solution and evaporated to dryness. To this crude mixture in THF (10 mL) was added TBAF (2.7 mL of 1.0 M THF solution, 2.7 mmol) and stirred at room temperature for 12 h. Saturated NH<sub>4</sub>Cl was added to the reaction mixture. The aqueous layer was extracted with EtOAc, and the organic layer was concentrated under reduced pressure to afford the crude product, which was purified by column chromatography (SiO<sub>2</sub>, 20% ethyl acetate in dichloromethane) to afford 0.38 g (87% yield) of **9**. <sup>1</sup>H-NMR (400 MHz, CD<sub>3</sub>COCD<sub>3</sub>)  $\delta$  8.03 (s, 2H), 6.69 (s, 1H), 6.53 (s, 1H), 6.34 (d, *J* = 2.0 Hz, 2H), 6.27 (t, *J* = 2.2 Hz, 1H), 4.59 (d, *J* = 5.6 Hz, 2H), 4.43 (s, 2H), 4.27 (t, *J* = 5.8 Hz, 1H), 3.88 (t, *J* = 6.4 Hz, 2H), 1.62-1.54 (m, 2H), 1.41 (s, 9H), 1.34-1.24 (m, 14H), 0.85 (t, *J* = 6.8 Hz, 3H); <sup>13</sup>C-NMR (100 MHz, CD<sub>3</sub>COCD<sub>3</sub>)  $\delta$  168.4, 158.0, 157.7, 156.5, 143.5, 136.8, 119.5, 110.3, 104.7, 103.5, 101.4, 94.1, 81.5, 68.8, 66.1, 64.4, 32.2, 29.70, 29.51, 29.32, 29.13, 28.93,

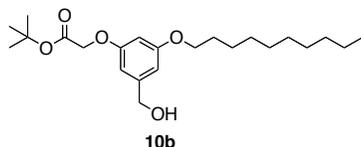
27.82, 26.32, 22.99, 14.03; EI/MS ( $m/z$ , r.i) : 502.3 ( $M^+$ , 20), 446 (40), 279 (40), 167 (45), 149 (100), 89 (30), 69 (45).

#### Synthesis of compound (10a):

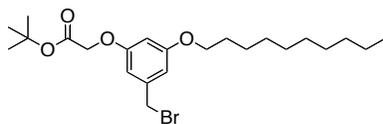


3,5-Dihydroxybenzyl alcohol (21.0 g, 150 mmol), potassium carbonate (20.7 g, 150 mmol), 18-Crown-6 (2.0 g, 7.5 mmol) and decyl iodide (32 mL, 150 mmol) were taken in 750 mL of acetone and refluxed for 12 h under argon atmosphere. The reaction mixture was allowed to cool and solvent was evaporated to dryness. The residue was partitioned between water and ethyl acetate. The organic layer was separated, the aqueous layer extracted with ethyl acetate. The combined organic layer was washed with brine and dried with anhydrous  $\text{Na}_2\text{SO}_4$  and evaporated to dryness. The residue was purified by silica gel column, eluting with EtOAc/hexane (40:60) to afford 13.0 g (31%) of **10a** as a colorless solid.  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  6.48 (s, 1H), 6.43 (s, 1H), 6.32 (t,  $J = 2.0$  Hz, 1H), 4.60 (s, 2H), 3.92 (t,  $J = 6.4$  Hz, 2H), 1.79-1.72 (quin, 2H), 1.45-1.27 (m, 14H), 0.88 (t,  $J = 6.6$  Hz, 3H);  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  160.4, 157.1, 142.7, 106.2, 105.4, 101.2, 68.1, 64.9, 31.8, 29.57, 29.41, 29.31, 29.19, 25.9, 22.6, 14.0; EI/MS ( $m/z$ , r.i): 280 ( $M^+$ , 55), 140 (100), 111 (12), 57 (8).

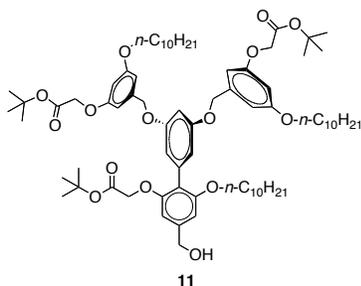
#### Synthesis of compound (10b):



Compound **10a** (11.53 g, 41.1 mmol) was dissolved in acetonitrile (125 mL). To this solution were added,  $\text{K}_2\text{CO}_3$  (6.8 g, 49.3 mmol),  $\text{NaI}$  (6.16 g, 41.1 mmol) and 18-Crown-6 (0.52 g, 2.0 mmol) followed by *tert*-butyl bromoacetate (6.0 mL, 41.1 mmol). The reaction mixture was refluxed for 36 h. It was then cooled to room temperature and solvent was evaporated to dryness. The residue was partitioned between water and  $\text{CH}_2\text{Cl}_2$ . The organic layer was separated, and the aqueous layer was extracted with  $\text{CH}_2\text{Cl}_2$ . The combined organic layer was dried over  $\text{Na}_2\text{SO}_4$  and evaporated to dryness. The crude product was purified by silica gel chromatography by elution with EtOAc/hexane (20:80) to afford 15.9 g of compound **10b** (98% yield).  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  6.54 (s, 1H), 6.47 (s, 1H), 6.39 (t,  $J = 2.2$  Hz, 1H), 4.61 (s, 2H), 4.49 (s, 2H), 3.92 (t,  $J = 6.4$  Hz, 2H), 1.79-1.72 (quin, 2H), 1.49 (s, 9H), 1.44-1.27 (m, 14H), 0.88 (t,  $J = 6.8$  Hz, 3H);  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.9, 160.3, 159.0, 143.4, 106.0, 104.5, 100.5, 82.2, 67.9, 65.5, 64.9, 31.7, 29.48, 29.46, 29.28, 29.22, 29.10, 27.9, 25.9, 22.5, 14.0; GC/MS ( $m/z$ , r.i): 394 ( $M^+$ , 100), 338 (50), 198 (75), 83 (32), 57 (35).

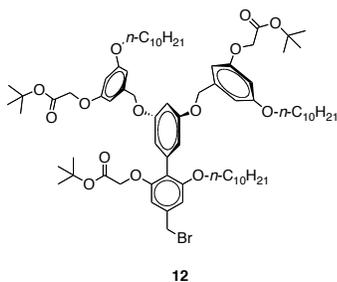
**Synthesis of compound (10):****10**

The alcohol **10b** (1.18 g, 3.0 mmol) was dissolved in dry THF (10 mL) under argon atmosphere. To this  $\text{PPh}_3$  (0.82 g, 3.15 mmol) was added. After 5 min *N*-bromosuccinimide (0.56 g, 3.15 mmol) was added in one portion. After stirring for 1 min, it was quenched with water and extracted with dichloromethane. The organic layer was evaporated to dryness and the residue purified by column chromatography ( $\text{SiO}_2$ , 5% ethyl acetate in hexanes) to afford the product **10**, 1.18 g (87% yield).  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  6.55 (s, 1H), 6.48 (s, 1H), 6.39 (t,  $J = 2.2$  Hz, 1H), 4.49 (s, 2H), 4.39 (s, 2H), 3.91 (t,  $J = 6.4$  Hz, 2H), 1.79-1.27 (m, 25H), 0.88 (t,  $J = 6.8$  Hz, 3H);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  167.6, 160.3, 159.0, 139.5, 108.5, 106.9, 101.5, 82.3, 68.0, 65.6, 33.4, 31.8, 29.47, 29.28, 29.24, 29.0, 27.9, 25.9, 22.6, 14.0; EI/MS ( $m/z$ , r.i.): 458 ( $\text{M}+2$ , 95), 456 ( $\text{M}^+$ , 95), 402 (36), 321 (42), 259 (37), 181 (46), 97 (17), 57 (100).

**Synthesis of compound (11, G1-OH):****11**

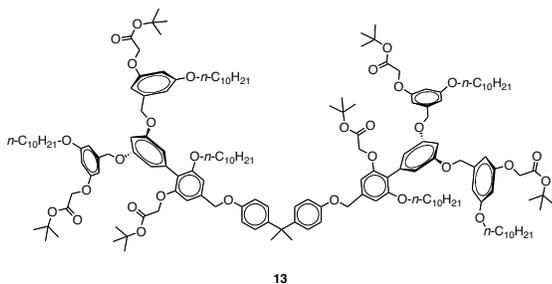
The monomer **9** (0.61 g, 1.23 mmol), potassium carbonate (1.69 g, 12.3 mmol), 18-Crown-6 (0.16 g, 0.61 mmol) and bromomethyl compound **10** (1.18 g, 2.5 mmol) in dry THF (15 mL) were heated at reflux and stirred vigorously under argon atmosphere for 40 h. The mixture was allowed to cool and evaporated to dryness under reduced pressure. The residue was partitioned between water and dichloromethane. The organic layer was separated and the aqueous layer extracted with dichloromethane. The combined organic layers were dried and evaporated to dryness. The residue was purified by silica gel column chromatography by elution with EtOAc/hexane (30:70) to afford 1.27 g (82% yield) of the product **11**.  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  6.70-6.41 (m, 11H), 4.95 (s, 4H), 4.67 (s, 2H), 4.49 (s, 4H), 4.44 (s, 2H), 3.94-3.88 (m, 6H), 1.77-1.20 (m, 75H), 0.90-0.84 (m, 9H);  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  168.1, 167.8, 160.3, 159.0, 158.9, 157.3, 156.0, 141.7, 139.5, 135.5, 119.2, 110.1, 106.8, 105.2, 104.6, 103.4, 101.2, 100.8, 82.2, 81.9, 69.7, 68.7, 67.9, 66.0, 65.6, 65.3, 31.80, 29.49, 29.46, 29.32, 29.25, 29.22, 29.01, 28.92, 27.9, 25.96, 25.91, 22.6, 14.0; MALDI-ToF: Calcd for  $\text{C}_{75}\text{H}_{114}\text{O}_{15}$ : 1254.82; Found: 1277.30 ( $\text{M}^+$ , 23).

### Synthesis of compound (12, G1-Br):



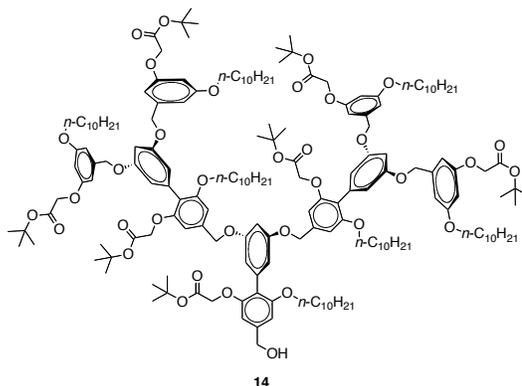
The alcohol **11** (3.25 g, 2.6 mmol) and PPh<sub>3</sub> (0.84 g, 3.23 mmol) were dissolved in dry THF (15 mL) under argon atmosphere. *N*-Bromosuccinimide (0.57 g, 3.32 mmol) was added in one portion. After stirring for 2 min, it was quenched with water and extracted with dichloromethane. The solvent was removed under reduced pressure and the residue was purified by silica gel column by elution with ethyl acetate/hexane (10:90) to afford 3.23 g (95% yield) of the product **12**. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  6.68-6.42 (m, 11H), 4.94 (s, 4H), 4.50-4.44 (m, 8H), 3.94-3.90 (m, 6H), 1.76-1.21 (m, 75H), 0.88-0.84 (m, 9H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  167.8, 167.7, 160.3, 159.0, 158.9, 157.2, 155.9, 139.4, 137.9, 135.1, 120.2, 109.9, 106.9, 106.8, 105.7, 105.2, 101.3, 100.8, 82.1, 82.0, 69.7, 68.7, 67.9, 66.0, 65.6, 33.7, 31.8, 29.49, 29.46, 29.29, 29.22, 29.17, 29.12, 28.9, 27.9, 25.95, 25.91, 22.5, 14.03; MALDI-ToF: Calcd for C<sub>75</sub>H<sub>113</sub>BrO<sub>14</sub>: 1316.73; Found: 1339.26 (M<sup>+</sup>, 23).

### Synthesis of compound (13, G1-dimer):



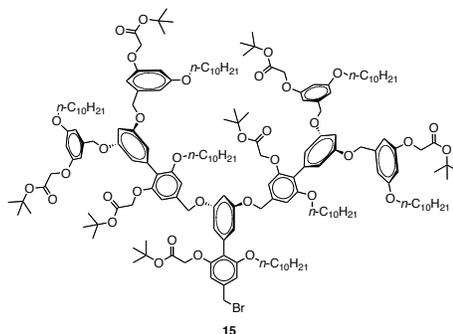
Bisphenol A (0.033 g, 0.14 mmol), potassium carbonate (0.27 g, 2.0 mmol), 18-Crown-6 (0.1 g, 0.4 mmol) and bromomethyl compound **12** (0.43 g, 0.32 mmol) in dry acetone (6 mL) was heated at reflux and stirred vigorously under argon atmosphere for 40 h. The work-up procedure used in the synthesis of **11** was followed. The residue was purified by silica gel column using EtOAc/hexane (15:85) eluent to afford 0.3 g (75%) of the product **13**. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.18-6.41 (m, 30H), 4.98 (s, 4H), 4.94 (s, 8H), 4.49 (s, 8H), 4.43 (s, 4H), 3.93-3.88 (m, 12H), 1.78-1.20 (m, 156H), 0.89-0.83 (m, 18H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  167.9, 167.7, 160.3, 159.0, 158.9, 157.2, 156.5, 155.9, 143.3, 139.4, 137.7, 135.4, 127.6, 119.5, 114.0, 110.0, 106.8, 105.3, 105.1, 104.0, 101.1, 100.8, 82.1, 81.8, 70.0, 69.7, 68.6, 67.9, 66.1, 65.5, 41.6, 31.7, 30.9, 29.46, 29.43, 29.26, 29.20, 29.16, 29.09, 28.93, 27.9, 25.9, 22.5, 14.0; MALDI-ToF: Calcd for C<sub>165</sub>H<sub>240</sub>O<sub>30</sub>: 2701.73; Found: 2722 (M<sup>+</sup>, 23).

### Synthesis of compound (14, G2-OH):



The monomer **9** (0.48 g, 0.96 mmol), potassium carbonate (0.8 g, 5.8 mmol), 18-Crown-6 (0.3 g, 1.16 mmol) and bromomethyl compound **12** (1.18 g, 2.5 mmol) in dry acetone (15 mL) were heated at reflux and stirred vigorously under argon atmosphere for 40 h. The work-up procedure used in the synthesis of **11** was followed. The residue was purified by silica gel column by elution with EtOAc/hexane (20:80) to afford 2.0 g (70%) of the product **14**.  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  6.74-6.41 (m, 27H), 4.98-4.93 (m, 12H), 4.68 (s, 2H), 4.48-4.43 (m, 14H), 3.93-3.88 (m, 14H), 1.78-1.18 (m, 175H), 0.88-0.82 (m, 21H);  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.9, 167.8, 167.7, 160.3, 158.99, 158.92, 157.3, 157.2, 155.9, 141.8, 139.4, 137.7, 135.7, 135.4, 119.5, 119.0, 110.0, 106.8, 105.5, 105.2, 104.6, 104.2, 103.2, 101.1, 100.8, 82.1, 81.87, 81.84, 70.0, 69.7, 68.6, 67.9, 66.1, 66.0, 65.5, 65.1, 31.7, 29.48, 29.44, 29.42, 29.25, 29.18, 29.09, 28.9, 27.8, 25.9, 22.3, 13.9; MALDI-ToF: Calcd for  $\text{C}_{179}\text{H}_{266}\text{O}_{35}$ : 2975.9; Found: 2999.93 ( $\text{M}^+$ , 23).

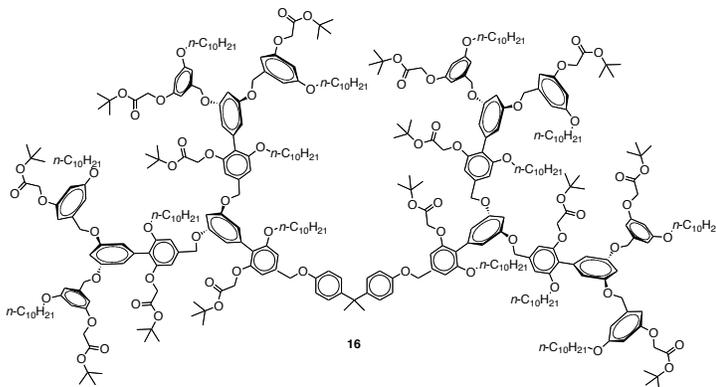
### Synthesis of compound (15, G2-Br):



The alcohol **14** (1.47 g, 0.49 mmol) and  $\text{PPh}_3$  (0.22 g, 0.86 mmol) were dissolved in dry THF (5 mL) under argon atmosphere. *N*-Bromosuccinimide (0.15 g, 0.86 mmol) was added in one portion. After stirring for 2 min, it was quenched with water and extracted with dichloromethane. The work-up procedure used in the synthesis of **12** was followed. The residue was purified by silica gel column using EtOAc/hexane (15:75) eluent to afford 1.31 g (87%) of the product **15**.  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  6.74-6.42 (m, 27H), 4.99-4.95 (m, 12H), 4.49-4.45 (m, 16H), 3.94-3.91 (m, 14H), 1.72-1.20 (m, 175H),

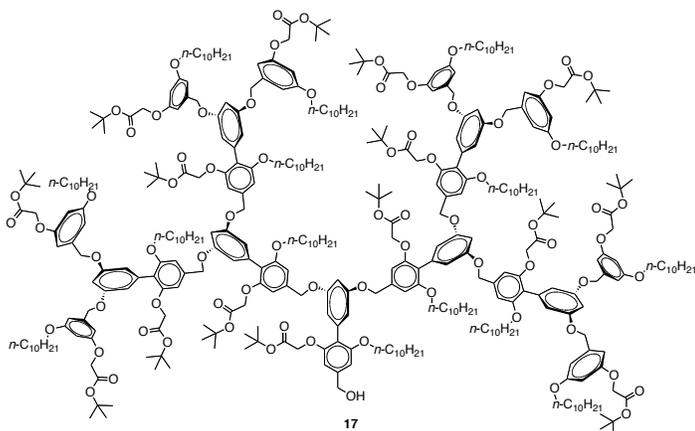
0.88-0.83 (m, 21H);  $^{13}\text{C}$ -NMR (100 MHz,  $\text{CDCl}_3$ )  $\square$  167.6, 167.48, 167.44, 160.1, 158.83, 158.79, 158.71, 157.06, 157.01, 155.73, 155.64, 139.3, 137.9, 137.6, 135.2, 135.1, 119.8, 119.3, 109.9, 106.7, 106.5, 105.5, 105.1, 104.8, 103.9, 101.1, 100.9, 100.5, 81.73, 81.68, 81.51, 69.7, 69.4, 68.4, 67.6, 65.8, 65.7, 65.3, 33.4, 31.6, 31.5, 29.32, 29.28, 29.25, 29.08, 29.01, 28.91, 28.81, 28.77, 27.6, 25.78, 25.74, 22.3, 13.8; MALDI-ToF: Calcd for  $\text{C}_{179}\text{H}_{265}\text{BrO}_{34}$ : 3037.82; Found: 3060.82 ( $\text{M}^+$ , 23).

### Synthesis of compound (16, G2-Dimer):



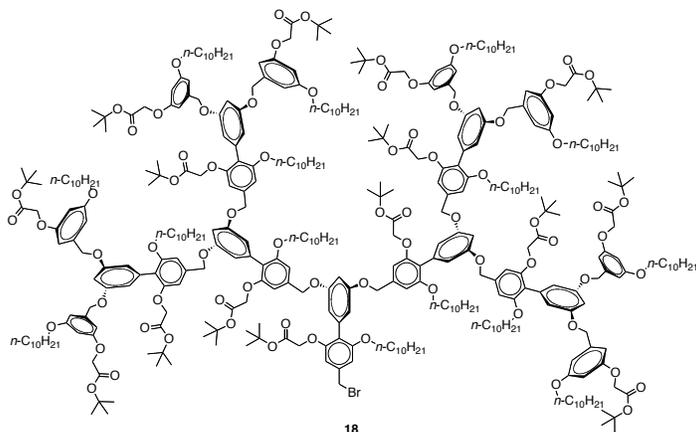
Bisphenol A (0.012 g, 0.054 mmol), potassium carbonate (0.045 g, 0.32 mmol), 18-Crown-6 (0.004 g, 0.016 mmol) and bromomethyl compound **15** (0.41 g, 0.13 mmol) in dry acetone (4 mL) were heated at reflux and stirred vigorously under argon atmosphere for 40 h. The work-up procedure used in the synthesis of **11** was followed. The residue was purified by silica gel column by elution with EtOAc/hexane (20:80) to obtain 0.27 g (80%) of **16**.  $^1\text{H}$ -NMR (400 MHz,  $\text{CDCl}_3$ )  $\square$  7.20-6.41 (m, 62H), 4.99-4.94 (m, 28H), 4.49-4.44 (m, 28H), 3.93-3.89 (m, 28H), 1.78-1.42 (m, 356H), 0.89-0.82 (m, 42H);  $^{13}\text{C}$ -NMR (100 MHz,  $\text{CDCl}_3$ )  $\square$  167.9, 167.8, 160.3, 159.09, 159.05, 159.00, 157.3, 156.6, 156.0, 155.9, 143.4, 139.5, 137.8, 137.7, 135.6, 135.5, 127.7, 119.6, 114.0, 110.1, 106.9, 105.6, 105.4, 105.3, 104.3, 104.2, 101.1, 100.8, 82.2, 82.0, 81.9, 70.1, 69.7, 68.7, 68.0, 66.1, 65.6, 41.7, 31.8, 31.0, 29.52, 29.50, 29.34, 29.26, 29.17, 29.05, 27.9, 25.99, 25.92, 22.6, 14.0; MALDI-ToF: Calcd for  $\text{C}_{373}\text{H}_{544}\text{O}_{70}$ : 6143.9; Found: 6166.9 ( $\text{M}^+$ , 23).

### Synthesis of compound (17, G3-OH):



The monomer **9** (0.064 g, 0.12 mmol), potassium carbonate (0.09 g, 0.64 mmol), 18-Crown-6 (0.009g, 0.03 mmol) and bromomethyl compound **15** (0.85 g, 0.28 mmol) in dry acetone (5 mL) were heated at reflux and stirred vigorously under argon atmosphere for 24 h. The work-up procedure used in the synthesis of **11** was followed. The residue was purified by silica gel column by elution with EtOAc/hexane (20:80) to afford 0.68 g (83%) of the product **17**.  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  6.78-6.41 (m, 59H), 5.01-4.94 (m, 28H), 4.68 (s, 2H), 4.49-4.45 (m, 30H), 3.93-3.90 (m, 30H), 1.77-1.19 (m, 375H), 0.89-0.82 (m, 45H);  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.9, 167.8, 167.7, 160.3, 158.99, 158.92, 157.2, 155.9, 141.8, 139.4, 137.8, 137.6, 135.7, 135.6, 135.4, 119.6, 119.5, 119.0, 110.0, 106.8, 105.6, 105.2, 104.3, 101.1, 100.8, 82.1, 81.89, 81.85, 70.0, 69.7, 68.6, 67.9, 66.1, 65.5, 65.1, 31.7, 29.44, 29.42, 29.24, 29.18, 29.08, 28.98, 27.8, 25.9, 22.5, 13.99; MALDI-ToF: Calcd for  $\text{C}_{387}\text{H}_{570}\text{O}_{75}$ : 6422.62; Found: 6422.27 (M+).

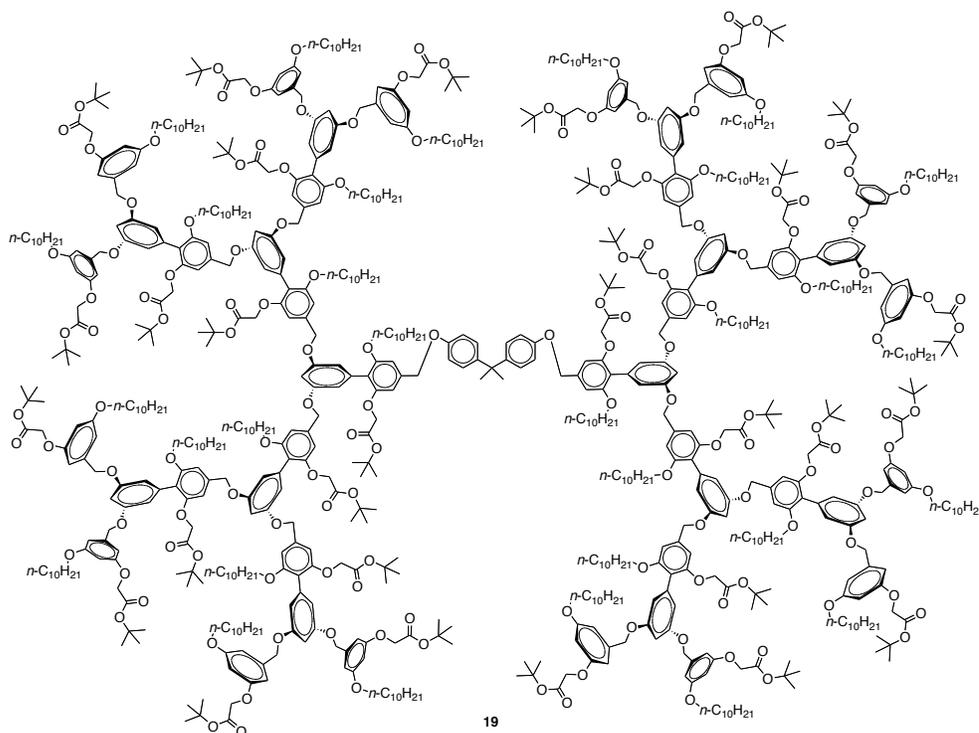
### Synthesis of compound (18, G3-Br):



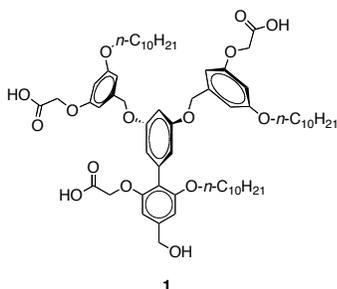
The alcohol **17** (0.46 g, 0.071 mmol) and  $\text{PPh}_3$  (0.074 g, 0.28mmol) were dissolved in dry THF (1.5 mL) under argon atmosphere. *N*-Bromosuccinimide (0.05 g, 0.28 mmol) was added in one portion. After stirring for 2 min, it was quenched with water and extracted with dichloromethane. The work-up procedure used in the synthesis of **12** was followed.

The residue was purified by silica gel column by elution with EtOAc/hexane (15:75) to obtain 0.35 g (76%) of the product **18**.  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  6.78-6.33 (m, 59H), 5.08-4.94 (m, 28H), 4.49-4.45 (m, 32H), 3.93-3.90 (m, 30H), 1.78-1.19 (m, 375H), 0.89-0.82 (m, 45H);  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.7, 167.6, 167.5, 160.1, 158.9, 158.7, 157.1, 155.8, 139.3, 137.8, 137.6, 135.5, 135.3, 135.2, 119.9, 119.4, 109.9, 106.6, 105.3, 104.9, 104.1, 101.0, 100.6, 81.8, 81.7, 81.6, 69.9, 69.5, 68.5, 67.7, 65.9, 65.4, 33.4, 31.6, 29.45, 29.34, 29.31, 29.14, 29.08, 28.98, 28.88, 27.80, 25.8, 22.4, 13.8; MALDI-ToF: Calcd for  $\text{C}_{387}\text{H}_{569}\text{BrO}_{74}$ : 6485.52; Found: 6489.98 ( $\text{M}^+$ ).

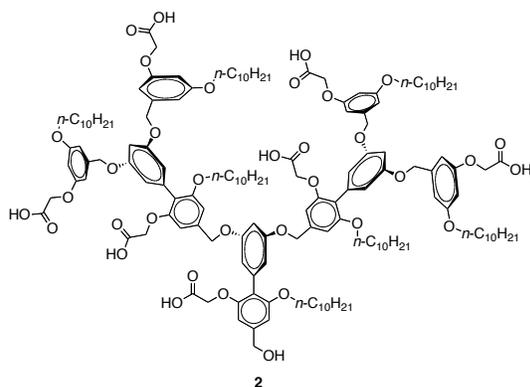
### Synthesis of compound (19, G3-dimer):



Bisphenol A (0.0048 g, 0.021 mmol), potassium carbonate (0.017 g, 0.12 mmol), 18-Crown-6 (0.0016 g, 0.0063 mmol) and bromomethyl compound **18** (0.34 g, 0.052 mmol) in dry acetone (3 mL) were heated at reflux and stirred vigorously under argon atmosphere for 30 h. The work-up procedure used in the synthesis of **11** was followed. The residue was purified by silica gel column by elution with EtOAc/hexane (18:82) to obtain 0.21 g (77% yield) of **19**.  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.20-6.41 (m, 126H), 4.98-4.93 (m, 60H), 4.48-4.44 (m, 60H), 3.93-3.90 (m, 60H), 1.78-1.19 (m, 756H), 0.88-0.81 (m, 90H);  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.99, 167.95, 167.8, 160.3, 159.1, 159.05, 159.01, 157.3, 156.6, 156.0, 155.9, 143.4, 139.5, 137.8, 137.7, 137.6, 135.7, 135.5, 127.7, 119.6, 114.0, 110.1, 106.9, 105.7, 105.3, 104.4, 101.1, 100.9, 82.25, 82.04, 82.01, 81.9, 70.1, 69.8, 68.7, 68.0, 66.1, 65.6, 41.7, 31.8, 31.0, 29.53, 29.51, 29.3, 29.2, 29.1, 29.0, 27.9, 25.9, 22.6, 14.0; MALDI-ToF: Calcd for  $\text{C}_{789}\text{H}_{1152}\text{O}_{150}$ : 13028.25; Found: 13051.25 ( $\text{M}^+$ , 23).

**Synthesis of compound (1, de-G1OH):**

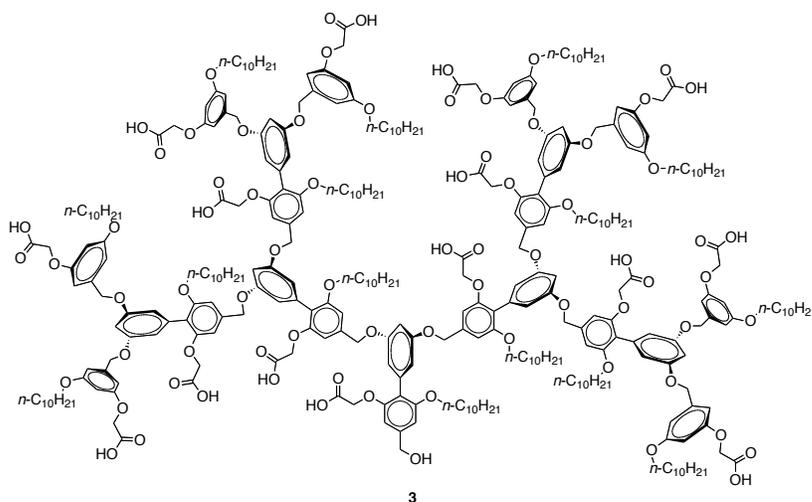
To a solution of alcohol **11** (0.12 g, 0.099 mmol) in tetrahydrofuran (6 mL) was added aqueous potassium hydroxide (0.17 g, 2.99 mmol) dissolved in water (1.5 mL). Methanol (3 mL) was then added to this two-phase system to give homogeneous solution. This mixture was then heated at reflux for 12 h. The reaction mixture was evaporated to dryness and the residue dissolved in water (10 mL) and the mixture heated at reflux for 24 h. After cooling to room temperature, the reaction mixture was acidified with 2N HCl. The precipitate formed was collected by vacuum filtration and dried to afford **1**. Yield: 0.095 g (95%). <sup>1</sup>H-NMR (400 MHz, CD<sub>3</sub>COCD<sub>3</sub>)  $\delta$  6.73-6.44 (m, 11H), 5.03 (s, 4H), 4.67-4.56 (m, 8H), 3.98-3.90 (m, 6H), 1.78-1.23 (m, 48H), 0.89-0.83 (m, 9H); <sup>13</sup>C-NMR (75 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  170.5, 170.2, 159.8, 159.1, 158.4, 156.4, 155.6, 143.7, 139.5, 135.8, 117.2, 110.4, 106.0, 105.5, 103.7, 102.8, 100.2, 69.0, 67.9, 67.4, 64.9, 63.0, 31.3, 29.14, 29.06, 29.01, 28.83, 28.76, 28.69, 25.5, 22.1, 13.9; MALDI-ToF: Calcd for C<sub>63</sub>H<sub>90</sub>O<sub>15</sub>: 1086.63; Found: 1086.97 (M<sup>+</sup>), 1110.37 (M+ +23).

**Synthesis of compound (2, de-G2OH):**

To a solution of alcohol **14** (0.10 g, 0.033 mmol) in tetrahydrofuran (5 mL) was added aqueous potassium hydroxide (0.13 g, 2.35 mmol) dissolved in water (1.2 mL). Methanol (2.5 mL) was then added to this two-phase system to give homogeneous solution. This mixture was then heated at reflux for 12 h. The reaction mixture was evaporated to dryness and the residue dissolved in water (10 mL) and the mixture heated at reflux for

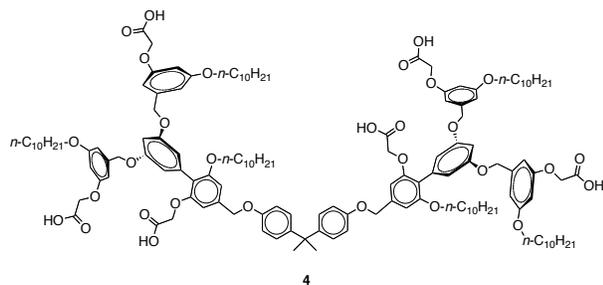
24 h. After cooling to room temperature, the reaction mixture was acidified with 2N HCl. The precipitate formed was collected by vacuum filtration and dried to afford **2**. Yield: 0.075 g (86%).  $^1\text{H-NMR}$  (400 MHz,  $\text{CD}_3\text{COCD}_3$ )  $\square$  6.89-6.46 (m, 27H), 5.11-5.04 (m, 12H), 4.71-4.63 (m, 16H), 4.00-3.94 (m, 14H), 1.78-1.22 (m, 112H), 0.87-0.83 (m, 21H);  $^{13}\text{C-NMR}$  (100 MHz,  $(\text{CD}_3)_2\text{SO}$ )  $\square$  170.3, 170.2, 170.0, 159.8, 158.9, 158.4, 158.6, 158.4, 156.6, 155.6, 139.5, 138.0, 135.5, 118.4, 110.2, 106.1, 105.8, 100.1, 69.0, 68.0, 67.4, 64.7, 64.5, 31.2, 29.06, 29.00, 28.95, 28.76, 28.69, 28.63, 25.5, 22.0, 13.9, 13.8; MALDI-ToF: Calcd for: 2583.47; Found: 2607.48 ( $\text{M}^+$ , 23).

### Synthesis of compound (**3**, de-G3-OH):



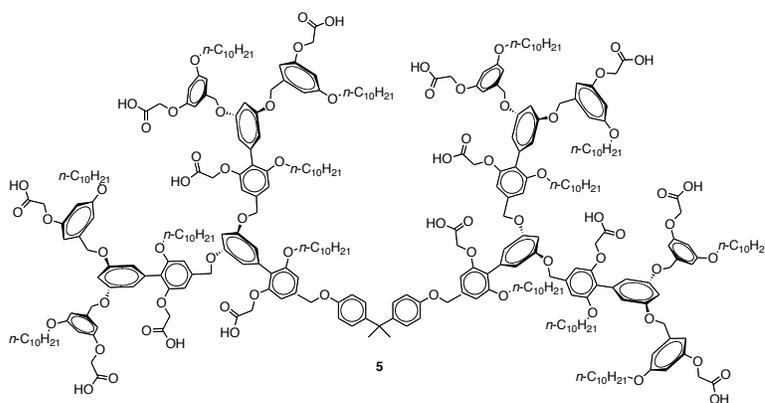
To a solution of alcohol **17** (0.16 g, 0.025 mmol) in tetrahydrofuran (6.8 mL) was added aqueous potassium hydroxide (0.21 g, 3.85 mmol) dissolved in water (1.7 mL). Methanol (3.5 mL) was then added to this two-phase system to give homogeneous solution. This mixture was then heated at reflux for 12 h. The reaction mixture was evaporated to dryness and the residue dissolved in water (20 mL) and the mixture heated at reflux for another 24 h. After cooling to room temperature, the reaction mixture was acidified with 2N HCl. The precipitate formed was collected by vacuum filtration and dried to afford **3**. Yield: 0.13 g (95%).  $^1\text{H-NMR}$  (400 MHz,  $\text{CD}_3\text{COCD}_3$ )  $\square$  6.90-6.45 (m, 59H), 5.12-5.03 (m, 28H), 4.70-4.63 (m, 32H), 3.99-3.93 (m, 30H), 1.78-1.21 (m, 240H), 0.88-0.82 (m, 45H);  $^{13}\text{C-NMR}$  (75 MHz,  $(\text{CD}_3)_2\text{SO}$ )  $\square$  170.2, 170.0, 159.8, 158.9, 158.6, 158.4, 156.6, 155.6, 139.5, 138.0, 135.5, 118.3, 110.2, 106.1, 105.8, 100.1, 69.0, 68.0, 67.4, 64.7, 64.5, 31.3, 29.13, 29.06, 29.01, 28.82, 28.76, 28.68, 25.5, 22.1, 13.94, 13.90; MALDI-ToF: Calcd for  $\text{C}_{327}\text{H}_{450}\text{O}_{75}$ : 5577.14; Found: 5576.69 ( $\text{M}^+$ ), 5598.34 ( $\text{M}^+$ , 23).

### Synthesis of compound (4, de-G1-Dimer):



To a solution of compound **13** (0.20 g, 0.075 mmol) in tetrahydrofuran (8 mL) was added aqueous potassium hydroxide (0.25 g, 4.55 mmol) dissolved in water (2 mL). Methanol (4 mL) was then added to this two-phase system to give homogeneous solution. This mixture was then heated at reflux for 12 h. The reaction mixture was evaporated to dryness and the residue dissolved in water (25 mL) and the mixture heated at reflux for another 24 h. After cooling to room temperature, the reaction mixture was acidified with 2N HCl. The precipitate formed was collected by vacuum filtration and dried to afford **4**. Yield: 0.17 g (97%). <sup>1</sup>H-NMR (400 MHz, CD<sub>3</sub>COCD<sub>3</sub>)  $\delta$  6.94-6.44 (m, 30H), 5.06-5.04 (m, 12H), 4.70 (s, 8H), 4.63 (s, 4H), 3.99-3.92 (m, 12H), 1.79-1.22 (m, 102H), 0.89-0.83 (m, 18H); <sup>13</sup>C-NMR (100 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  170.2, 170.0, 159.8, 158.9, 158.4, 156.5, 156.1, 155.6, 142.8, 139.5, 138.1, 135.5, 127.4, 118.3, 114.2, 110.1, 106.1, 105.8, 105.2, 104.1, 100.4, 100.1, 69.3, 69.0, 68.0, 67.5, 64.7, 64.6, 41.2, 31.3, 31.2, 30.7, 29.06, 29.01, 28.95, 28.77, 28.69, 28.64, 28.52, 25.51, 22.08, 13.91, 13.89; MALDI-ToF: Calcd for C<sub>141</sub>H<sub>192</sub>O<sub>30</sub>: 2365.35; Found: 2364.34 (M<sup>+</sup>), 2387.32 (M<sup>+</sup>, 23).

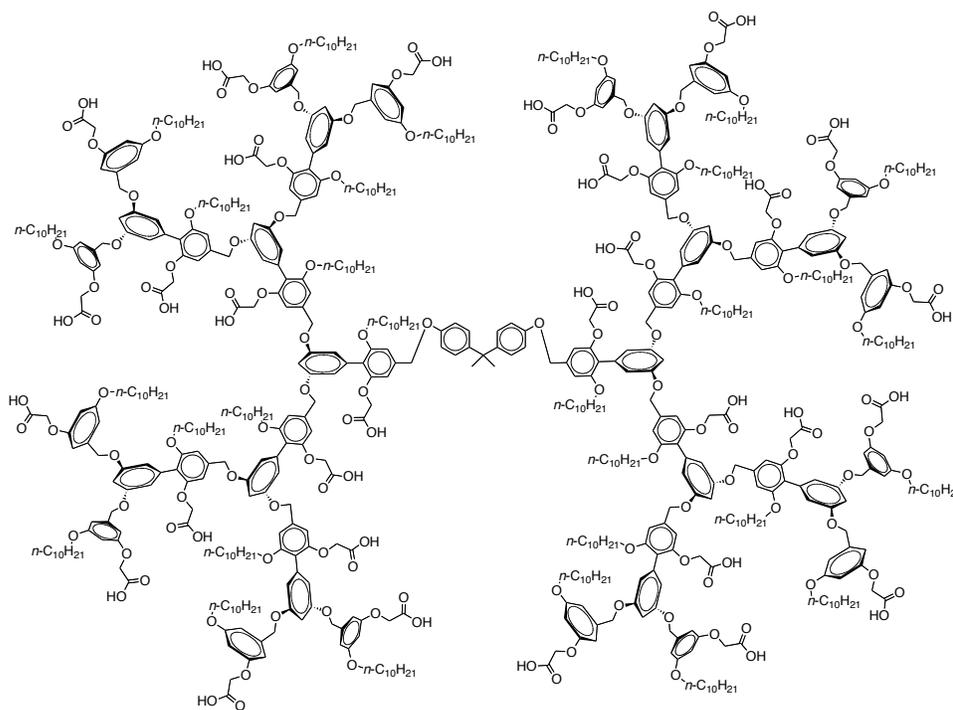
### Synthesis of compound (5, de-G2-dimer):



To a solution of compound **16** (0.14 g, 0.024 mmol) in tetrahydrofuran (6 mL) was added aqueous potassium hydroxide (0.19 g, 3.4 mmol) dissolved in water (1.5 mL). Methanol (3 mL) was then added to this two-phase system to give homogeneous solution. This mixture was then heated at reflux for 12 h. The reaction mixture was evaporated to dryness and the residue dissolved in water (20 mL) and the mixture heated at reflux for

24 h. After cooling to room temperature, the reaction mixture was acidified with 2N HCl. The precipitate formed was collected by vacuum filtration and dried to afford **5**. Yield: 0.11 g (92%).  $^1\text{H-NMR}$  (400 MHz,  $\text{CD}_3\text{COCD}_3$ )  $\delta$  7.18-6.44 (m, 62H), 5.10-5.03 (m, 28H), 4.70-4.63 (m, 28H), 3.99-3.93 (m, 28H), 1.78-1.21 (m, 230H), 0.87-0.82 (m, 42H);  $^{13}\text{C-NMR}$  (100 MHz,  $(\text{CD}_3)_2\text{SO}$ )  $\delta$  170.25, 170.20, 170.02, 159.8, 158.9, 158.6, 158.4, 156.6, 156.1, 155.6, 142.8, 139.5, 138.1, 138.0, 135.8, 135.5, 127.4, 118.4, 114.1, 110.2, 106.1, 105.8, 105.1, 104.1, 100.3, 100.1, 69.3, 69.0, 68.0, 67.4, 64.7, 64.5, 41.2, 31.2, 30.7, 29.07, 29.02, 28.96, 28.78, 28.71, 28.65, 25.52, 22.0, 13.89, 13.86. ; MALDI-ToF: Calcd for  $\text{C}_{317}\text{H}_{432}\text{O}_{70}$ : 5359.02; Found: 5358.26 ( $\text{M}^+$ ), 5380.14 ( $\text{M}^+$ , 23).

### Synthesis of compound (**6**, de-G3-dimer):



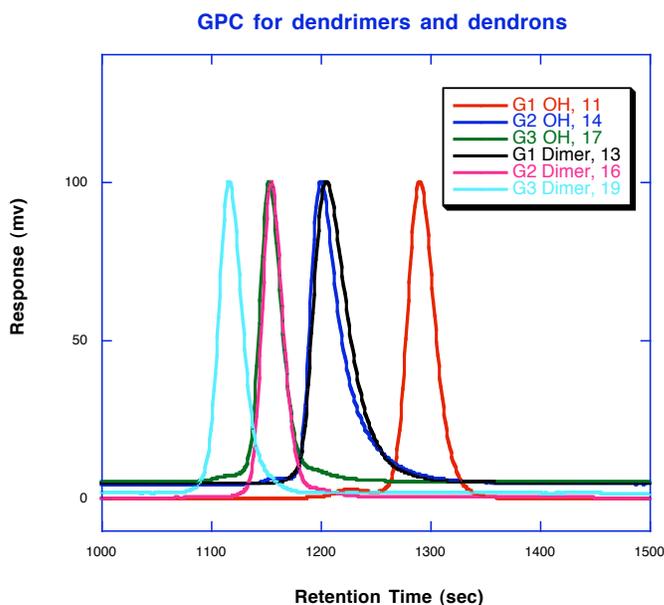
6

To a solution of compound **19** (0.15 g, 0.011 mmol) in tetrahydrofuran (6 mL) was added aqueous potassium hydroxide (0.2 g, 3.5 mmol) dissolved in water (1.5 mL). Methanol (3 mL) was then added to this two-phase system to give homogeneous solution. This mixture was then heated at reflux for 12 h. The reaction mixture was evaporated to dryness and the residue dissolved in water (25 mL) and the mixture heated at reflux for another 24 h. After cooling to room temperature, the reaction mixture was acidified with 2N HCl. The precipitate formed was collected by vacuum filtration and dried to afford **6**. Yield: 0.12 g (92%).  $^1\text{H-NMR}$  (400 MHz,  $\text{CD}_3\text{COCD}_3$ )  $\delta$  7.18-6.45 (m, 126H), 5.12-5.03 (m, 60H), 4.69-4.65 (m, 60H), 3.98-3.95 (m, 60H), 1.77-1.21 (m, 486H), 0.88-0.82 (m, 90H);  $^{13}\text{C-NMR}$  (100 MHz,  $(\text{CD}_3)_2\text{SO}$ )  $\delta$  170.2, 170.1, 170.0, 159.8, 158.9, 158.6, 158.4, 156.6, 155.6, 139.5, 138.2, 138.1, 138.0, 135.6, 135.5, 127.4, 118.5, 118.4, 114.1, 110.2, 106.1, 105.8, 105.2, 104.1, 100.1, 100.5, 69.4, 69.0, 68.0, 67.4, 64.8, 64.5, 41.2, 31.3, 30.9, 29.08, 29.02, 28.9, 28.79, 28.72, 28.66, 25.5, 22.0, 13.87, 13.82 ; MALDI-ToF: Calcd for  $\text{C}_{677}\text{H}_{928}\text{O}_{150}$ : 11458.5; Found: 11458.84 ( $\text{M}^+$ ).

### Sample preparation for UV-Visible Spectroscopy and DLS measurements:

The UV-Visible absorption spectra were taken in a spectrophotometer scanning from 300-800 nm. For normal micelle studies all the compounds **1-6** were first put in a round bottom flask along with de-ionized water to make  $10^{-4}$  M solution. Since the compounds 1-6 were not soluble in water due to the presence of the carboxylic acid groups, 1.5-2 equivalents of KOH was added to ensure solubility. The solutions were sonicated for  $\sim 3$  hours at  $50^{\circ}\text{C}$  to get a clear solution of the dendrimers. From these,  $10^{-5}$  and  $10^{-6}$  M solutions were also made by dilution. To 5 mL of each of these solutions,  $\sim 10$ mg of Reichardt's dye was added and sonicated for 3 more hours at  $50^{\circ}\text{C}$  and then filtered to get a clear solution of the dye encapsulated dendrimer in water and spectra taken. For the inverted micelle studies, the dendrimers **1-6** were dissolved in toluene to make  $10^{-4}$  M solution and to ensure solubility sonicated for  $\sim 2$  hours, at  $50^{\circ}\text{C}$ . To 5 mL clear solution of the dendrimers,  $\sim 5$  mg of Proflavine.HCl was added and sonicated for 3 hours at  $50^{\circ}\text{C}$ . After the sonication the solutions were filtered and spectra taken.

The sample preparations for the DLS experiments are same as the UV-Visible spectroscopy. A digital correlator and a goniometer were used for the DLS measurements. The light source was a solid-state laser system, operating at 514 nm. The temperature was kept constant at  $25^{\circ}\text{C}$ . Dust was eliminated by filters with  $0.22\ \mu\text{m}$  pore size for aqueous solutions and  $0.20\ \mu\text{m}$  pore size for toluene solutions. All the measurements were done at a correlation time of 1.30 minutes. The particle sizes taken are average of at least five readings.



2.084  
2.073  
2.067  
2.061  
2.056  
2.050  
2.045  
2.039  
1.786  
1.770  
1.753  
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1.717  
1.634  
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1.598  
1.583  
1.464  
1.444  
1.427  
1.297  
1.290  
1.233  
0.892  
0.876  
0.857  
0.839  
0.131

3.905  
3.920  
3.936  
3.954  
3.970  
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4.569  
4.603  
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5.037  
5.624  
6.440  
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6.564  
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6.720  
6.725  
6.739

Compound 1 (De G10H)

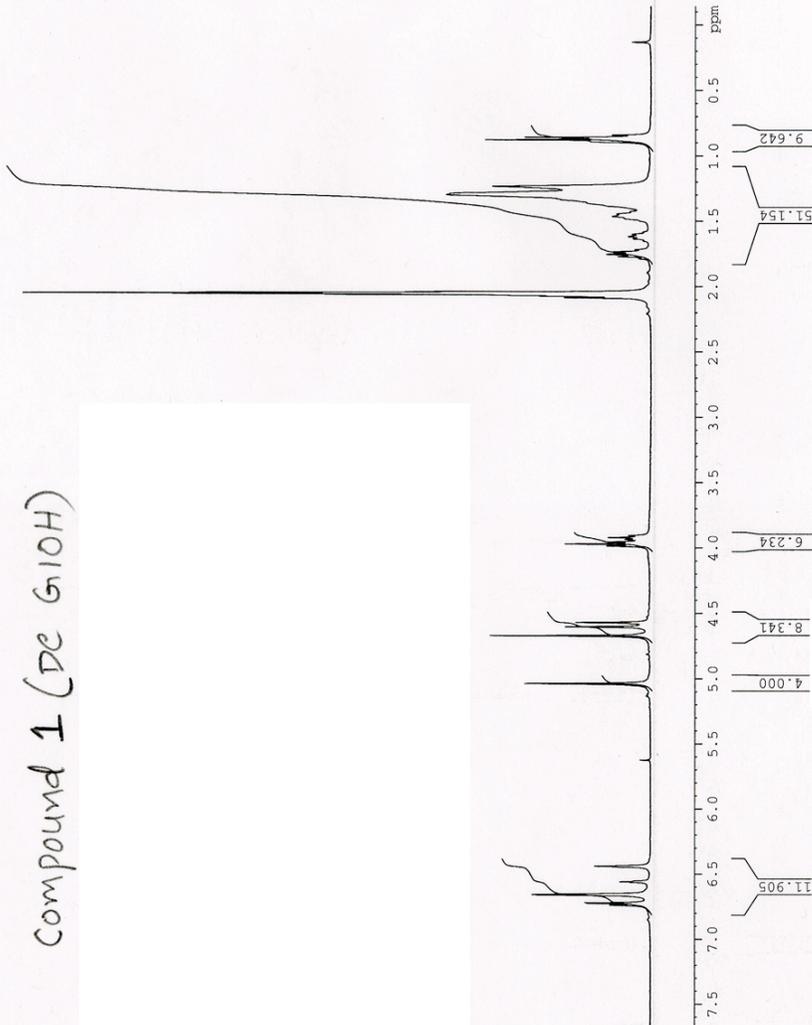
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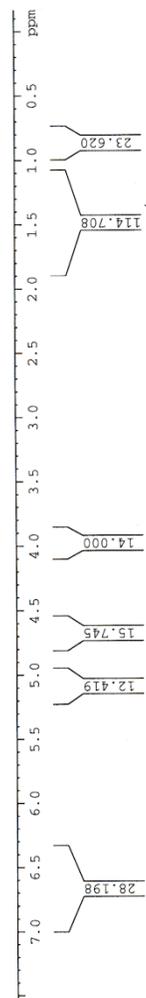
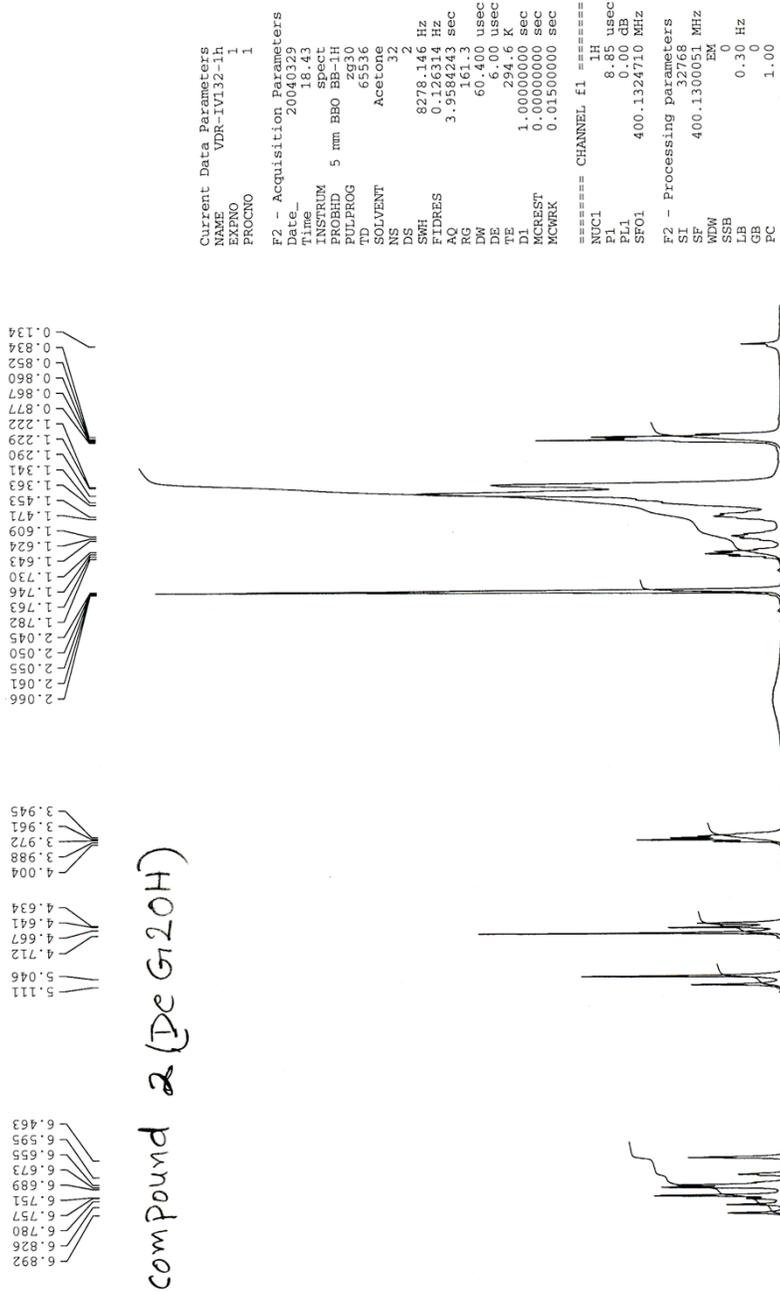
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6.841  
6.821  
6.787  
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Compound 3 (DE 93-01)

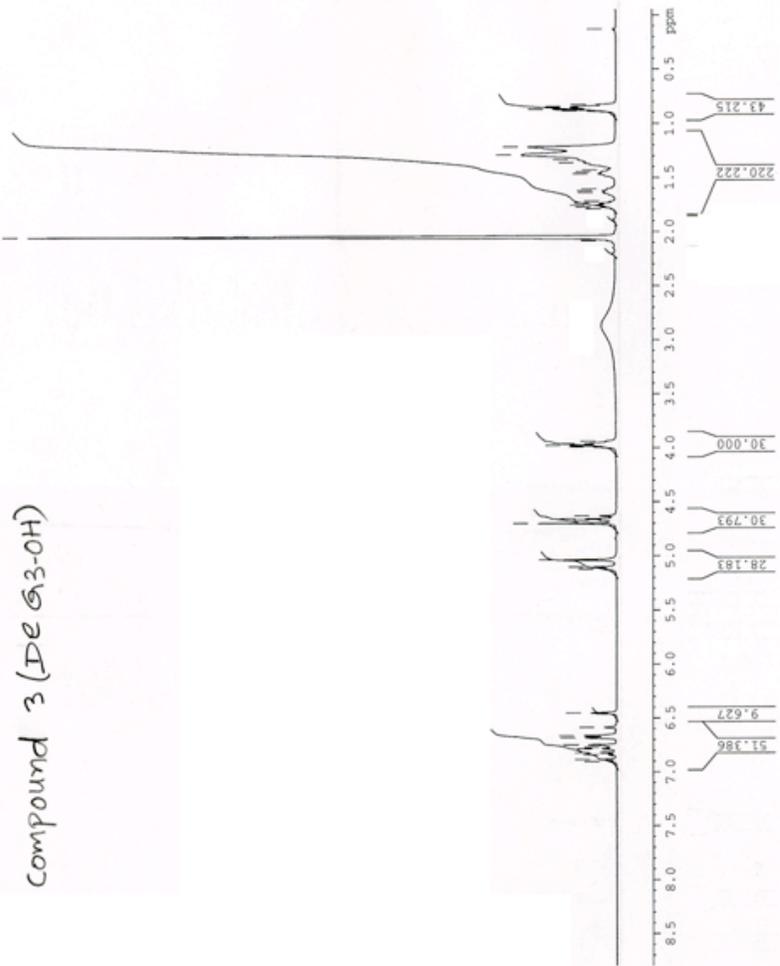
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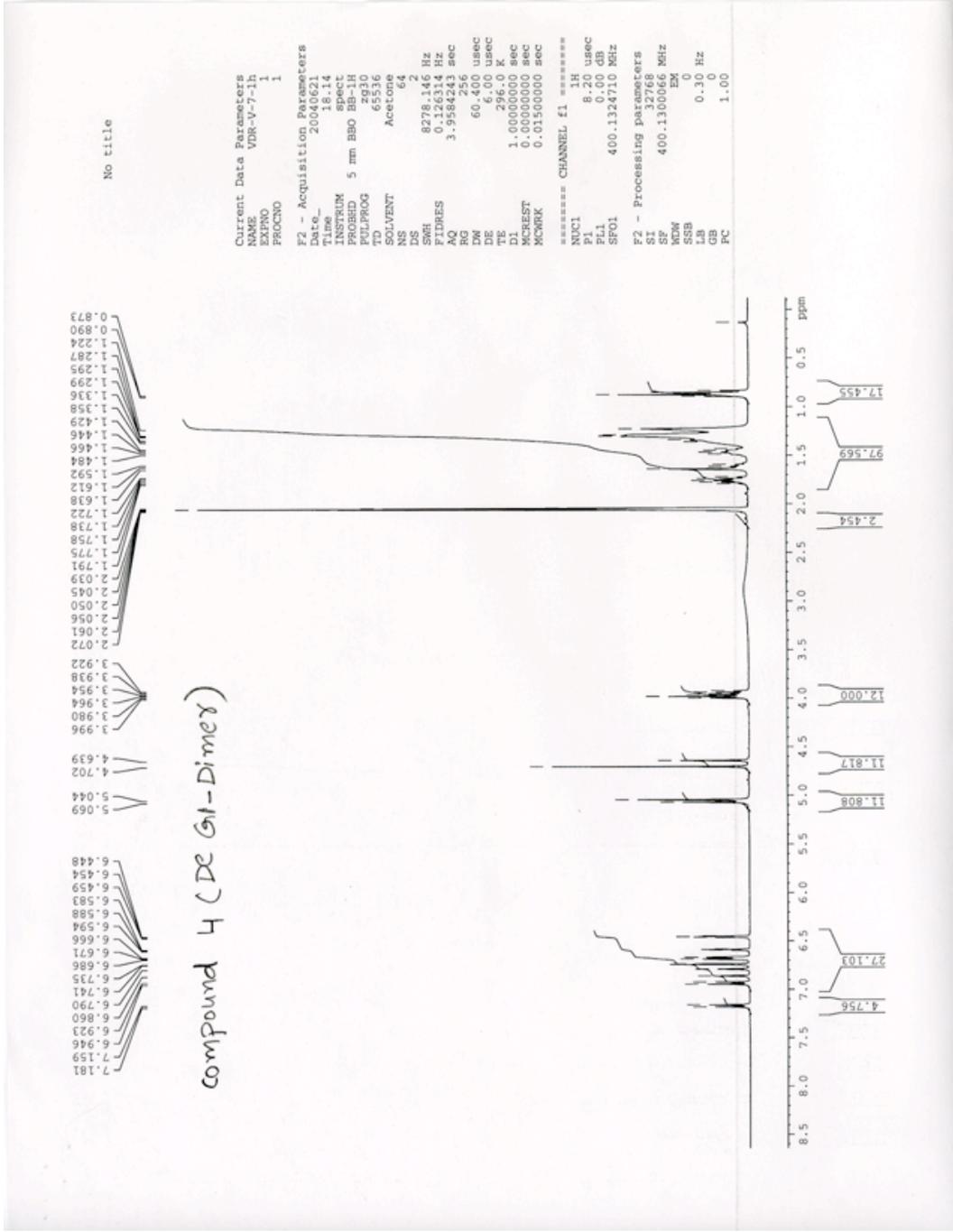
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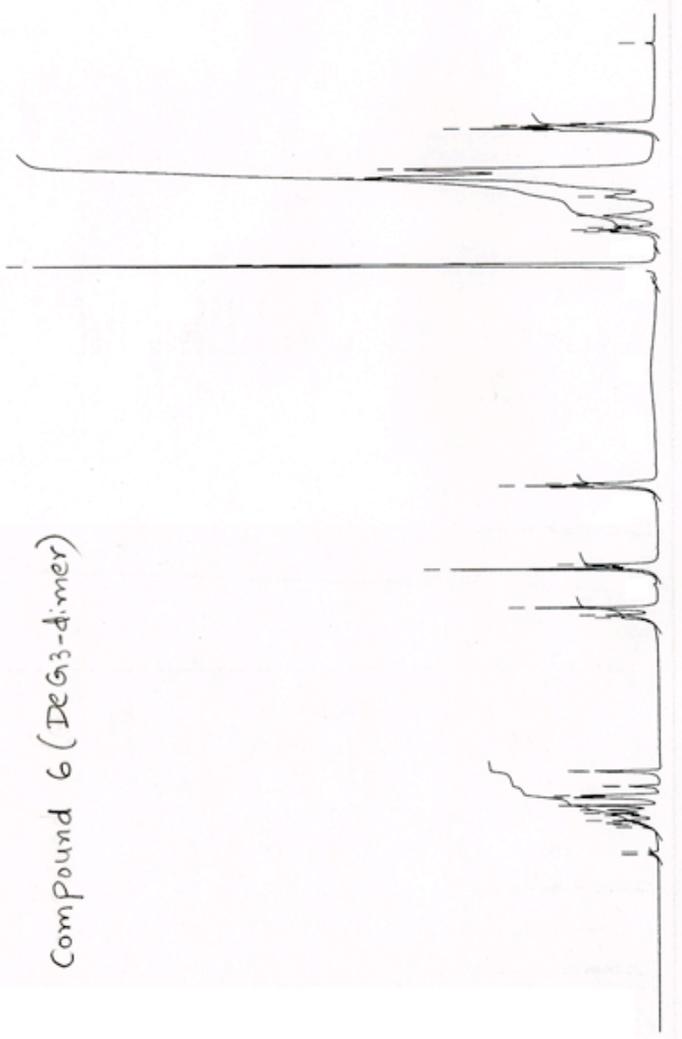
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Compound 6 (DEG3-dimer)



Current Data Parameters  
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