Supporting Information

for

Modular Synthesis of Supramolecular DNA Amphiphiles through Host-guest Interactions and their Self-assembly into DNA-decorated Nanovesicles

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Synthesis of guest molecules (1 & 2) and host DNA (DNA-β-CD)

The guest molecules 1, 2 and host DNA (DNA-β-CD) were synthesized as per the following schemes.

**Synthesis of 1**

![Synthetic scheme for 1](image)

Scheme S1. Synthetic scheme for 1.


Synthesis of 2

\[
\begin{align*}
\text{R4} + \text{R6} + \text{R7} & \rightarrow \text{R8} \\
\text{C}_{12}H_{2}Br, \text{THF} & \hspace{1cm} \text{K}_2\text{CO}_3, 60 ^\circ\text{C}, 24 \text{ h} \\
\end{align*}
\]

\[
\begin{align*}
\text{R9} + \text{G4} & \rightarrow \text{CuSO}_4\cdot5\text{H}_2\text{O}, \text{Sodium ascorbate} \\
\text{t-BuOH}:\text{H}_2\text{O} (1:1), 70 ^\circ\text{C}, 72 \text{ h} \\
\end{align*}
\]

Synthesis of R4

\[
\begin{align*}
\text{R1} \rightarrow \text{R2} & \rightarrow \text{R3} \\
\text{NaBH}_4, \text{EtOH}, \text{THF} & \hspace{1cm} 0 ^\circ\text{C}, 6 \text{ h} \\
\text{HBr in acetic acid (30\%)} & \hspace{1cm} \text{DCM, rt, 8 h} \\
\end{align*}
\]

\[
\begin{align*}
\text{R4} \rightarrow \text{R3} & \rightarrow \text{R5} \\
\text{NaN}_3 & \hspace{1cm} \text{DMF, 60 ^\circ\text{C}, 1 h} \\
\end{align*}
\]

Synthesis of R6

\[
\begin{align*}
\text{R5} \rightarrow \text{R6} & \rightarrow \text{R7} \\
\text{Paraformaldehyde, TFA} & \hspace{1cm} \text{rt, 15 min} \\
\end{align*}
\]

Synthesis of G4

\[
\begin{align*}
\text{G1} + \text{G2} & \rightarrow \text{G3} & \rightarrow \text{G4} \\
\text{Et}_3\text{N}, 180 ^\circ\text{C} & \hspace{1cm} \text{overnight} \\
\text{Br} & \hspace{1cm} \text{dry DMF, NaH, 0 ^\circ\text{C}} \\
\end{align*}
\]

Scheme S2. Synthetic scheme for 2.
Synthesis of DNA-β-CD

Synthesis of D3

\[
\begin{align*}
\text{D1} & \quad + \quad \text{D2} \\
\rightarrow & \quad \text{D3} \\
1. & \text{DCM, 0 °C, 1 h} \\
2. & \text{rt, 2 h}
\end{align*}
\]

Synthesis of β-CD-N₃ and DNA-β-CD

Scheme S3. Synthetic scheme for DNA-β-CD.

Synthesis of P2: To an ice-cold solution of 3,4,5-trimethoxy aniline (10 g, 54.64 mmol) in a mixture of water (120 mL) and sulphuric acid (8 mL), aqueous solution of sodium nitrite (36.49 g in 60 mL water) was added drop wise. After the addition of NaNO₂ was complete, the reaction mixture was poured into an aqueous solution of potassium iodide (13.85 g in 30 mL water) at 50 °C and was magnetically stirred for 30 min. Then the reaction mixture was allowed to come to room temperature, followed by the addition of saturated solution of sodium sulphite, to neutralize excess iodine until no change in color of the reaction mixture...
was observed. The resulting aqueous solution was extracted with diethyl ether and saturated brine solution. The organic layer was dried over anhydrous sodium sulphate, filtered and solvent was removed to get crude product as brown solid, which was further purified by column chromatography using petroleum ether:ethyl acetate (90:10) to get desired product as white solid (92%). TLC (petroleum ether:ethyl acetate, 90:10): R<sub>f</sub> = 0.4; M.P. 86 °C; <sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>OD), δ (ppm): 3.70 (s, 6H), 3.20 (s, 3H), 6.87 (s, 2H); <sup>13</sup>C NMR (125 MHz, CD<sub>3</sub>OD), δ (ppm): 59.43, 63.61, 89.61, 118.97, 142.06, 157.91; GC-MS (EI)-m/z of C<sub>9</sub>H<sub>11</sub>IO<sub>3</sub>: 293.97 (calcd.), 294 (expt).

**Synthesis of P3:** P<sub>2</sub> (5 g, 17 mmol) was dissolved in 50 mL of freshly distilled dichloromethane. Solution was cooled to -78 °C followed by the drop wise addition of boron tribromide (1.0 M in DCM, 100 mL) using an addition funnel. After the addition of BBr<sub>3</sub> was complete, the reaction mixture was allowed to stir at -78 °C for 30 min more and later stirred for 24 h at room temperature. It was quenched with ice water and was further stirred for 30 min. The resulting solution was extracted with ethyl acetate and washed with saturated brine. The organic layer was dried over sodium sulphate, filtered and solvent was removed to get brown oil, which was further purified by column chromatography using dichloromethane:methanol (90:10) to get desired product as brown solid (70%). TLC (dichloromethane:methanol, 90:10): R<sub>f</sub> = 0.5; M.P. 89 °C; <sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>OD), δ (ppm): 6.54 (s, 2H); <sup>13</sup>C NMR (125 MHz, CD<sub>3</sub>OD), δ (ppm): 80.35, 117.50, 134.77, 148.26; GC-MS (EI)-m/z of C<sub>6</sub>H<sub>5</sub>IO<sub>3</sub>: 251.92 (calcd.), 252 (expt).

**Synthesis of P4:** P<sub>3</sub> (6.3 g, 25 mmol) was dissolved in dry DMF and degassed with nitrogen for 15 min, followed by the addition of potassium carbonate (58.65 g, 425 mmol) and was further stirred for 30 min at room temperature. Then 1-bromo dodecane (36 mL, 150 mmol) was added slowly using syringe and the reaction mixture was allowed to stir for 7 h at 60 °C. After cooling the reaction mixture to room temperature, dimethylformamide was removed in rotatory evaporator. The compound was dissolved in dichloromethane and extracted with DCM/water mixture several times. The collective organic layer was dried over anhydrous sodium sulphate, filtered and solvent was removed to give crude product, which was further purified by column chromatography using petroleum ether:dichloromethane (95:5) to get desired product as white solid (45%). TLC (petroleum ether:dichloromethane, 95:5): R<sub>f</sub> = 0.3;
M.P. 80 °C; ¹H NMR (500 MHz, CDCl₃), δ (ppm): 0.80 (t, J = 7.1 Hz, 9H), 1.19-1.22 (m, 48H), 1.34-1.39 (m, 6H), 1.61-1.67 (m, 2H), 1.68-1.73 (m, 4H), 3.84 (t, J = 6.4 Hz, 6H), 6.76 (s, 2H); ¹³C NMR (125 MHz, CDCl₃), δ (ppm): 14.13, 21.71, 26.05, 26.11, 29.30, 29.38, 29.41, 29.60, 29.64, 29.68, 29.71, 29.75, 29.76, 30.28, 31.95, 69.33, 73.45, 85.64, 116.24, 138.40, 153.96; GC-MS (EI)-m/z of C₄₂H₇₇IO₃: 756.49 (calcld.), 756 (expt).

**Synthesis of P5:** Solution of P₄ (8 g, 10.57 mmol) in freshly distilled dry THF (45 mL) and dry triethylamine (29.6 mL) was degassed with nitrogen for 15 min. Bis(triphenylphosphine)palladium(II)dichloride (0.315 g, 0.53 mmol), copper(I) iodide (0.2095 g, 1.1 mmol) and trimethylsilylacetylene (2.3 mL, 15.9 mmol) were added to the degassed solution, which turned dark green as soon as the addition was complete. The reaction mixture was stirred overnight at 60 °C. After the completion of reaction, solvent was removed to get crude product as brown liquid which was further purified by column chromatography using petroleum ether:dichloromethane (90:10) to get product as white solid (85%). TLC (petroleum ether:dichloromethane, 90:10): Rf = 0.5; M.P. 91 °C; ¹H NMR (500 MHz, CDCl₃), δ (ppm): 0.16 (s, 9H), 0.81 (t, J = 6.5 Hz, 9H), 1.19-1.26 (m, 48H), 1.24-1.35 (m, 6H), 1.62-1.65 (m, 2H) 1.68-1.72 (m, 4H), 3.87 (t, J = 6.5 Hz, 6H), 6.58 (s, 2H); ¹³C NMR (125 MHz, CDCl₃), δ (ppm): 0.98, 14.07, 21.66, 26.04, 26.06, 26.89, 29.31, 29.34, 29.36, 29.56, 29.61, 29.63, 29.67, 29.70, 29.72, 30.27, 31.90, 69.10, 92.49, 105.47, 110.55, 117.42, 139.35, 152.85; GC-MS (EI)-m/z of C₄₇H₈₆O₃Si: 726.63 (calcld.), 727 (expt).

**Synthesis of P6:** To a solution of P₅ (6.15 g, 8.45 mmol) in dichloromethane (42 mL) and methanol (42 mL), potassium carbonate (5.83 g, 42.25 mmol) was added and stirred at room temperature for 4 h. After the completion of reaction, distilled water was added to the reaction mixture, and was extracted with dichloromethane. The organic layer was dried over anhydrous sodium sulphate, filtered and solvent was removed to get the desired product as white solid (96%). TLC (petroleum ether:dichloromethane, 95:5): Rf = 0.5; M.P. 91 °C; ¹H NMR (500 MHz, CDCl₃), δ (ppm): 0.81 (t, J = 6.7 Hz, 9H), 1.19-1.30 (m, 51H), 1.36-1.39 (m, 6H), 1.62-1.68 (m, 2H), 1.69-1.72 (m, 4H), 2.91 (s, 1H), 3.88 (t, J = 4.2 Hz, 6H), 6.61 (s, 2H); ¹³C NMR (125 MHz, CDCl₃), δ (ppm): 14.13, 22.69, 26.07, 26.09, 29.32, 29.37, 29.39, 29.59, 29.63, 29.66, 29.70, 29.73, 29.75, 30.31, 31.93, 31.94, 69.18,
73.53, 75.72, 84.05, 110.76, 116.40, 139.61, 152.96; GC-MS (EI)-m/z of $C_{44}H_{78}O_3$: 654.59 (calcd.), 654 (expt).

**Synthesis of P7:** Solution of P6 (5 g, 7.63 mmol) in freshly distilled dry tetrahydrofuran (33 mL) and dry triethylamine (21.4 mL) was degassed with nitrogen for 15 min. Bis(triphenylphosphine)palladium(II)dichloride (0.27 g, 0.38 mmol), copper(I) iodide (0.145 g, 0.76 mmol) and (4-iodophenylethynyl)trimethylsilane (2.52 g, 8.39 mmol) was added to the degassed solution, which turned dark green as soon as the addition was complete. The reaction mixture was stirred overnight at 60 °C. After the completion of reaction, solvent was removed to get crude product as brown liquid which was further purified by column chromatography using petroleum ether:dichloromethane (90:10) as eluent to get product as white solid (90%). TLC (petroleum ether : dichloromethane, 90:10): $R_f = 0.4$; M.P. 70 °C; $^1$H NMR (500 MHz, CDCl$_3$), δ (ppm): 0.15 (s, 9H), 0.82 (t, $J = 6.5$ Hz, 9H), 1.19-1.34 (m, 48H), 1.35-1.40 (m, 6H), 1.63-1.68 (m, 2H), 1.69-1.75 (m, 4H), 3.90 (t, $J = 6.55$ Hz, 6H), 6.64 (s, 2H), 7.35 (s, 4H); $^{13}$C NMR (125 MHz, CDCl$_3$), δ (ppm): 0.95, 15.13, 23.73, 27.11, 27.96, 30.38, 30.40, 30.43, 30.63, 30.67, 30.69, 30.73, 30.77, 31.36, 32.96, 70.22, 26, 74.59, 88.80, 92.78, 97.22, 105.72, 111.25, 118.36, 123.77, 124.50, 132.31, 132.91, 140.39, 154.07; GC-MS (EI)-m/z of $C_{55}H_{90}O_3Si$: 826.66 (calcd.), 827 (expt).

**Synthesis of P8:** To a solution of P7 (5 g, 6.04 mmol) in dichloromethane (30 mL) and methanol (30 mL), potassium carbonate (4.17 g, 30.2 mmol) was added and stirred at room temperature for 4 h. After the completion of reaction, distilled water was added to the reaction mixture, and was extracted with dichloromethane. The organic layer was dried over anhydrous sodium sulphate, filtered and solvent was removed to get the desired product as white solid (87%). TLC (petroleum ether:dichloromethane, 90:10): $R_f = 0.5$; M.P. 68 °C; $^1$H NMR (500 MHz, CDCl$_3$), δ (ppm): 0.81 (t, $J = 6.5$ Hz, 9H), 1.19-1.30 (m, 48H), 1.37-1.43 (m, 6H), 1.65-1.68 (m, 2H), 1.71-1.77 (m, 4H), 3.09 (s, 1H), 3.90 (t, $J = 6.5$ Hz, 6H), 6.65 (s, 2H), 7.38 (s, 4H); $^{13}$C NMR (125 MHz, CDCl$_3$), δ (ppm): 14.13, 25.07, 25.08, 28.32, 28.35, 28.38, 28.58, 28.63, 28.65, 28.68, 28.71, 28.73, 28.74, 29.31, 30.91, 30.93, 68.17, 72.55, 77.79, 82.29, 86.55, 90.81, 109.21, 116.24, 120, 68, 122.88, 130.35, 131.03, 138.37, 152.03; GC-MS (EI)-m/z of $C_{52}H_{82}O_3$: 754.62 (calcd.), 755 (expt).
**Synthesis of P9:** Solution of P8 (3.7 g, 4.9 mmol) in freshly distilled dry tetrahydrofuran (21 mL) and dry triethylamine (13.7 mL) was degassed with nitrogen for 15 min. Bis(triphenylphosphine)palladium(II)dichloride (0.17 g, 0.245 mmol), copper(I) iodide (0.09 g, 0.49 mmol) and 4-iodobenzylalcohol (1.26 g, 5.39 mmol) was added to the degassed solution, which turned dark green as soon as the addition was complete. The reaction mixture was stirred overnight at 60 °C. After the completion of reaction, solvent was removed to get crude product as brown liquid which was further purified by column chromatography using petroleum ether:chloroform (50:50) to get product as yellow solid (36%). TLC (petroleum ether : chloroform, 50:50): R_f = 0.2; M.P. 118 °C; 1H NMR (500 MHz, CDCl_3), δ (ppm): 0.82 (t, J = 6.5 Hz, 9H), 1.19-1.27 (m, 51H), 1.38-1.47 (m, 6H), 1.65-1.69 (m, 2H), 1.70-1.76 (m, 4H), 3.90 (t, J=6.5 Hz, 6H), 4.64 (s, 2H), 6.66 (s, 2H), 7.28 (d, J = 8 Hz, 4H), 7.45 (d, J = 4.5 Hz, 2H); 13C NMR (125 MHz, CDCl_3), δ (ppm): 14.13, 22.71, 26.10, 29.35, 29.38, 29.41, 29.61, 29.66, 29.68, 29.72, 29.75, 30.33, 31.95, 31.96, 64.96, 69.18, 73.58, 87.86, 89.21, 91.04, 91.73, 110.19, 117.38, 122.30, 122.89, 123.24, 126.86, 131.45, 131.53, 131.81, 139.30, 153.04; GC-MS (EI)-m/z of C_{59}H_{88}O_4: 860.66 (calcd.), 861 (expt.).

**Synthesis of 1:** To an ice-cold solution of 1-adamantane carboxylic acid (0.35 g, 1.97 mmol) in dry dichloromethane (25 mL), oxalyl chloride (0.22 mL) was added dropwise, followed by the addition of a drop of dimethylformamide. Then the reaction mixture was allowed to stir for 2 h at room temperature. After the completion of reaction, excess oxalyl chloride was removed by purging nitrogen. To a magnetically stirred solution of P9 (0.5 g, 0.58 mmol) in freshly distilled dry tetrahydrofuran (25 mL), dry triethylamine (0.16 mL) was added, subsequently the above freshly prepared acid chloride was added dropwise at room temperature. Finally a pinch of 4-dimethylaminopyridine was added and the reaction mixture was stirred at room temperature for 12 h. On completion of reaction, it was quenched with ice-cold water and extracted with chloroform. The organic layer was dried over anhydrous sodium sulphate, filtered and solvent was dried to give crude product which was further purified by column chromatography using petroleum ether:chloroform (90:10) to get desired product as yellow solid (42%). TLC
(petroleum ether:chloroform, 90:10): R<sub>f</sub> = 0.5; M.P. 132 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>), δ (ppm): 0.81 (t, J = 7 Hz, 9H), 1.19 (m, 49H), 1.37-1.42 (m, 6H), 1.64-1.68 (m, 8H), 1.71-1.76 (m, 4H), 1.85-1.86 (m, 6H), 1.95 (bs, 3H), 3.91 (t, J = 6.5 Hz, 6H), 5.03 (s, 2H), 6.66 (s, 2H), 7.25 (d, J = 8.5 Hz, 2H), 7.42-7.45 (m, 6H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>), δ (ppm): 14.12, 22.70, 26.09, 27.95, 29.35, 29.37, 29.40, 29.60, 29.65, 29.67, 29.71, 29.75, 30.33, 31.94, 31.95, 36.49, 38.85, 40.82, 65.30, 69.19, 73.57, 87.84, 90.89, 110.21, 117.35, 122.68, 122.83, 123.30, 127.64, 131.45, 131.54, 131.74, 136.95, 153.05. MALDI-TOF MS-m/z of C<sub>70</sub>H<sub>103</sub>O<sub>5</sub>: [M+H]<sup>+</sup> 1023.77 81 (calcd.); 1023.81 (expt).

**Synthesis of 2**

**Synthesis of R<sub>2</sub>:** Solution of R<sub>1</sub> (10 g, 74.55 mmol) in ethanol (140 mL) and THF (200 mL) was cooled to 0 °C. After slow addition of NaBH<sub>4</sub> (0.70 g, 18.63 mmol), it was stirred for six hours by maintaining temperature at 0 °C. After completion of reaction, it was acidified with 2M HCl to pH 5. Solvent was evaporated, residue obtained was dissolved in ethylacetate (100 X 3) was extracted from water (400 mL), Organic phase was washed with water, dried over anhydrous sodium sulphate and the solvent was evaporated to get a clear oil which was further purified by column chromatography using DCM:MeOH (96:4) as eluent to get desired product (80%). TLC (DCM:MeOH, 96:4): R<sub>f</sub> = 0.5; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>), δ (ppm): 1.81 (bs, 1H), 4.74 (d, J = 5.0 Hz, 2H), 7.47 (d, J = 8.0 Hz, 2H), 7.82 (d, J = 8.0 Hz, 2H), 9.94 (s, 1H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>), δ (ppm): 64.61, 126.98, 130.03, 135.76, 147.73, 191.95. GC-MS (EI)-m/z of C<sub>8</sub>H<sub>8</sub>O<sub>2</sub>: 136.05 (calcd.), 136 (expt).

**Synthesis of R<sub>3</sub>:** To a solution of R<sub>2</sub> (7.65 g, 56.17 mmol) in DCM (60 mL), 30% HBr in acetic acid (31 mL) was added slowly and was stirred at room temperature overnight. After solvent evaporation residue obtained was purified by column chromatography using petroleum ether:DCM (90:10) as eluent to get R<sub>3</sub> as white solid (95%). TLC (petroleum ether:DCM, 50:50): R<sub>f</sub> = 0.48; M.P. 100 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>), δ (ppm): 4.44 (s, 2H), 7.49 (d, J = 7.50 Hz, 2H), 7.80 (d, J = 8.0 Hz, 2H), 9.94 (s, 1H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>), δ (ppm): 31. 96, 129.68, 130.18, 136.14, 144.26, 191.51. GC-MS (EI)-m/z of C<sub>8</sub>H<sub>7</sub>BrO: [M]<sup>+</sup> 197.90 (calcd.), 197.90 (expt), [M+2]<sup>+</sup> 199.90 (calcd.), 199.90 (expt).
Synthesis of R4: To a solution of R3 (7.5 g, 37.55 mmol) in dry DMF (50 mL), NaN₃ (4.88 g, 75.11 mmol) was added and was stirred at 60 °C for an hour. Reaction mixture was allowed to cool to room temperature, DMF was removed under reduced pressure and the residue was dissolved in DCM. It was extracted from water, organic phase was dried over anhydrous sodium sulphate, solvent was evaporated to get crude product which was further purified by column chromatography using petroleum ether:DCM (90:10) as eluent to get desired product R4 as colourless oil (90%). TLC (petroleum ether:DCM, 50:50): Rf = 0.40; ¹H NMR (500 MHz, CDCl₃), δ (ppm) = 4.39 (s, 2H), 7.43 (d, J = 7.50, 2H), 7.84 (d, J = 7.50, 2H), 9.96 (s, 1H). ¹³C NMR (125 MHz, CDCl₃), δ (ppm) = 54.29, 128.50, 130.24, 136.19, 142.13, 191.66. GC-MS (EI)-m/z of C₈H₇N₃O: 161.058 (calcd.), 161 (expt).

Synthesis of G3: To a solution of G1 (5.0 g, 23.2 mmol) in triethylamine (10 mL), tetraethylene glycol (G2) (94.7 g, 488mmol) was added. The reaction mixture was stirred overnight at 180 °C. After completion, the reaction mixture was allowed to cool to room temperature. Subsequently it was extracted with DCM, washed with 2M HCl (20 mL), and once with brine (20 mL). The organic layer was dried on sodium sulphate and the solvent was removed under reduced pressure. Then the crude product was obtained was purified using column chromatography using DCM:MeOH (95:5) as eluent to get desired product as yellow oil (78%).TLC (DCM:MeOH, 95:5); Rf = 0.3; ¹H NMR (500 MHz, CDCl₃) δ ppm: 1.50-1.57 (m, 6H), 1.68 (bs, 6H), 2.07 (bs, 3H), 3.53-3.54 (m, 6H), 3.59-3.60 (m, 8H), 3.66 (t, J = 4.1 Hz, 2H); ¹³C NMR (125 MHz, CDCl₃) δ ppm: 29.50, 35.43, 40.39, 40.48, 58.52, 60.73, 69.25, 69.50, 69.58, 69.61, 70.27, 71.48, 71. 64; GC-MS (EI)-m/z of C₁₈H₃₂O₅: 328.22 (calcd.); 328 (expt.).

Synthesis of G4: A solution of G3 (1.0 g, 3.04 mmol) in dry DMF (7 mL) was cooled to 0 °C, NaH (0.182 g, 3.65 mmol) was added and stirred for 30 min. subsequently propargyl bromide (0.434 g, 6.36 mmol) was added. Reaction mixture was stirred at 0 °C for 6 h. It was allowed to reach room temperature, and was quenched with ice cold water, extracted with DCM, washed with water and brine and solvent was removed under reduced pressure to get the crude product which was further purified using column chromatography using DCM:MeOH (98:2) as eluent to get desired product as yellow oil (80%); TLC
(DCM:MeOH, 98:2), R<sub>f</sub> = 0.3. ¹H NMR (500 MHz, CDCl<sub>3</sub>) δ ppm: 1.50-1.57 (m, 6H), 1.67 (s, 6H), 2.06 (s, 3H), 2.34 (s, 1H), 3.50-3.51 (m, 4H), 3.57-3.62 (m, 12H), 4.13 (s, 2H); ¹³C NMR (125 MHz, CDCl<sub>3</sub>) δ ppm: 30.53, 36.48, 41.50, 58.43, 59.28, 69.15, 70.43, 70.61, 70.62, 70.64, 71.30, 72.26, 74.48, 79.69. GC-MS (El)-m/z of C<sub>20</sub>H<sub>32</sub>O<sub>5</sub>: 352.225 (calcd.); 351 (expt).

**Synthesis of R6:** A solution of paraformaldehyde (2.0 g, 66.6 mmol) suspended in 115.6 mL of freshly distilled pyrrole (1.66 mol) was degassed for 5 min. Then TFA (0.5 mL, 6.66 mmol) was added and stirred up to 10 min. After the completion of reaction, trimethylamine was added to quench the reaction mixture and then excess pyrrole was removed by vacuum distillation. The product was purified by column chromatography using DCM as eluent to obtain desired product as colourless solid. M.P. 68.9 ºC; TLC (DCM), R<sub>f</sub> = 0.72; ¹H NMR (500 MHz, CDCl<sub>3</sub>) δ ppm: 3.91 (s, 2H), 5.96 (s, 2H), 6.07 (s, 2H), 6.57 (s, 2H), 7.82 (bs, 2H); ¹³C NMR (125 MHz, CDCl<sub>3</sub>) δ ppm: 28.69, 105.33, 107.40, 116.20, GC-MS (EI)-m/z of C<sub>9</sub>H<sub>10</sub>N<sub>2</sub>: 146.08 (calcd.); 146 (expt.).

**Synthesis of R8:** To a solution of 3, 5-dihydroxybenzaldehyde (0.85 g, 6.20 mmol), R<sub>4</sub> (1.0 g, 6.20 mmol) and R<sub>6</sub> (1.81 g, 4.40 mmol) in DCM:MeOH (20:5, 600 mL), was added BF<sub>3</sub>.OEt<sub>2</sub> (2.0 mL) under nitrogen at room temperature and was stirred in dark for 12 hr. To this mixture DDQ (4.22 g, 18.61 mmol), was added and the reaction mixture was stirred for an additional 12 h at room temperature. After that the reaction mixture was concentrated to volume of 50 mL and then filtered through silica gel using DCM:MeOH (97:3) as eluent. Without further purification, the product was dissolved in 10% MeOH/DCM containing Zn(OAc)<sub>2</sub> (1.303 g, 5.936 mmol) and then stirred for 12 h at room temperature. Solvent was removed under reduced pressure and the reaction mixture was purified by column chromatography with DCM:MeOH (97:3), to get desired product as reddish purple solid (15%). M.P. >300 ºC; TLC (DCM:MeOH, 96:4), R<sub>f</sub> = 0.41; ¹H NMR (500 MHz, CD<sub>3</sub>OD) δ ppm: 4.69 (s, 2H), 6.68 (s, 1H), 7.14 (s, 2H), 7.74 (d, J = 6.8 Hz, 2H), 8.21 (d, J = 7.0 Hz, 2H), 8.92 (d, J = 3.9 Hz, 2H), 9.11 (d, J = 3.6 Hz, 2H), 9.34 (s, 4H), 10.19 (s, 2H); ¹³C NMR (125 MHz, CD<sub>3</sub>OD) δ ppm: 54.41, 29.42, 47.08, 47.25, 47.42, 47.59, 47.76, 47.88, 47.93, 48.05, 48.10, 48.22, 54.41, 58.71, 101.38, 105.24, 114.59, 124.15, 126.21, 127.00, 129.24, 131.04, 131.17, 134.67, 137.13, 143.45, 145.42, 148.60, 149.69, 152.95, 155.99, 160.63. MALDI-TOF MS-m/z of C<sub>33</sub>H<sub>22</sub>N<sub>7</sub>O<sub>2</sub>Zn: [M+H]<sup>+</sup> 612.11 (calcd.); 612.10 (expt.).
Synthesis of R9: In dry THF (5 mL), mixture of 1-bromododecane (0.8 mL, 3.9 mmol), R8 (0.12 g, 0.194 mmol), anhydrous K$_2$CO$_3$ (0.268 g, 1.94 mmol) and 18-crown-6 (0.01 g, 0.039 mmol) were refluxed under nitrogen for 24. The product was extracted with DCM, washed with water and dried on anhydrous sodium sulphate and solvent was removed under reduced pressure. The residue was purified by column chromatography on silica gel using petroleum ether:DCM (80:20) as eluent to obtain bright red colour solid (70%). M.P. 86 °C; TLC (petroleum ether:DCM, 80:20), R$_f$ = 0.5; $^1$H NMR (500 MHz, CDCl$_3$) δ ppm: 0.77 (t, J = 7.0 Hz, 6H), 1.18-1.29 (m, 25H), 1.38-1.43 (m, 10H), 1.77-1.81 (m, 5H), 4.06 (t, J = 2.5 Hz, 4H), 4.50 (s, 2H), 6.83 (t, J = 5.0 Hz, 1H), 7.35 (d, J = 2.5 Hz, 2H), 7.58 (d, J = 8.0 Hz, 2H), 8.17 (d, J = 8.0 Hz, 2H), 9.00 (d, J = 4.5 Hz, 2H), 9.19 (d, J = 4.5 Hz, 2H), 9.34 (t, J = 4.0 Hz, 4H), 10.21 (s, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$) δ ppm: 14.06, 22.65, 26.13, 29.31, 29.45, 29.59, 29.60, 29.64, 31.89, 54.85, 68.44, 101.01, 106.25, 114.55, 119.19, 120.14, 126.43, 131.75, 131.79, 132.25, 132.71, 134.58, 134.93, 142.76, 144.27, 149.47, 149.64, 149.88, 150.07, 158.37. MALDI-TOF MS-m/z for C$_{57}$H$_{71}$N$_7$O$_2$: [M-Zn+2H]$^+$ 885.56 (calcld.); 885.59 (expt).

Synthesis of 2: To a solution of R9 (0.053 g, 0.059 mmol) suspended in t-BuOH/water 1:1 mixture (10 mL) was added, CuSO$_4$·5H$_2$O (0.0029 g, 0.011 mmol), sodium ascorbate (0.0094 g, 0.047 mmol) and G4 (0.043 g, 0.119 mmol ), and stirred at 70 °C for 72 h. After completion of reaction, it was allowed to cool to room temperature, solvent was removed under reduced pressure, and residue was dissolved in DCM. Organic phase was washed with brine, dried over anhydrous sodium sulphate and solvent was removed to get the crude product which was further purified through column chromatography using DCM:MeOH (97:3) to get desired product as red sticky solid (70%); TLC (DCM:MeOH, 97:3), R$_f$ = 0.3; $^1$H NMR ( 500 MHz, CDCl$_3$) δ ppm : 0.79 ( t, J = 7.0 Hz, 6H), 1.18-1.39 ( m, 39H), 1.43-1.66 ( m, 33H), 1.81 ( m, 4H), 1.99 ( bs, 3H), 2.06 ( bs, 2H), 2.68 ( bs, 2H), 3.18 ( bs, 2H), 3.36-3.57 ( m, 18H), 4.09 ( t, J = 6.50 Hz, 4H), 4.62 ( s, 2H), 6.69 ( bs, 1H), 6.84 ( bs, 2H), 6.81 ( s, 1H), 7.92 ( d, J = 7.0 Hz, 2H), 8.80 ( d, J = 4.0 Hz, 2H), 9.17 ( d, J = 4.0 Hz, 2H), 9.33-9.36 ( m, 4H), 10.24 ( s, 2H). $^{13}$C NMR (125 MHz, CDCl$_3$) δ ppm: 14.06, 24.58, 28.07, 28.23, 28.34, 28.57, 28.68, 29.01, 29.48, 30.91, 31.73, 35.43, 40.46, 58.27, 66.70, 66.94, 68.94, 69.63, 69.73, 69.95, 70.29,
71.28, 89.13, 101.86, 104.07, 109.03, 111.66, 113.26, 119.59, 123.59, 129.09, 134.35, 142.22, 145.35, 149.41, 152.70, 157.41. MALDI-TOF MS-m/z for C_{77}H_{101}N_{7}O_{7}ZnK [M+K]^+: 1338.66 (calcd.); 1338.84 (expt.).

**Synthesis of D3:** To a stirred solution of *p*-toluenesulfonyl chloride (5.0 g, 26.22 mmol) in dry dichloromethane (25 mL), a solution of imidazole (3.6 g, 57.68 mmol) in dry dichloromethane (25 mL) was added drop wise over a period of 1 h at 0 °C under nitrogen. The resulting mixture was allowed to cool to room temperature and was stirred vigorously further for 2 h. The reaction mixture was then filtered. The filtrate was concentrated under reduced pressure, and then purified by column chromatography using dichloromethane as eluent to give a white crystalline solid (90%). TLC (DCM), R_f = 0.6, ^1H NMR (500 MHz, CDCl_3, δ ppm): 2.30 (s, 3H), 6.94 (s, 1H), 7.15 (s, 1H), 7.23 (d, J = 8.2 Hz, 2H), 7.70 (d, J = 8.2 Hz, 2H), 7.87 (s, 1H); ^13C NMR (125 MHz, CDCl_3, δ ppm : 21.79, 117.52, 127.44, 130.51, 131.48, 135.02, 136.73,146.42. MS (EI)-m/z of C_{10}H_{10}N_{2}O_{2}S: 222.04 (calcd.), 222 (expt).

**Synthesis of D5:** D4 (19.0 g, 16.74 mmol) and D3 (4.83 g, 21.76 mmol) were mixed in deionized water (190 mL) with vigorous stirring for 4 h at room temperature. Then gradually added 50 mL of aqueous NaOH solution 20% (W/V) to the reaction mixture and continued stirring for an additional 10 min. Filtered off the insoluble solid and neutralized the filtrate to pH 7-6 with dilute HCl, then the solution was saturated with ammonium chloride upon which a white thick precipitate was observed. The precipitate was filtered in sintered funnel and was subsequently washed with cold water (50 mL) and acetone (50 mL). The residue was allowed to dry in vacuum pump for 1 h and was further recrystallized with hot water to give a desired product as a white powder (15%). ^1H NMR (500 MHz, DMSO-d_6, δ ppm): 2.48 (s, 3H), 3.20-3.64 (m, 40H), 4.16-4.19 (m, 1H), 4.30-4.34 (m, 2H), 4.43-4.48 (m, 5H), 4.75 (bs, 2H), 4.81-4.83 (m, 5H), 5.62-5.81 (m, 14H), 7.43 (d, J = 8.2 Hz, 2H), 7.74 (d, J = 8.2 Hz, 2H); ^13C NMR (125 MHz, DMSO-d_6, δ ppm): 21.75, 60.45, 72.60, 72.71, 72.90, 72.97, 73.27, 73.61, 81.31, 81.96, 82.05, 82.21, 101.82, 102.47, 102.77, 128.12, 130.44, 133.21, 145.36. MALDI-TOF MS-m/z of C_{49}H_{76}O_{37}Na: [M+Na]^+: 1311.36 (calcd.); 1311.46 (expt.).
Synthesis of D6:[S2] To a stirring suspension of D5 (2.0 g, 1.554 mmol) in 200 mL of water, sodium azide (2.01 g, 31.028 mmol) was added and the mixture was refluxed overnight. After the completion of reaction, the mixture was cooled to room temperature and filtered the mixture. Subsequently the reaction mixture was concentrated under reduced pressure, followed by the addition of acetone (300 mL) to the mixture and a white precipitate was observed. The precipitate was filtered in sintered funnel and subsequently washed with acetone (5 X 10 mL) then dried in vacuum. Recrystallized the white solid in hot water and dried in vacuum at 60 °C overnight to give desired product as white crystalline solid (53%). 1H NMR (500 MHz, DMSO-d6, δ ppm): 3.31-3.76 (m, 43H), 4.47-4.55 (m, 6H), 4.83-4.88 (m, 7H), 5.63-5.75 (m, 14H); 13C NMR (125 MHz, DMSO-d6, δ ppm): 60.48, 60.68, 70.73, 72.57, 72.74, 72.94, 73.34, 73.41, 73.59, 79.69, 81.95, 82.08, 82.40, 83.52, 101.13, 102.48, 102.82. MALDI-TOF MS-m/z of C42H70N3O34: [M+H]+ 1160.38 (calcd.); 1159.94 (expt.).

Synthesis of modified DNAs: Oligonucleotides were synthesized on 1 μmol scale with a CPG of loading density 1000 Å, as the solid support using conventional phosphoramidite chemistry. Natural oligonucleotides were synthesized using the standard protocols. Modified phosphoramidites, 5'-dimethoxytrityl-5-(octa-1,7-diynyl)-2'-deoxyuridine, 3'-(2-cyanoethyl)-(N,N-diisopropyl)-phosphoramidite (C8-alkyne-dU) and 6-(4,4'-dimethoxy-4'-methylsulfonyl-tritylaminohexyl-(2-cyanoethyl)-(N,N-diisopropyl)-phosphoramidite (C6-amine) were introduced at the 5'-end using the standard protocols with an extended coupling time of 30 minutes. In the case of alkyne modified DNA the trityl-off oligonucleotides were cleaved off the resin and was deprotected by treatment with concentrated NH4OH (28 %, 1 mL) at room temperature for 24 h. C8-alkyne modified DNA was further used for click reaction. In the case of C6-amine modified DNA, trityl-on oligonucleotides was deprotected by treatment with concentrated NH4OH (28 %, 1 mL) at room temperature for 24 h was subsequently purified by High Performance Liquid Chromatography (HPLC) using ammonium acetate buffer (20 mM, pH 6.5) and acetonitrile.
as eluents. Purified DNA was treated with 1 mL of 20:80 acetic acid-water mixture for the removal of DMS(O)MT group for 1 h at room temperature. Solution will become hazy due to the release of DMS(O)MT alcohol, which is not soluble in water. DMS(O)MT alcohol was removed by extracting the solution with ethyl acetate where DNA will be in the aqueous layer, which was collected, concentrated and used directly for further reactions.

**Synthesis of DNA-β-CD:** To 113.4 μL of D6 (100 mM, 11.34 μmol, 25 eq.), 113.4 μL of a freshly prepared solution containing Cu(I)Br (100 mM, 11.34 μmol, 25 eq.) and TBTA (200 mM, 22.68 μmol, 50 eq.) in DMSO:t-BuOH (3:1) was added. The mixture was degassed using three cycles of freeze-pump-thaw method. To this degassed solution, 5'-alkyne modified DNA solution (100 μL, 0.5 mM, 0.45 μmol) in water was added. The mixture was then vortexed and stirred at 60 °C for 24 hours. The reaction mixture was transferred into a 2 mL vial and DMSO was removed in speed vacuum concentrator and was further diluted with water, filtered using 0.45 μm filter size (PVDF membrane, Millipore Ultrafree MC) and was analysed using 20 % denaturing PAGE.

**Purification of DNA-β-CD:** The DNA strands were loaded into a 20% denaturing PAGE and was electrolysed (400 V, 75 mA, 50 W, 1 h 45min). After staining the gel with Ethidium bromide, it was viewed using a UV transilluminator. The gel was visualized under UV and the band corresponding to the β-CD conjugated DNA strand was cut out with a surgical scalpel. The cut out gel blocks were transferred into clean vials, crushed with a glass rod, mixed with 1 mL elution buffer [ammonium acetate (500 mM), magnesium acetate (10 mM), 0.5 M EDTA (pH 8.0)] and shaken at 1200 rpm overnight at room temperature. The filtrate was filtered out through centrifugal filters (0.45 μm filter size PVDF membrane, Millipore Ultrafree MC) at 8000 rpm for 6 minutes. Elution procedure was repeated for the residue for once again with 500 μL elution buffer. The final DNA filtrate was concentrated to ~200 μL. 1 mL n-butyl alcohol was added to the solution and vortexed for 2 min, before being centrifuged at 8000 rpm for 3 min. The upper layer (butanol) was discarded, and the lower aqueous layer remixed with 1 mL absolute ethanol and was stored overnight at -30 °C. The solution was centrifuged at 13000 rpm for 30 minutes at 4 °C and the precipitate re-suspended in 500 μL ice-cold 70 % ethanol, after which it was stored in -30 °C for 3-4 hr. It was centrifuged again at 13000 rpm for 10 minutes at 4 °C and ethanol was discarded. Solvent was completely removed from the pellet by keeping it in the speed vac. 200 μL of Milli-Q water was added to the pellet, it was vortexed to dissolve and characterized using ESI-MS.
DNA1-β-CD: 12897.076 (calcd.); 12895.560 (expt.) and DNA2-β-CD: 9807.076 (calcd.); 9807.934 (expt.).

Synthesis of DNA modified gold nanoparticle: DNA functionalized gold nanoparticles (~20 nm) were synthesized using the strategy reported by Yan and Liu et al. using lipoic acid-modified oligonucleotide.[S1] To 100 µL of amine modified DNA solution (0.16 µmol), 100 µL of sodium carbonate/bicarbonate buffer (pH 9), lipoic acid ester (0.004 g, 16.3 µmol) dissolved in 200 µL of DMF, were added and the reaction mixture was vortexed overnight at room temperature. After the reaction, unreacted ester was precipitated by adding 200 µL of water into the reaction mixture. Then it was filtered and then purified using reverse phase HPLC using ammonium acetate and acetonitrile as eluents. Lipoic acid conjugated DNA thus obtained was used for the surface modification of Au-NPs. For this, tris(2-carboxyethyl)phosphine hydrochloride (0.0012 g, 3.9 µmol) dissolved in 10 µL of 0.5 M tris buffer (pH 7) was added to lipoic acid labelled DNA (0.618 µmol) solution and vortexed for 1 h at room temperature. After purification using Glen gel pak 1.0 desalting columns, it was concentrated to 100 µL. Then 10 µL of 0.5XTBE (88 mmol trizma base, 89 mmol boric acid, 2 mM EDTA pH 8.0 ) buffer, AuNP (57 µL, 0.195 nmol) were added into the DNA (0.019 µmol) solution and vortexed at room temperature for 40 h. Then, 1 µL of 4M NaCl solution was added at an interval of 3 hrs. After 40 h, reaction mixture was centrifuged at 6000 rpm for 1 h and the colourless supernatant was removed. The red pellet was resuspended in 1 mL of water, centrifuged at 6000 rpm and the supernatant was removed. Concentration of these Au-NP-DNA conjugates was estimated from optical absorbance at ~520 nm, and used for further experiments.

Fig. S1 a) Native polyacrylamide gel (20%) of DNA1-β-CD & C8-alkyne modified DNA after staining with ethidium bromide solution. Retardation in electrophoretic mobility of DNA1-β-CD in comparison to C8-alkyne modified DNA confirms the conjugation. b) absorption spectrum of DNA1-β-CD. [DNA1-β-CD] = 1 µM.
Calculation of coupling efficiency

Coupling efficiency was calculated using the absorption spectral changes. Initially, absorption of DNA1-β-CD/1 conjugates was recorded. In order to remove any unconjugated DNA1-β-CD the solution was filtered using 30 KDa Amicon centrifugal filters (Milipore UFC5030BK) at 4000 rpm for 3 minutes. This was repeated for 15 times and absorption of the filtrate was recorded, which corresponds to the absorption of any unconjugated DNA1-β-CD. The self-assembled DNA1-β-CD/1 would remains in the residue.

Absorbance of DNA1-β-CD/1 at 260 nm before filtration = 0.411

Concentration of DNA1-β-CD/1 before filtration \( = 1.11 \times 10^{-6} \text{ M (} \varepsilon = 369600 \text{ cm}^{-1}\text{M}^{-1} \) 
\( = 5.55 \times 10^{-10} \text{ moles} \)

This corresponds to both conjugated (DNA1-β-CD/1) and unconjugated DNA (DNA1-β-CD)

Filtrate contains only DNA1-β-CD which are not conjugated with 1

Absorbance of filtrate at 260 nm \( = 0.048 \)

Concentration of unconjugated DNA1-β-CD \( = 1.298 \times 10^{-7} \text{ M} \)
\( = 1.298 \times 10^{-10} \text{ moles} \)

No. of moles conjugated DNA (DNA1-β-CD/1) \( = 5.55 \times 10^{-10} - 1.298 \times 10^{-10} \)
\( = 4.252 \times 10^{-10} \text{ moles} \)

Efficiency of coupling
\[
\frac{\text{No. moles of conjugated DNA1} - \beta - \text{CD}}{\text{Total no. of moles of DNA1} - \beta - \text{CD}} \times 100
\]
\[
\frac{4.252 \times 10^{-10}}{5.55 \times 10^{-10}} \times 100
\]
\( = 76.6 \% \)
Fig. S2 a) Temperature dependent emission spectrum of a) 1 in THF ($\lambda_{max} = 310$ nm) and b) 2 in THF ($\lambda_{max} = 420$ nm). This experiment shows the effect of temperature on the emission of 1 and 2.

Fig. S3 a) CD spectrum of a) DNA1-β-CD/1 and b) DNA1-β-CD/2. [DNA1-β-CD/1], [DNA1-β-CD/2] = 1 μM.

Fig. S4 Fluorescence spectra of calcein encapsulated in DNA1-β-CD/2 vesicle and calcein in vesicle-free solution ($\lambda_{ex} = 470$ nm).
Fig. S5 a) & b) Additional AFM images for DNA1-β-CD/1 vesicles (z-scale = 10 nm). Fitted histograms of c) size, and d) height distribution for DNA1-β-CD/1 vesicles. [DNA1-β-CD/1] = 1 μM. Histograms for the calculation of average size and height were plotted using about 400 random vesicles from different mica surfaces. Exactly, 378 and 427 vesicles were used for the construction of histograms for size and height, respectively.
Fig. S6 a) & b) Additional AFM images for DNA1-β-CD/2 vesicles (z-scale = 15 nm). Fitted histograms of c) size, and d) height distribution for DNA1-β-CD/2 vesicles. [DNA1-β-CD/2] = 1 μM. Exactly, 293 and 341 vesicles were used for the construction of histograms for size and height, respectively.

Fig. S7 AFM image of DNA1-β-CD/1 vesicle formed at room temperature.
Fig. S8 Additional TEM images of a) & b) DNA1-β-CD/1 and c)-f) DNA1-β-CD/2 vesicles. SEM images of DNA1-β-CD/2 vesicles. [DNA1-β-CD/1], [DNA1-β-CD/2] = 1 μM.

Fig. S9 TEM image for DNA2-β-CD/1 vesicles.
Fig. S10 Fluorescence microscopic image of a) DNA1-β-CD/1 and b) DNA1-β-CD/2 vesicles formed in serum. The corresponding TEM images of c) DNA1-β-CD/1 and d) DNA1-β-CD/2.

Fig. S11 Proposed scheme showing the membrane of [DNA1-β-CD/1] and [DNA1-β-CD/2] vesicles. Completely extended helical conformation for ssDNA, extended conformations for alkyl and glycol chains, and interdigitation of the alkyls chains were assumed for the membrane thickness calculations. Accordingly, membrane thicknesses of ~35 nm and ~37 nm were obtained for DNA1-β-CD/1 and DNA1-β-CD/2 vesicle, respectively.
Fig. S12 a-d) Additional TEM images for Au-NP (~20 nm) decorated DNA1-β-CD/2 vesicles. [DNA1-β-CD/2], [Au-NP] = 1 μM (0.5 × TBE buffer, NaCl = 50 mM, pH 7.5).
Fig. S13 Absorption spectral changes of AuNPs in the presence of DNA1-β-CD/2 vesicle. NPs are coated with a) non-complementary DNA (NC-DNA) and b) without DNA (bare). c) & d) The corresponding emission spectral changes and e) & f) the corresponding TEM images.
Fig. S14 Additional fluorescence microscopy images for a) & b) DNA1-β-CD/1 vesicles, and c) & d) DNA1-β-CD/2 vesicles. [DNA1-β-CD/1], [DNA1-β-CD/2] = 1 μM.
Fig. S15 Stern-Volmer plot of quenching of DNA1-β-CD/2 vesicle emission with the addition of ~20 nm Au-NP.
Fig. S16 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of P2.
Fig. S17 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of P3.
Fig. S18 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of P4.
Fig. S19 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of P5.
Fig. S20 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of P6.
Fig. S21 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of P7.
Fig. S22 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of P8.
Fig. S23 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of P9.
Fig. S24 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of 1.
Fig. S25 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of R8.

Fig. S26 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of R9.
Fig. S27 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of 2.

![NMR spectra of 2](image1)

Fig. S28 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of R2.
Fig. S29 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of R3.
Fig. S30 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of R4.
Fig. S31 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of R6.
Fig. S32 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of G3.
Fig. S33 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of G4.
Fig. S34 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of D3.
Fig. S35 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of D5.
Fig. S36 $^1$H (top) and $^{13}$C-NMR (bottom) spectra of D6.
References
