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 $^1$H NMR spectra of mPEG-NHS
**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:
\[ M_{A1} + M_{\text{Linker}} + M_{Me} + n \times M_{\text{CH}_2\text{CH}_2\text{O}} = 7038 + 44 + 15 + (n \times 44) \]
\[ = 7097 + n \times 44 \]

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

\[ M_{A3} = 7593 \]

[PEG-A3+H]+ = 7652 + n × 44

\( n = 50 \), requires 9852, found 9840
## Buffers and Solutions

### Table S2: Solutions and buffers used herein

<table>
<thead>
<tr>
<th>Solution</th>
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| 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 µL 0.5 M EDTA (pH 8)  
  26.5 µL 7.5 % Orange G  
  51.3 µL water |
| Denaturing PAGE gel (15%)       | 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 |
| Provides 7.5 mL of gel suitable for casting 1 0.75 mm thick minigel | |
| 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%)           | 3.75 mL 40% acrylamide/bis-acrylamide 29/1  
  0.75 mL 10 × TBE  
  3 mL water |
| Provides 7.5 mL of gel suitable for casting 1 0.75 mm thick minigel | |
| 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 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.