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# Structural shift of DNA template between hairpin and dimer tunes the emission color of DNA-templated AgNCs

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#### **Supplementary Information**

Figures 1-11



Supplementary figure 1. Emission spectra of 6C-27a-3bp (3.75 µM). The spectra were recorded by exciting from 300-720

nm in 20 nm steps. The spectral homogeneity in emission maximum indicates the presence of single type of AgNCs.



Supplementary figure 2. Emission spectra of 6C-217-11bp ( $3.75 \mu$ M). The spectra were recorded by exciting from 300-720 nm in 20 nm steps. The spectral heterogeneity in emission maximum indicates the presence of one type of AgNCs, with one being the dominant at Ex/Em 480/590 nm.



Supplementary figure 3. Emission spectra of 6C-159-8bp ( $3.75 \mu M$ ). The spectra were recorded by exciting from 300-720 nm in 20 nm steps. The spectral homogeneity in emission maximum indicates the presence of single type of AgNCs.



Supplementary Figure 4. Emission spectra of 6C-159-11bp (3.75  $\mu$ M). The spectra were recorded by exciting from 300-720 nm in 20 nm steps. The spectral heterogeneity in emission maximum indicates the presence of at least two types of AgNCs, with one being dominant at Ex/Em 480/590 nm. The second emission peak with Ex/Em at 580/660 nm can also be seen. Another peak appears at Near Infrared emission at Ex/Em 620/710 nm but this could not be visualized on the gel.



Supplementary Figure 5. Emission spectra of 6C-159-13bp ( $3.75 \mu$ M). The spectra were recorded by exciting from 300-720 nm in 20 nm steps. The spectral heterogeneity in emission maximum indicates the presence of at least two types of AgNCs, with one being the dominant at Ex/Em 480/590 nm. The second emission peak with Ex/Em at 580/660 nm can also be seen.

Full Emission Spectrum of DNA/AgNCs of 6C-159-21bp 100000 -380 80000 -400 -420 Emission Intensity (A.U.) -440 -460 60000 -480 -500 **—**540 40000 -580 ----600 -620 640 20000 **—660 —**680 ---700 **—**720 0 350 400 450 500 550 600 650 700 750 800 850 Wavelength (nm

Supplementary Figure 6. Emission spectra of 6C-159-21bp (3.75  $\mu$ M). The spectra were recorded by exciting from 300-720 nm in 20 nm steps. The spectral heterogeneity in emission maximum indicates the presence of at-least two types of AgNCs, with one being the dominant at Ex/Em 480/590 nm. The second emission peak corresponds to Ex/Em 580/660 nm.



Supplementary Figure 7. A) Emission spectra of 9A-6C-30T (3.75  $\mu$ M). The spectra were recorded by exciting from 300-720 nm in 20 nm steps. The dominant AgNC emits at Ex/Em 480/590 nm. B) Emission spectra of 9A-6C-30T-v8 (3.75  $\mu$ M). The spectra were recorded by exciting from 300-720 nm in 20nm steps. The spectral heterogeneity in emission maximum indicates the presence of two types of AgNCs, with one being the dominant at Ex/Em 480/590 nm and second one with Ex/Em at 580/660 nm.



Supplementary Figure 8. A) Emission spectra of 6C-30T-30A ( $3.75 \mu$ M). The spectra were recorded by exciting from 300-720 nm in 20 nm steps. The spectral heterogeneity in emission maximum indicates the presence of two types of AgNCs, with one being the dominant at Ex/Em 480/590 nm. B) The minor emission peak corresponds to Ex/Em 580/660 nm has been enlarged from A. C) Native gel electrophoresis of the DNA/AgNCs templates 6C-30T-30A. Samples were prepared either untreated or added with AgNO<sub>3</sub> only or with AgNO<sub>3</sub> and NaBH<sub>4</sub> before running the gel electrophoresis experiment. The DNA bands were visualized either with SG or AgNCs or both. SD: self-dimer DNA, H/L: anchor-loop DNA template, SG: SYBR Gold dye.

+SG



Supplementary Figure 9: Native gel electrophoresis of the 9A-6C-30T DNA/AgNCs templates with 2X SYBR Gold compare to Figure 2B for visualization of only DNA template structure without addition of A. Samples were prepared either untreated or added with AgNO<sub>3</sub> only or with AgNO<sub>3</sub> and NaBH<sub>4</sub> before running the gel electrophoresis experiment. The DNA bands were visualized either with SYBR Gold (SG), native AgNCs fluorescence, or both. SD: self-dimer DNA, H/L: hairpin-loop, cH/L: compact hairpin-loop.



Supplementary Figure 10: miRNA detection by 6C-159-13bp under varying salt and buffer conditions.

A) miRNA detection was performed in the presence of 20 mM Tris Acetate buffer (pH 7.5) and 20 mM NaNO<sub>3</sub> Emission intensity was measured at Ex/Em 460/590 nm. B) miRNA detection was performed in the presence of 20 mM NaNO<sub>3</sub>. Emission intensity was measured at Ex/Em 560/640 nm