

Synthesis and Self-assembly of a DNA Molecular Brush

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Supporting Information

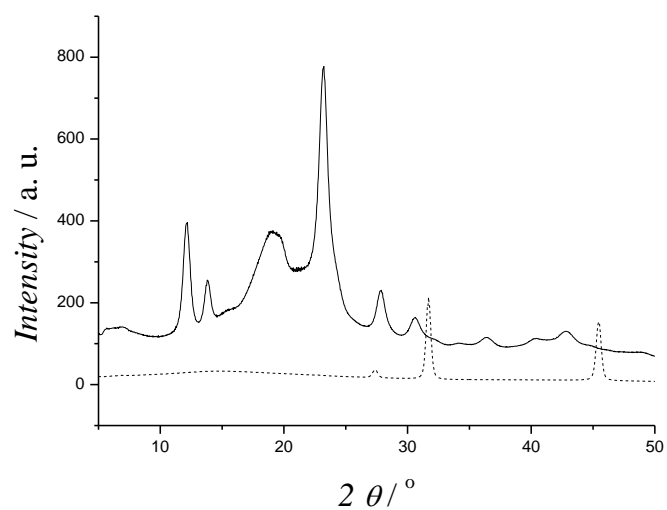


Figure S1. X-ray diffraction curve of freeze-dried precipitate of PBOX, prior to (dashed line) and subsequent to crystallization (solid line) of a 1 wt% polymer solution in ethanol–water 55:45 (w/w) at room temperature

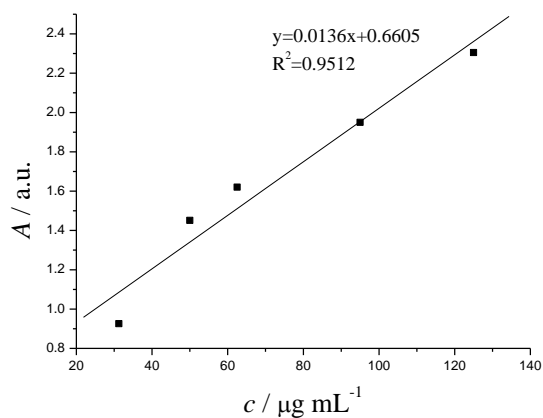


Figure S2. Absorbance calibration curve of the nucleic acid sequence recorded at 268 nm.

UV-Vis grafting density estimation. PBOX absorbance at 268 nm is negligible

For a representative quantification of the grafting density: absorbance value at 268;

$$A_{268} = 1.809$$

Thus, concentration is equal to;

$$x = (1.809 - 0.6605) / 0.0136 = 84.5 \mu\text{g mL}^{-1}$$

Concentration for measurement; 0.1 mg mL^{-1} , volume; 1mL

$$m_{\text{DNA}} = 84.5 \mu\text{g}$$

$$M_{\text{PBOX}} = 5381.45 \text{ g mol}^{-1}$$

$$M_{\text{DNA}} = 3709.9 \text{ g mol}^{-1}$$

$$m_{\text{PBOX}} = 100 - 84.5 = 15.5 \mu\text{g}$$

$$n_{\text{PBOX}} = 15.5 \times 10^{-6} / 5381.45 = 2.9 \text{ nmol}$$

$$m_{\text{DNA}} = 84.5 \mu\text{g}$$

$$n_{\text{DNA}} = 84.5 \times 10^{-6} / 3709.9 = 22.8 \text{ nmol}$$

$$n_{\text{DNA}} / n_{\text{PBOX}} = 7.86 \approx \mathbf{8 \text{ DNA strands for one PBOX chain}}$$

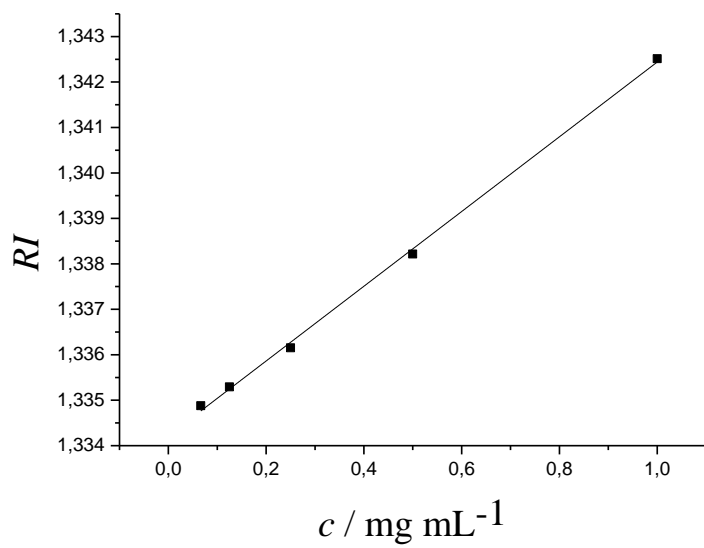


Figure S3. Refractive index (RI) dependence on concentration (c): $\frac{dn}{dc} = 0.0082 \text{ cm}^3 \text{g}^{-1}$

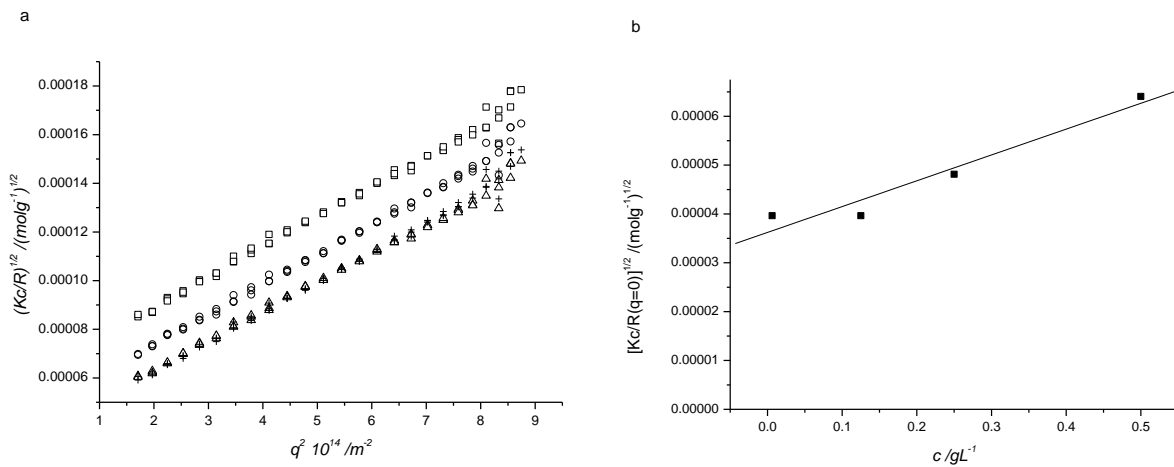


Figure S4. Berry analysis of the scattered intensity as assessed by static light scattering a) angle dependence for \square) 0.5, \circ) 0.25, Δ) 0.125 et $+$) 0.00625 g L^{-1} ; b) concentration dependence subsequent to 0 angle extrapolation

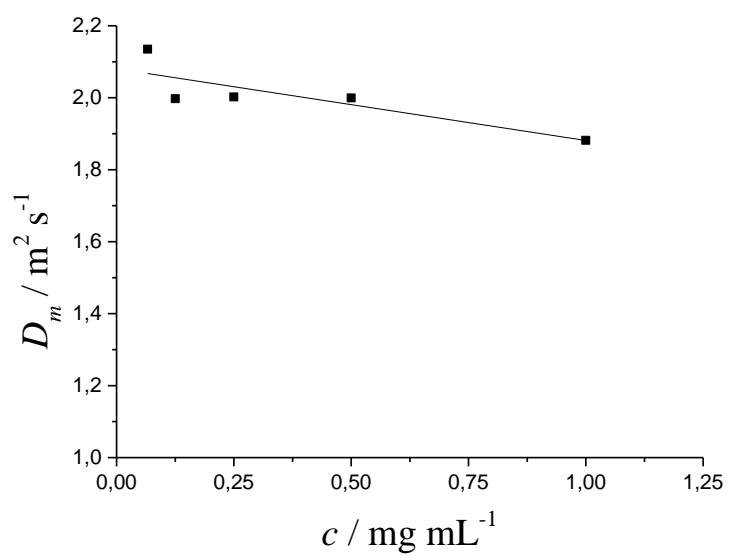


Figure S5. Concentration dependence of the mutual diffusion coefficient as measured by dynamic light scattering

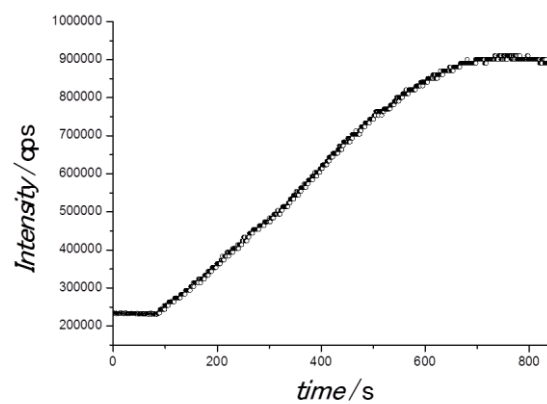


Figure S6. Time course of the fluorescein fluorescence intensity subsequent to encapsulation (concentration) and release by addition of sodium azide

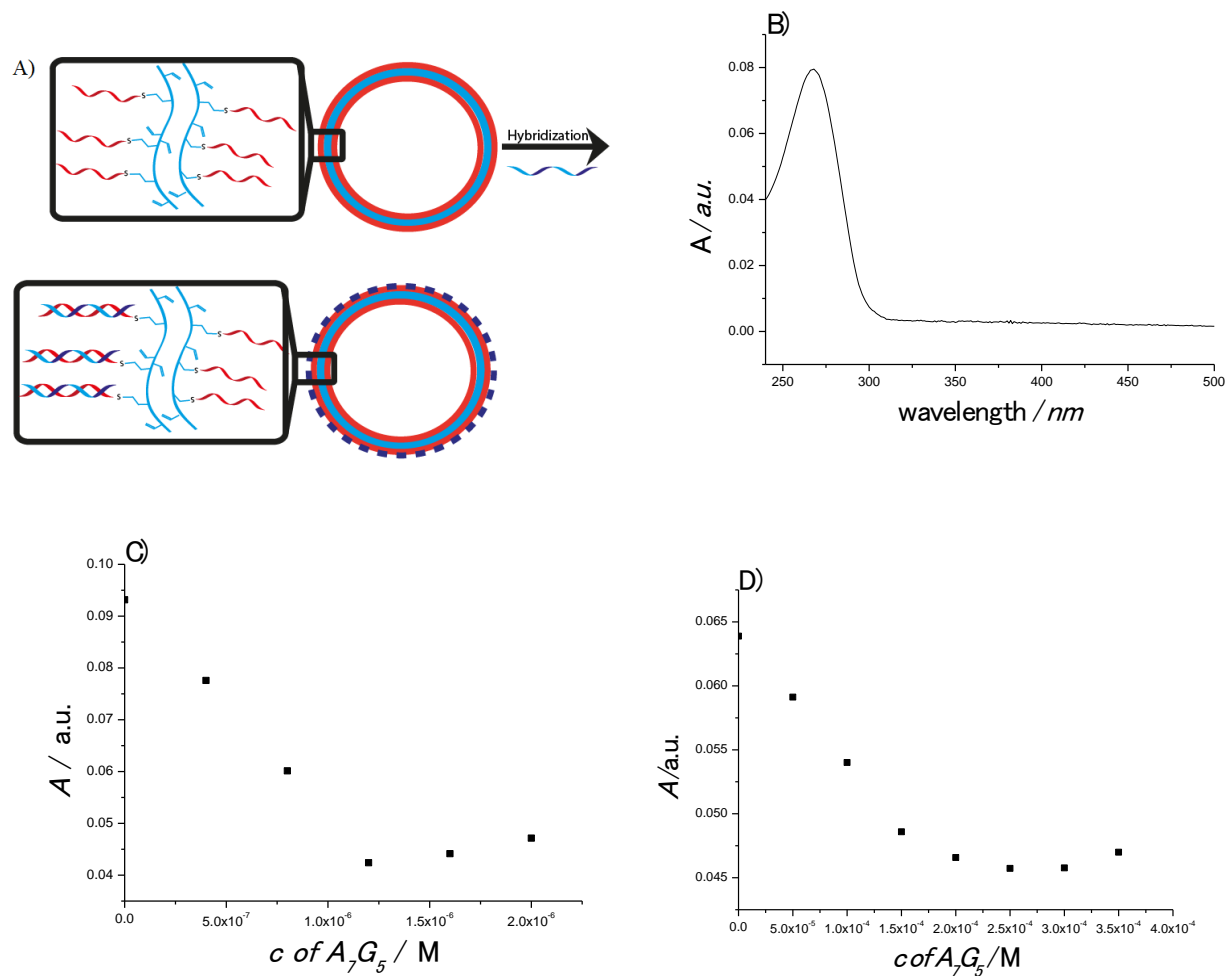


Figure S7. A) Schematic representation of hybridization. B) Representative spectrum which rules out hindrance owing to scattering C) Titration upon hybridization (maximum absorbance at 268 nm) D) Control hybridization of free C_5T_7 with A_7G_5 . Efficiency 100%: all complementary sequences did hybridize

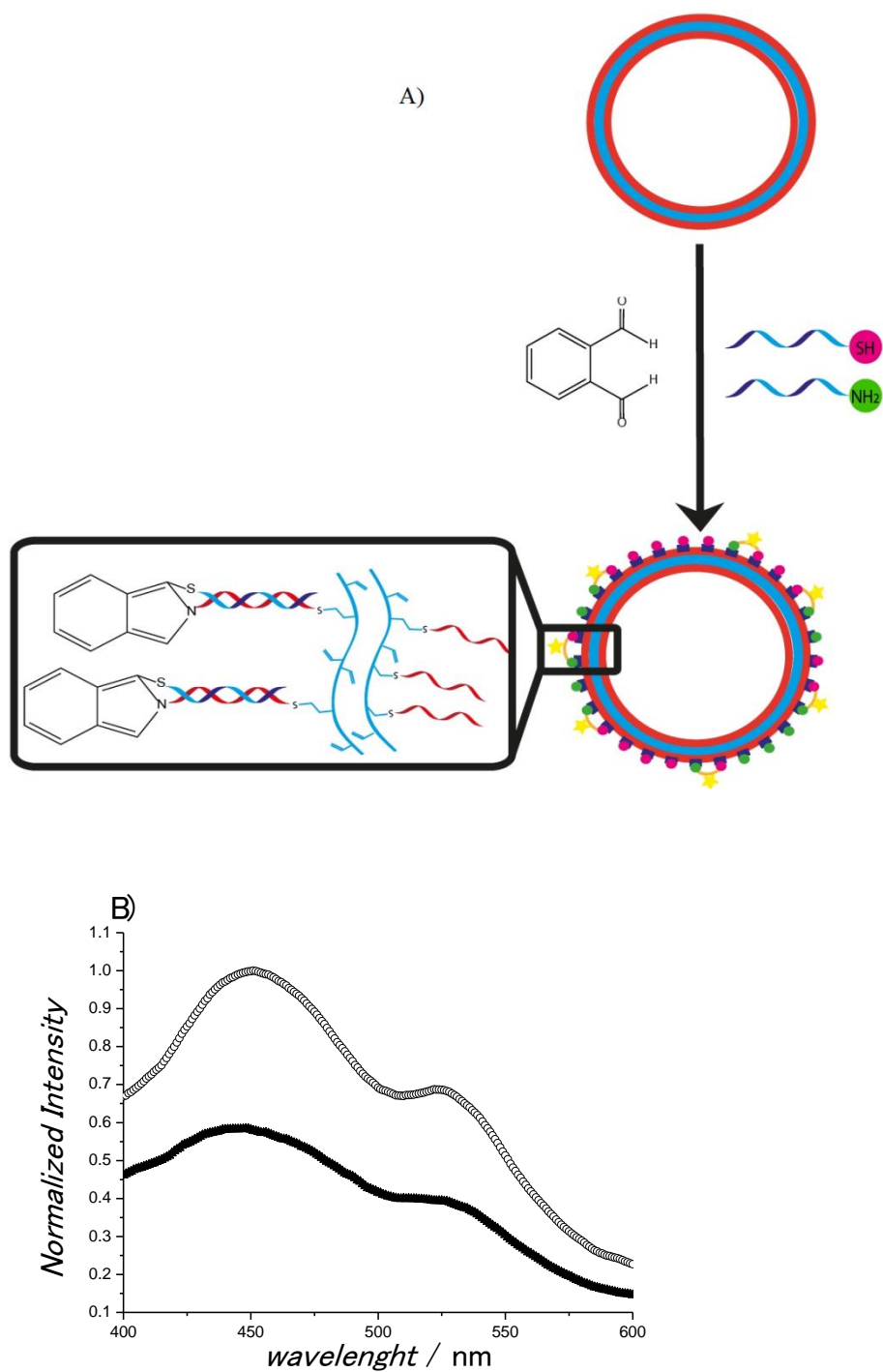


Figure S8. A) Schematic representation of isoinдол reaction; B) Fluorescence spectroscopy upon isoinдол formation at the surface of PBOX spheres, ▲) initial stage of reaction, ○) reaction completed

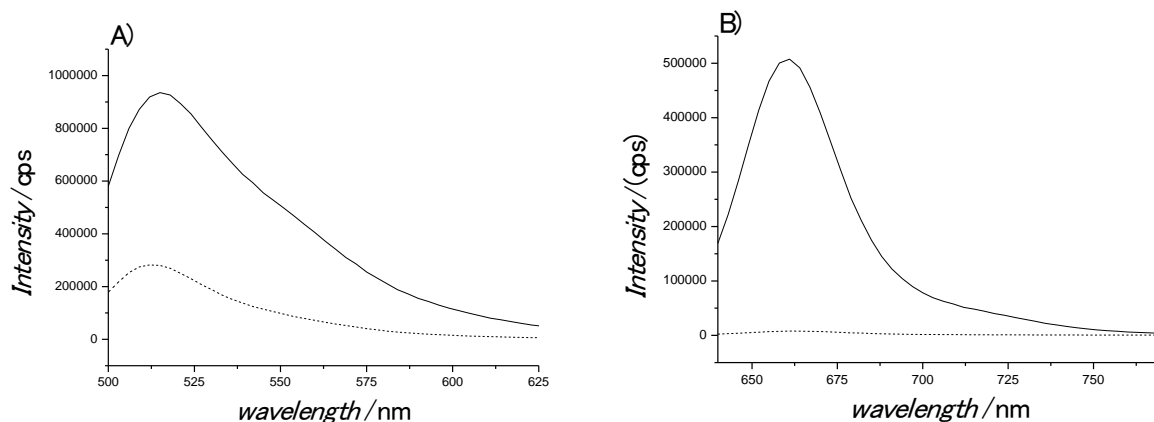


Figure S9. Fluorescence intensity spectra upon speciation (solid line: before washing; dotted line: after washing) of a solution of PBOX-g-DNA self-assembled structures incubated with the complementary sequence stained with A) FITC which hybridizes with the nucleic acid grafts engaged in self-assembly and B) the non-complementary sequence labeled with Cy5 which remains in solution before washing (background). Subsequent to washing, the complementary sequence stained with FITC hybridizes with the PBOX-g-DNA composing the self-assembled structure, being the non-complementary sequence removed during the washing process (no background).

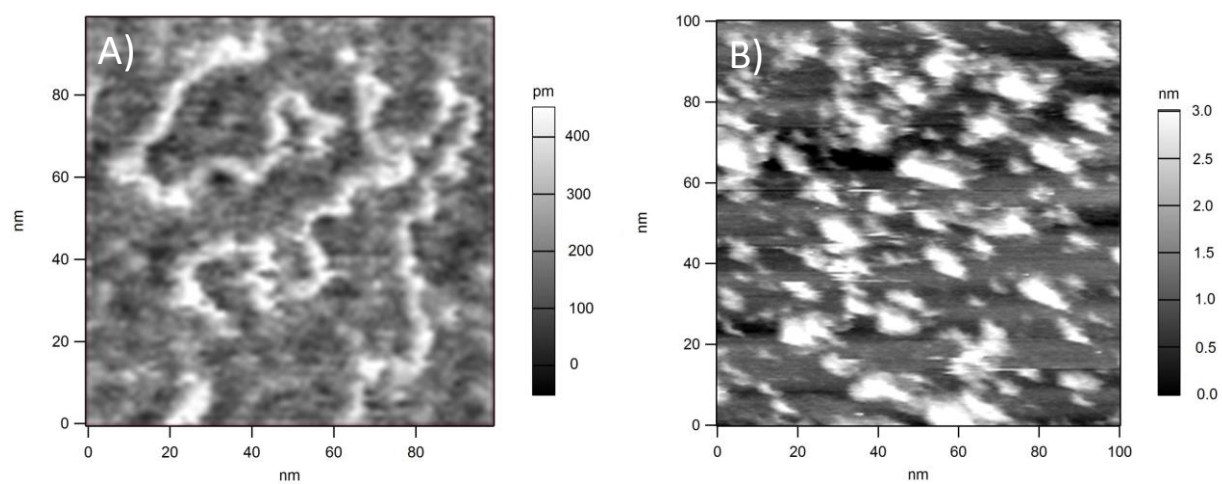
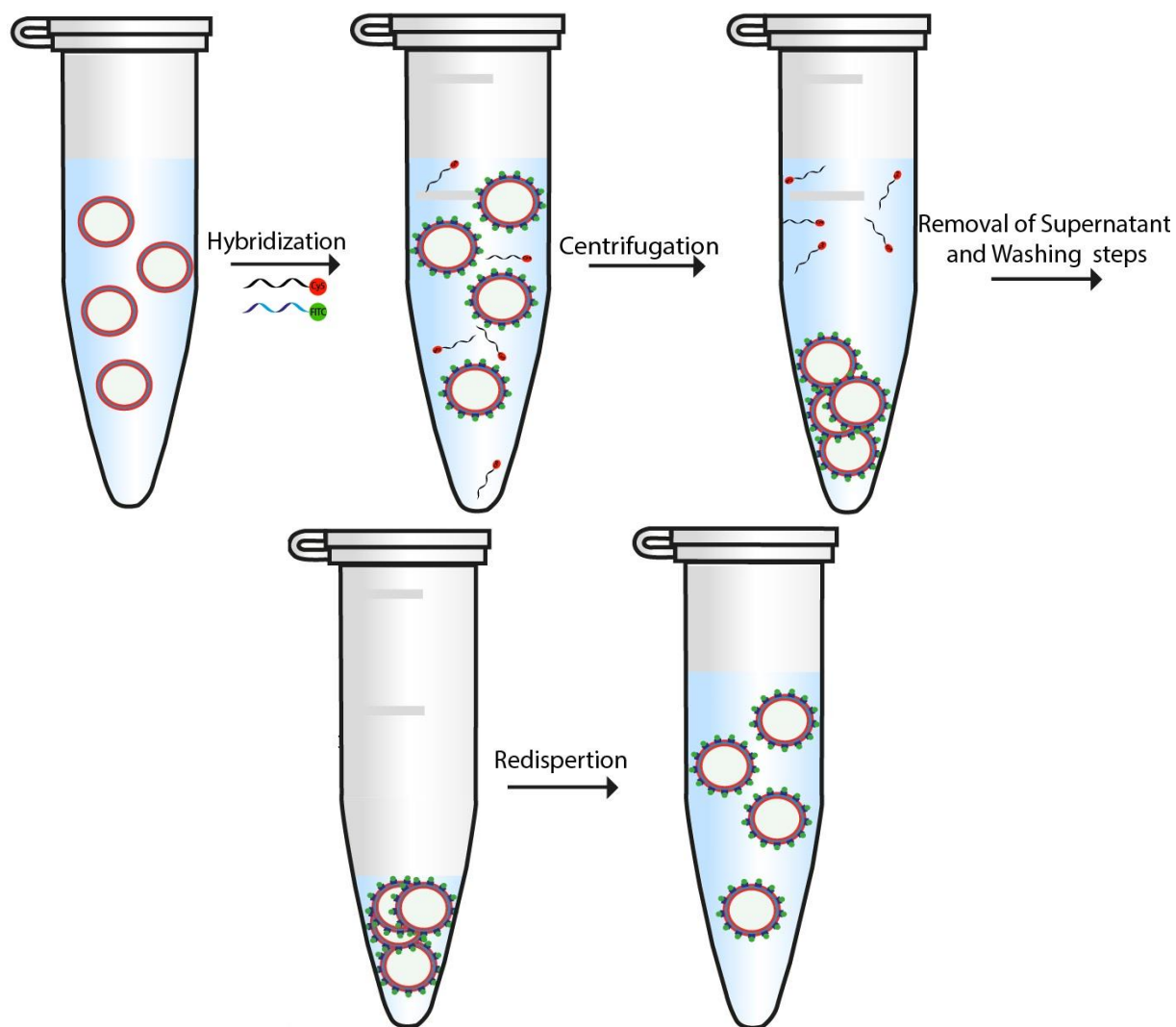


Figure S10. Atomic force microscopy imaging of A) molecularly dissolve PBOX polymer chains adsorbed on mica B) PBOX-g-DNA copolymer adsorbed on mica



Scheme S1. Procedure for sorting out nucleotides sequences with the use of PBOX-g-DNA spheres.

Wavenumber (cm ⁻¹)	Assignments
920	Vinyl C=CH ₂
970	P-O in (R-O) ₂ -PO ₂ upper band
1064	P=O in (R-O) ₂ -PO ₂ lower band
1226	P=O in (R-O) ₂ -PO ₂ upper band
1471	N-H stretching
1652	C=O amide I

Table S1: Significant FTIR vibration bands and their corresponding wavenumbers