

SUPPORTING INFORMATION

Hg²⁺ detection with rational design of DNA-templated fluorescent silver nanoclusters.

Liam Yourston¹, Polikron Dhoqina², Nolan Marshall¹, Rujani Mahmud¹, Ethen Kuether¹, Alexey V. Krasnoslobodtsev^{1*}

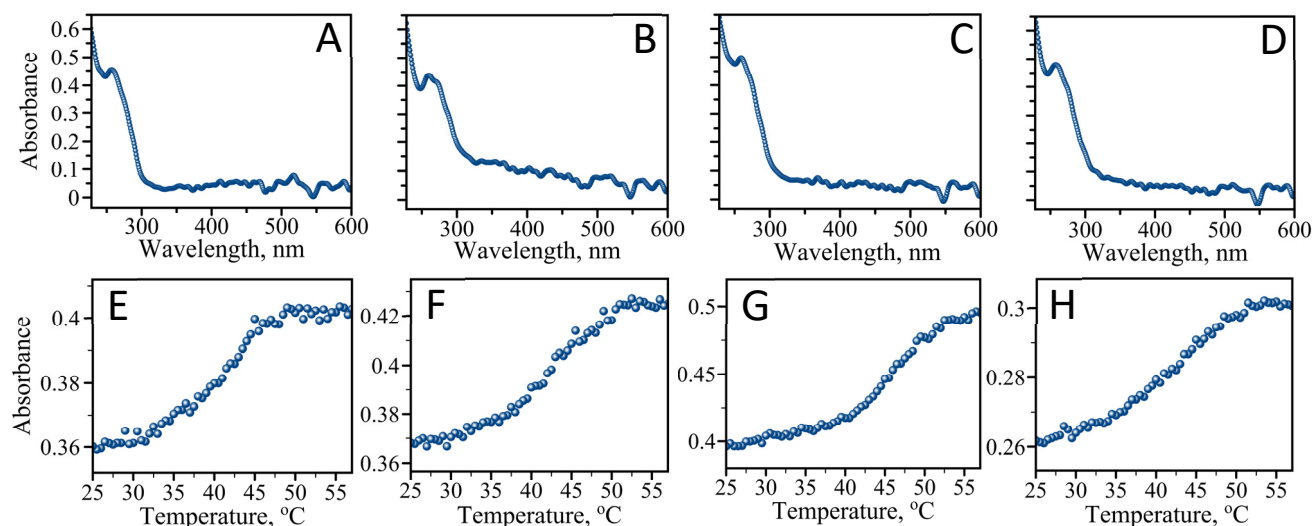
¹Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182, USA

²Department of Physics, Faculty of Natural Sciences, University of Tirana, Tirana 1001, Albania

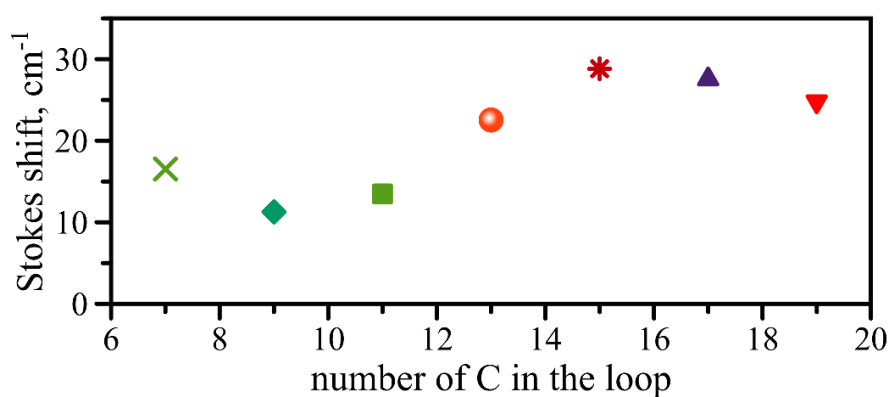
SEQUENCES USED IN THIS PROJECT

All oligonucleotides were purchased from IDT, Inc. Names denote the numbers of cytosines and thymines in each hairpin loop, underlined below.

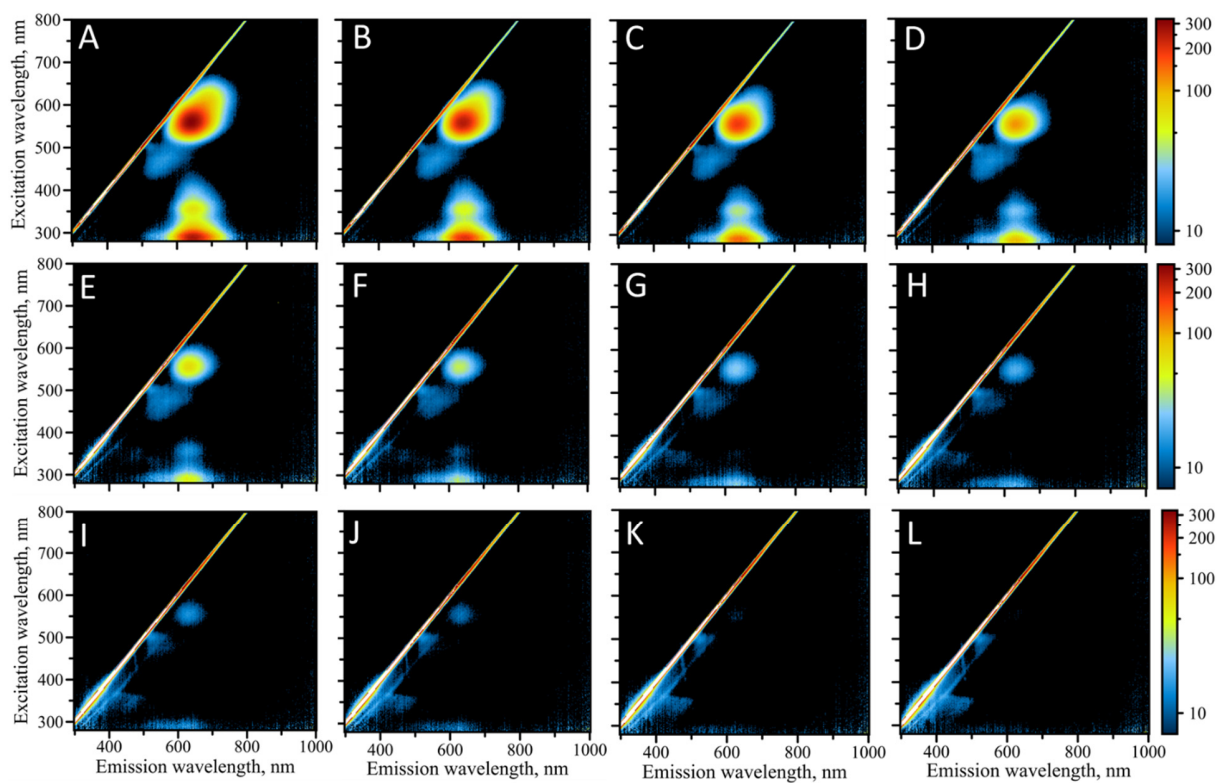
HL-C₇: 5'- TATCCGTCCCCCCCCACGGATA
 HL-C₉: 5'- TATCCGTCCCCCCCCACGGATA
 HL-C₁₁: 5'- TATCCGTCCCCCCCCACGGATA
 HL-C₁₃ (HL-T₀C₁₃): 5'- TATCCGTCCCCCCCCACGGATA
 HL-C₁₅: 5'- TATCCGTCCCCCCCCACGGATA
 HL-C₁₇: 5'- TATCCGTCCCCCCCCACGGATA
 HL-C₁₉: 5'- TATCCGTCCCCCCCCACGGATA
 HL-T₂C₁₁: 5'- TATCCGTTTCCCCCCCCCTACGGATA
 HL-T₄C₉: 5'- TATCCGTTTCCCCCCCCCTTACGGATA
 HL-T₆C₇: 5'- TATCCGTTTTCCCCCCTTTACGGATA



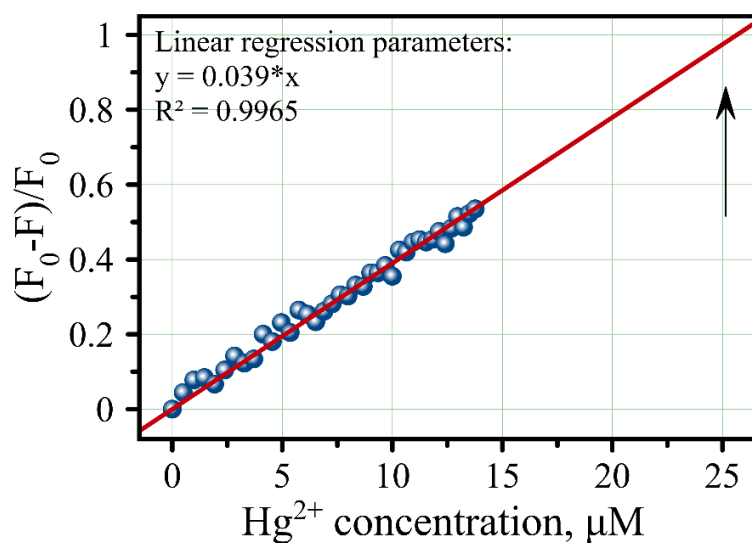
SI Figure S1. UV-vis characterization of AgNC@HL-T_mC_n designs. Top panel – UV-vis absorption spectra: A) AgNC@HL-T₀C₁₃, B) AgNC@HL-T₂C₁₁, C) AgNC@HL-T₄C₉, D) AgNC@HL-T₆C₇. Bottom panel – melting curves measured as change in A₂₆₀: E) AgNC@HL-T₀C₁₃, F) AgNC@HL-T₂C₁₁, G) AgNC@HL-T₄C₉, H) AgNC@HL-T₆C₇.



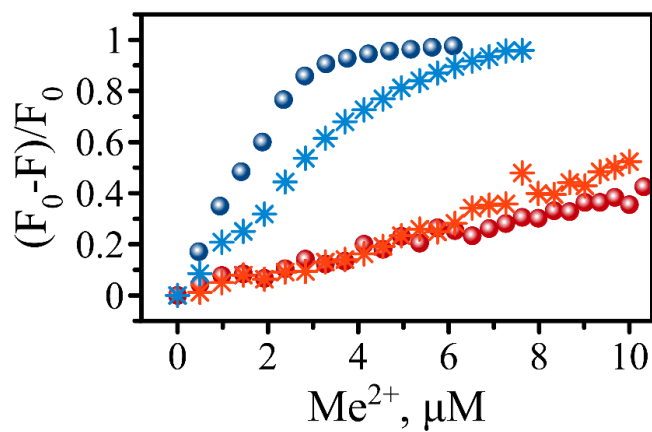
SI Figure S2. The trend of Stokes shift expressed in units of energy, cm⁻¹.



SI Figure S3. Titration of AgNCs@HL-C₁₃ with different ratios of C_{AgNC}/C_{Hg2+}. A) 1/0, B) 1/0.076, C) 1/0.15, D) 1/0.23, E) 1/0.38, F) 1/0.46, G) 1/0.54, H) 1/0.69, I) 1/0.77, J) 1/0.85, K) 1/0.92, L) 1/1. C_{AgNC@HL-C13} was kept the same at 6.2 μM.



SI Figure S4. Linear regression analysis of quenching data points for AgNC@HL-T₆C₇. The plot represents the best fit with $R^2=0.9965$, intercept 0 and slope of 0.039. Red line was also extrapolated to $(F_0-F)/F_0 = 1$ where complete quenching is expected to occur, thus setting up the upper limit of monitorable Hg^{2+} concentration.



SI Figure S5. Comparative graph of quenching data points for AgNC@HL-T₀C₁₃ (blue) and AgNC@HL-T₆C₇ (red). Circles represent data points obtained for quenching with Hg^{2+} and stars represent data points obtained for quenching with Cu^{2+} .