

Programmed assembly of polymer–DNA conjugate nanoparticles with optical readout and sequence-specific activation of biorecognition.

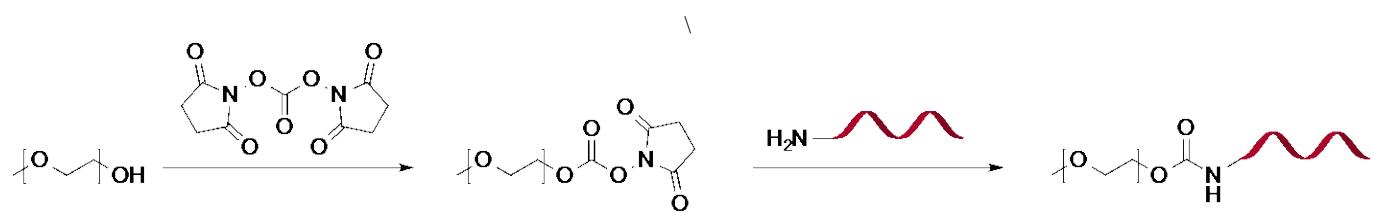
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Synthesis of PEGylated DNA strands



Scheme 1 Synthesis of mPEG-NHS and PEGylated oligonucleotides.

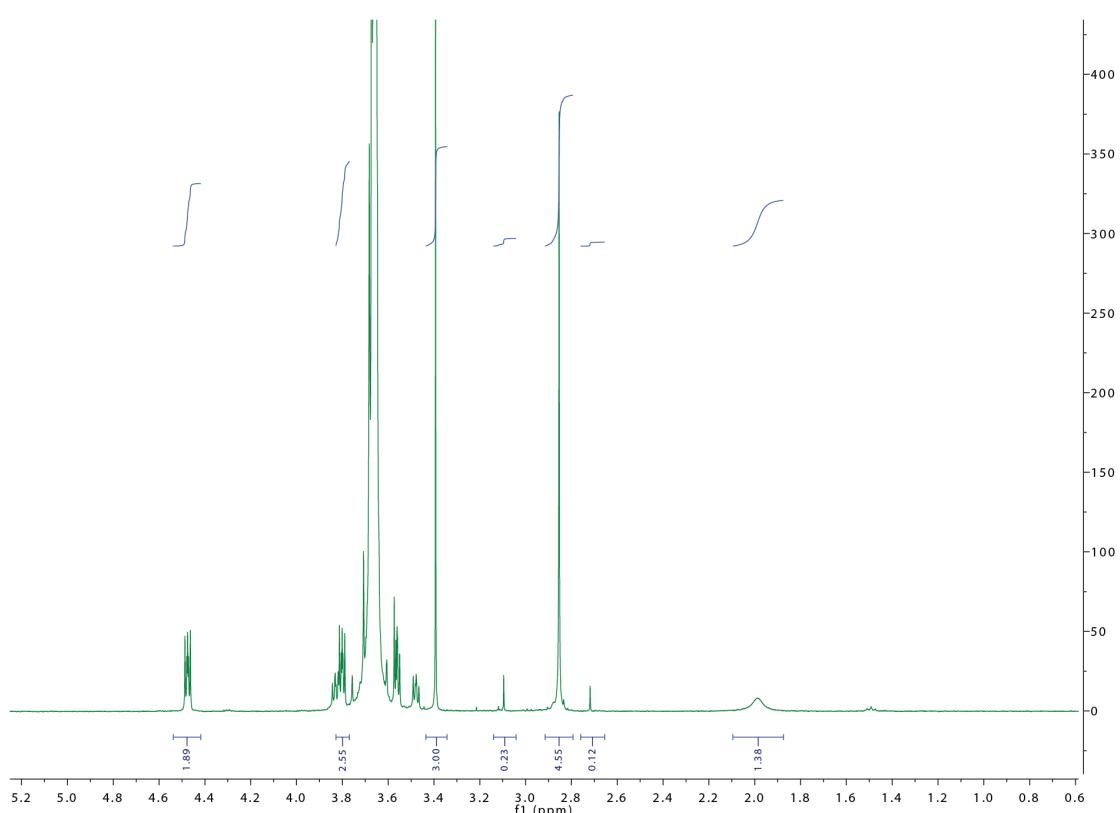


Figure S1 ^1H NMR spectra of mPEG-NHS

HPLC Analysis

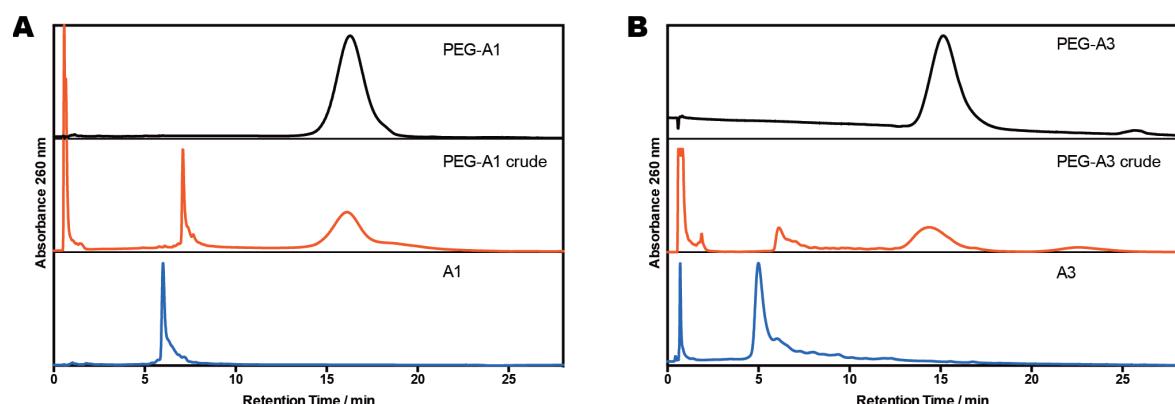


Figure S2 HPLC analysis of oligonucleotides before and after PEGylation and subsequent purification. **A.** Oligonucleotide A1; **B.** oligonucleotide A3.

MALDI analysis

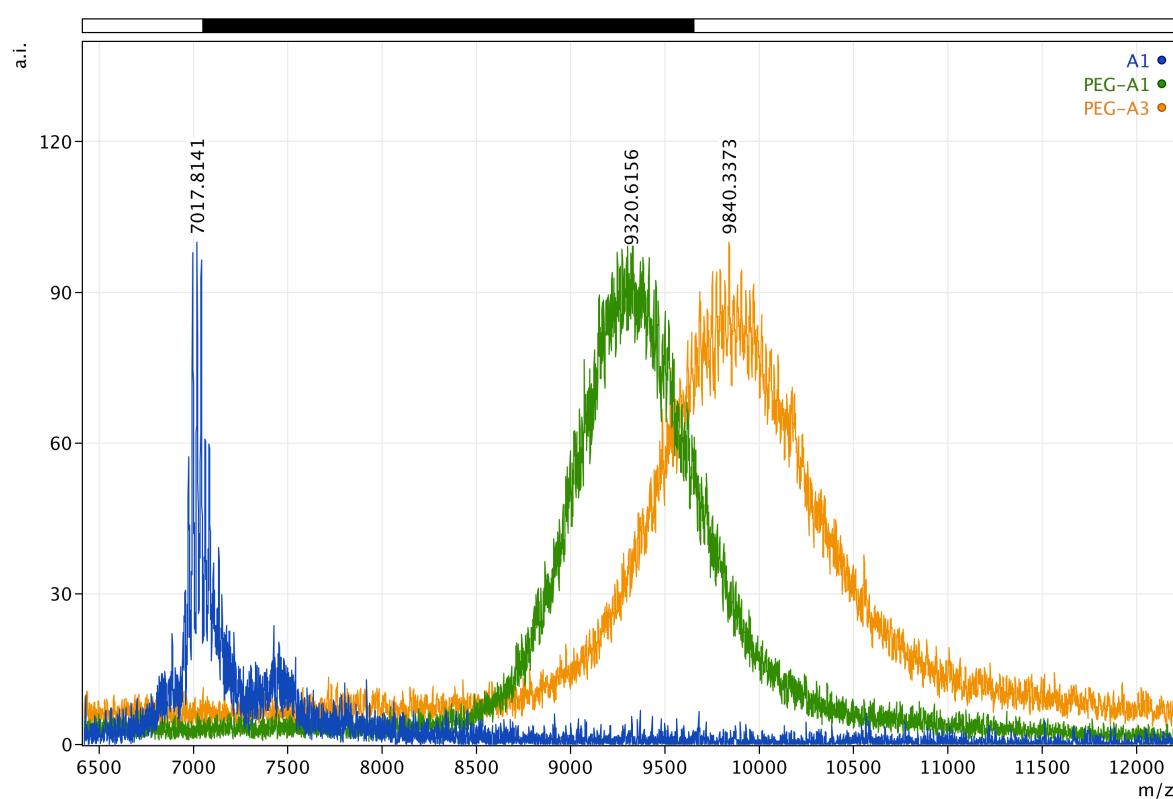


Figure S3 MALDI-TOF mass spectrometry of oligonucleotides before and after PEGylation. Spectrum of A3 prior to PEGylation is not shown as the unmodified oligonucleotide would not ionise successfully.

Oligo A1 m/z 7017, [M+H]⁺ requires 7038.

Mass expected for conjugation of PEG to A1:

$$\begin{aligned} M_{A1} + M_{\text{Linker}} + M_{\text{Me}} + n \times M_{\text{CH}_2\text{CH}_2\text{O}} &= 7038 + 44 + 15 + (n \times 44) \\ &= 7097 + n \times 44 \end{aligned}$$

If n = 51, then [PEG-A1+H]⁺ requires 9341, found 9320.

$$M_{A3} = 7593$$

$$[\text{PEG-A3+H}]^+ = 7652 + n \times 44$$

$$n = 50, \text{ requires } 9852, \text{ found } 9840$$

Buffers and Solutions

Table S2 Solutions and buffers used herein

Solution	Components
Hybridization buffer	10 mM tris-HCl 50 mM NaCl 1 mM EDTA Dissolved in DNase free water and adjusted to pH 7.5.
Denaturing loading buffer	900 µL formamide 22.2 uL 0.5 M EDTA (pH 8) 26.5 uL 7.5 % Orange G 51.3 uL water
Denaturing PAGE gel (15%) Provides 7.5 mL of gel suitable for casting 1 0.75 mm thick minigel	2.82 mL 40% acrylamide/bis-acrylamide 29/1 3.6 g urea 0.75 mL 10 × TBE 0.85 mL water 37.5 µL 10 wt% ammonium persulfate 3.75 µL TEMED
Native loading buffer	100 µL glycerol 100 µL 10 × TBE 800 µL water For the ladder 20 µL of 7.5% Orange G was added with a equal reduction in the volume of water added
Native PAGE gel (20%) Provides 7.5 mL of gel suitable for casting 1 0.75 mm thick minigel	3.75 mL 40% acrylamide/bis-acrylamide 29/1 0.75 mL 10 × TBE 3 mL water
Methylene blue staining solution	200 mg methylene blue 100 mL 10 × TBE 900 mL water
Stains-All solution (0.1%)	20 mg Stains-All 20 mL formamide
Destaining buffer	30 mL 20 mM tris buffer pH 8 10 mL propan-2-ol
Stains-All staining solution	5 mL 0.1% Stains-All solution 20 mL destaining buffer

Dynamic light-scattering (DLS)

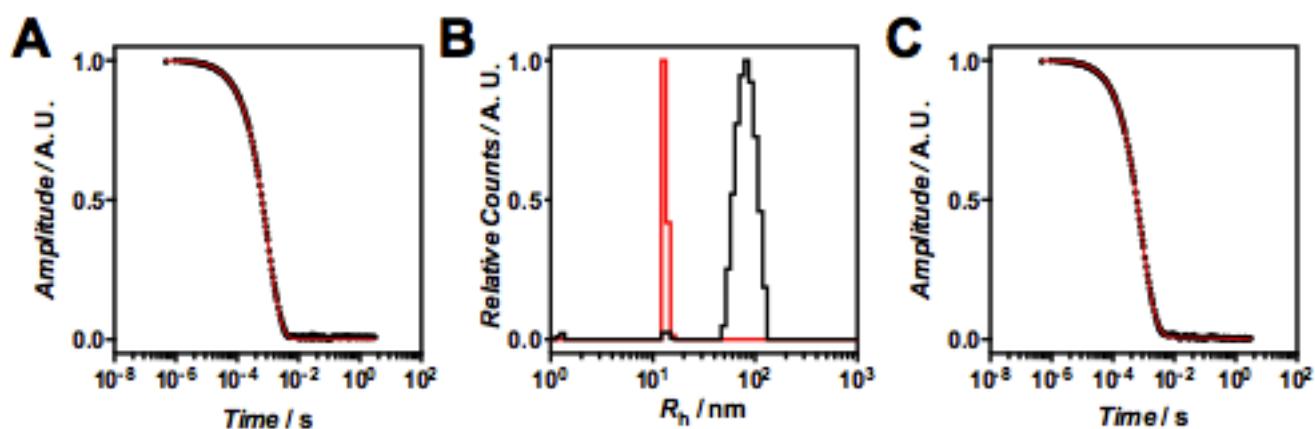


Figure S4 **A.** Correlation curve for DLS of hybrid PEG-A1:B1. **B.** Dynamic light-scattering of oligo B1. Intensity (black line) and number (red line) distributions. **C.** Correlation curve for DLS of oligo B1.

Transmission electron microscopy

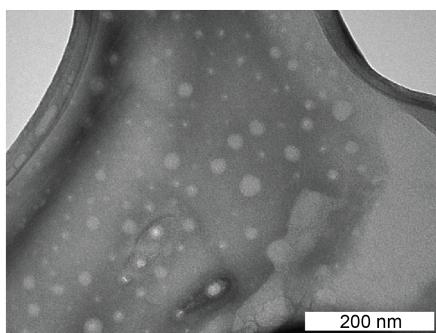


Figure S5. Transmission electron micrograph of oligo B1 stained with sodium phosphotungstate.

Stability assay

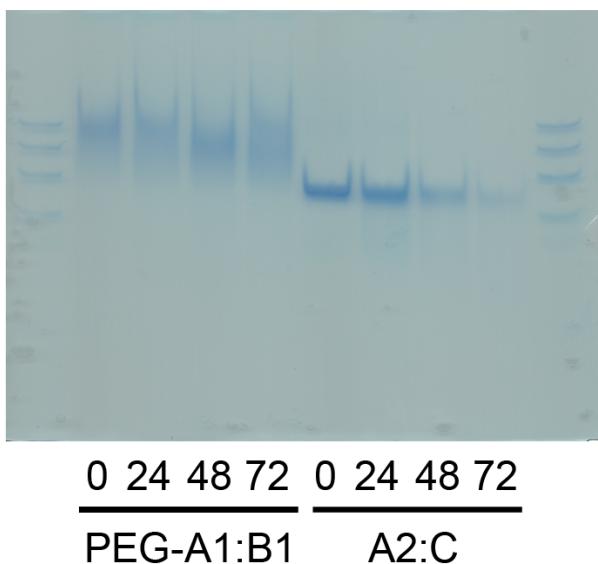


Figure S6 Stability assay analyzed by PAGE. Lanes 1–4: PEG-A1:B1 after 0, 24, 48 and 72 h incubation. Lanes 5–8: A2:C after 0, 24, 48 and 72 h incubation

Strand displacement assays

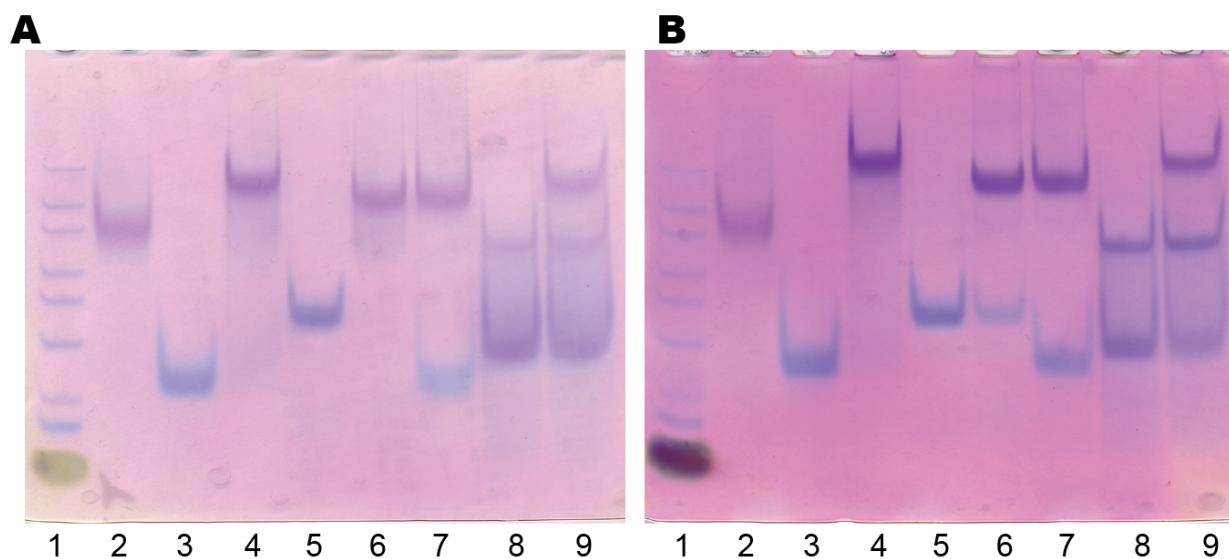


Figure S7 Strand displacement analyzed by PAGE. **A.** Lanes: 1) Ladder, 2) PEG-A1, 3) B2, 4) PEG-A1:B2, 5) C, 6) PEG-A1:C, 7) PEG-A1:B2 + C, 8) D, 9) PEG-A1:B2 + D. **B.** Lanes: 1) Ladder, 2) PEG-A3, 3) B3, 4) PEG-A3:B3, 5) C, 6) PEG-A3:C, 7) PEG-A3:B3 + C, 8) D, 9) PEG-A3:B3 + D.

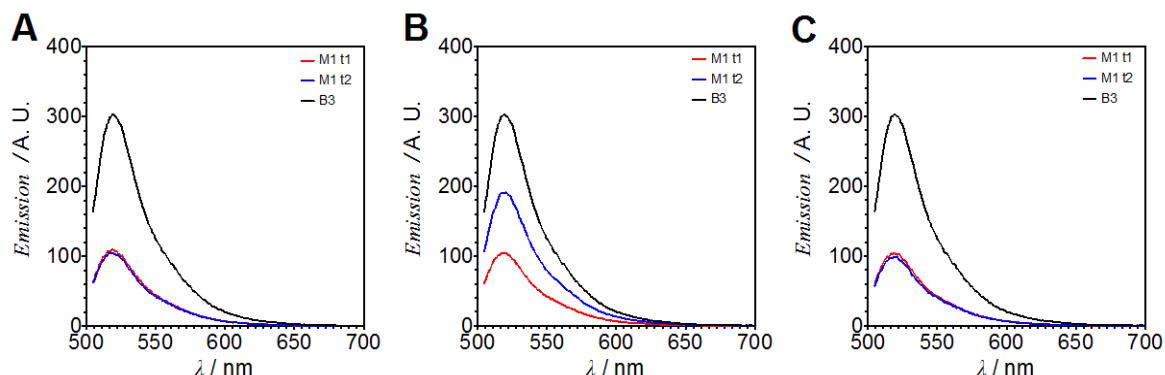


Figure S8 Fluorescence emission spectra of hybrid PEG-A3:B3 before (t1) and after (t2) dilution/displacement. The spectrum of B3 is provided for comparison. **A.** addition of buffer; **B.** addition of 1 equivalent of strand C; **C.** addition of 1 equivalent of strand D.