

Supplemental Material for

Structural Insights into DNA-Stabilized Silver Clusters

Danielle Schultz¹, Robert G. Brinson³, Neşe Sari³, Jeffrey A. Fagan², Christina Bergonzo³, Nancy J. Lin¹ and Joy P. Dunkers¹

¹Biomaterials Group, Biosystems and Biomaterials Division, National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, Maryland

²Polymers and Complex Fluids Group, Materials Measurement Science Division, National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, Maryland

³Institute for Bioscience and Biotechnology Research, National Institute of Standards and Technology and the University of Maryland, 9600 Gudelsky Drive, Rockville, Maryland

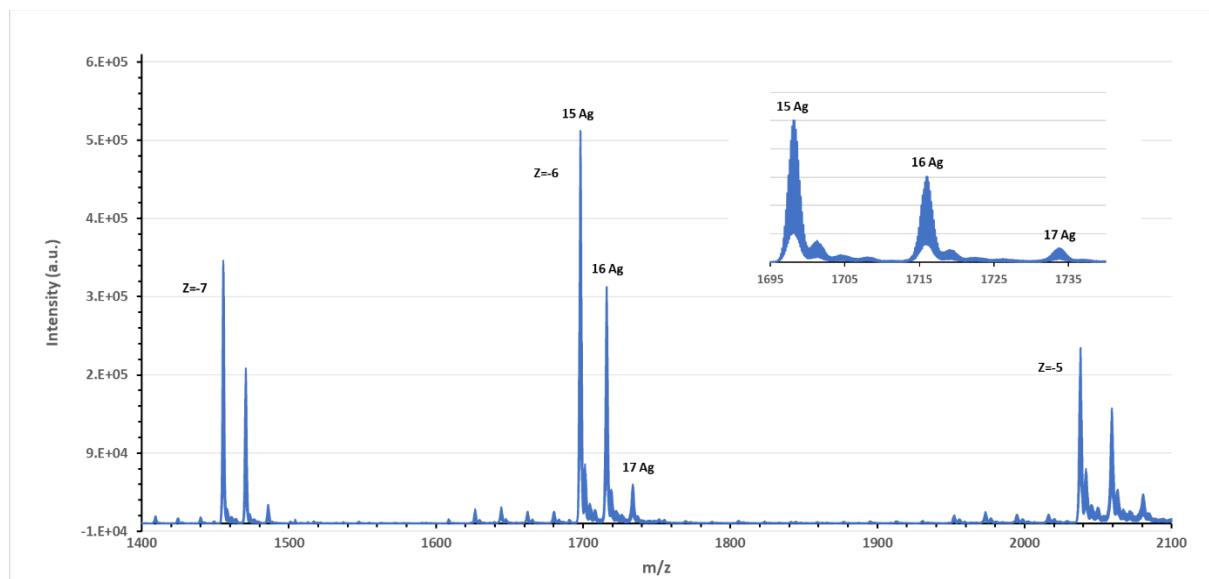
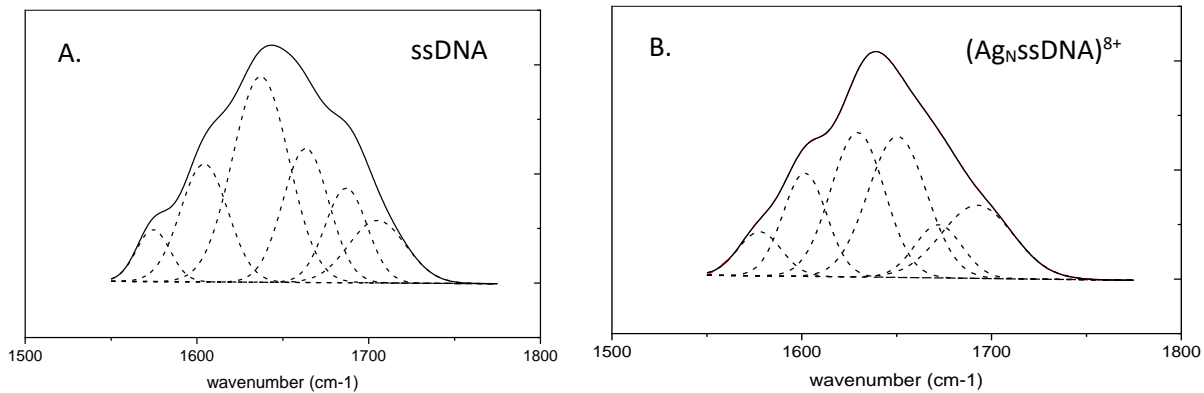


Figure S1. Mass spectrum of the $(\text{Ag}_{\text{NssDNA}})^{8+}$ complex showing the DNA complex with $\text{Ag}_{15}:\text{Ag}_{16}:\text{Ag}_{17}$ abundances of 7.1:4.9:1. The predominant species has a net charge of +8.



ssDNA (cm ⁻¹)	(Ag _N ssDNA) ⁸⁺ (cm ⁻¹)
1700	1692
1689	1672
1661	1650
1634	1629
1604	1601
1574	1577

Figure S2: Gaussian peak fit to base region and resulting peak positions of liquid ssDNA (A) and (Ag_NssDNA)⁸⁺ (B). There are theoretically a minimum of 14 vibrational modes in this region. However, only 6 unique peaks were fit that could contain multiple modes. Addition of Ag resulted in red shift of all peaks and changes in relative intensities.

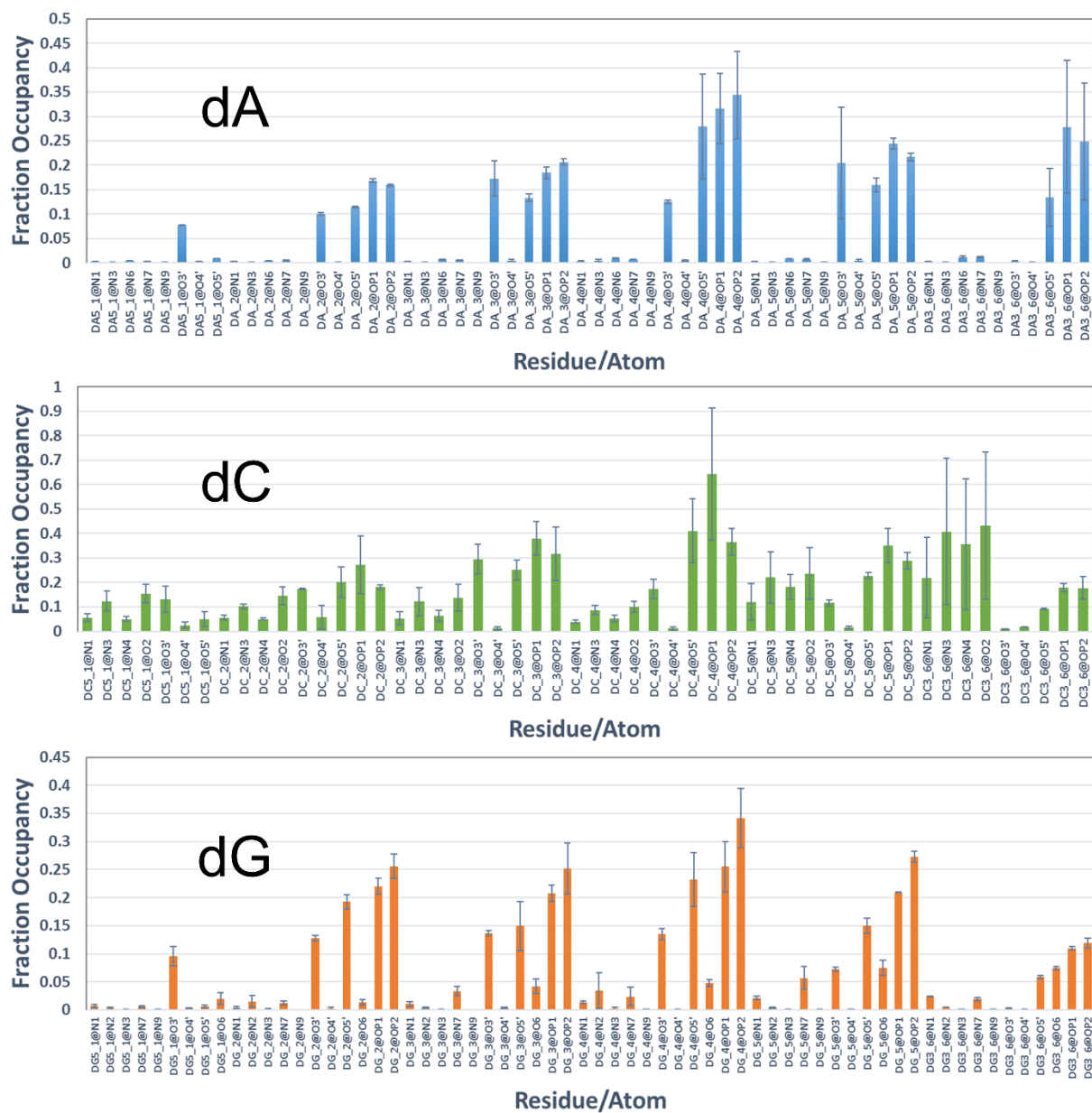


Figure S3. Average fraction occupancies per atom for Ag(I) associated with dA, dC, and dG ssDNA. Averages and standard deviations are reported for two independent simulations with different starting conformations of ssDNA and different (randomized) ion positions. Note the different y-axis scales for fraction occupancy.

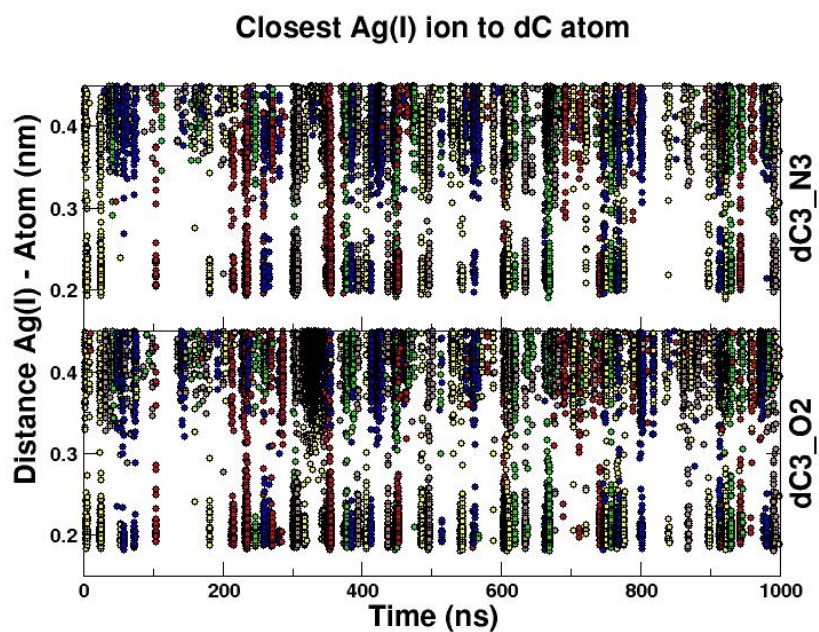


Figure S4. Plot showing distance between Ag(I) and N3 (top) or O2 (bottom) of dC3 vs. time. Distances less than 0.45 nm (where 0.4 nm cutoff for “bound” ions) are shown. Different colors indicate different Ag(I) ions in the simulation. It is clear that for some binding events, the same ion is bound to O2 and N3, and for other binding events there is only one ion associated with the dC atom.

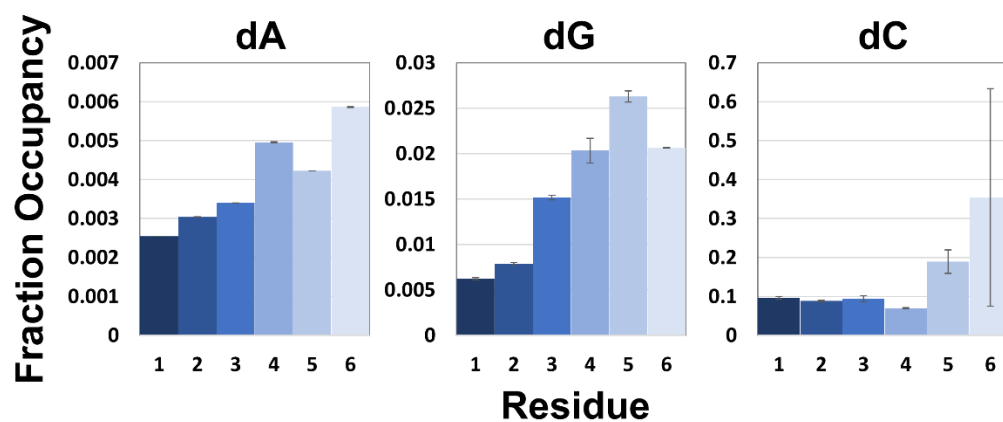


Figure S5. Average base atom occupancies per residue (1-6) for Ag(I) associated with dA, dC, and dG ssDNA. Averages are over all base oxygen and nitrogen atoms for two simulations. Error bars represent the sum of squares of base atom standard deviations between two runs. Note the different scales for the y-axis values.

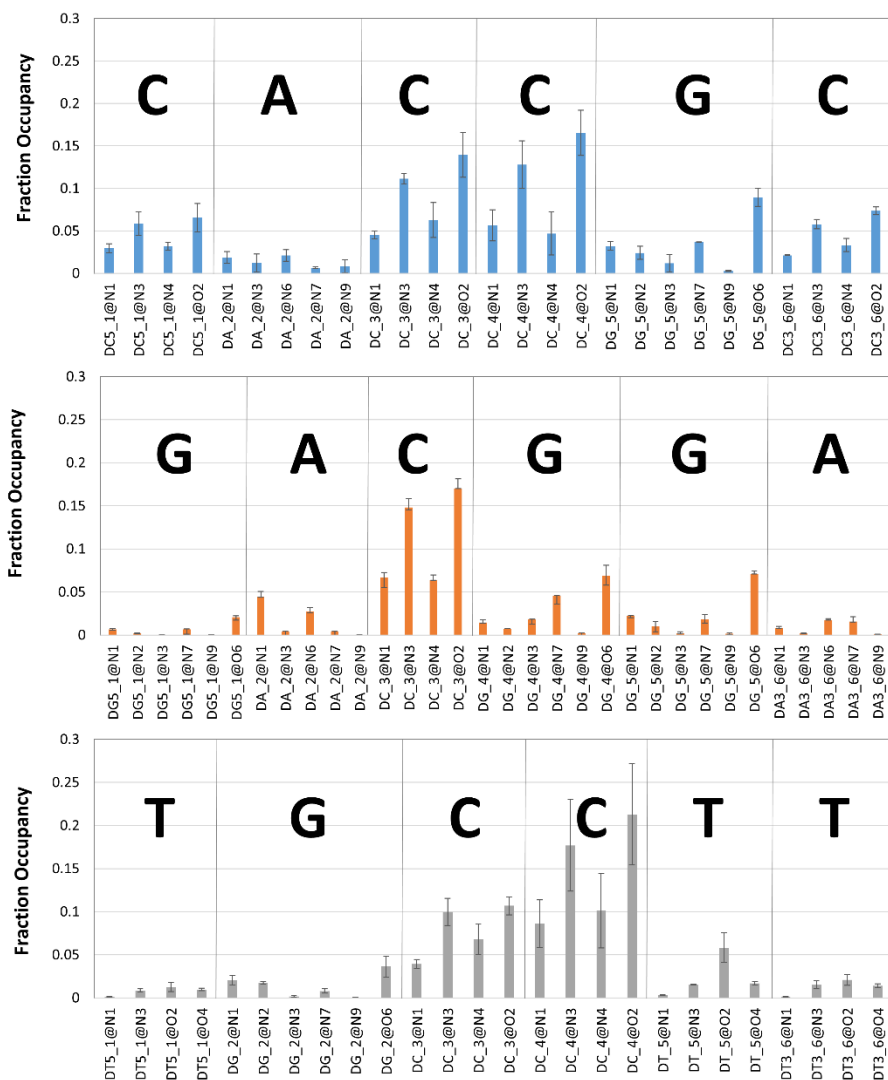


Figure S6. Average base atom occupancies for Ag(I) associated with CACCGC, GACGGG, and TGCCT oligomers of ssDNA. Averages are over all base oxygen and nitrogen atoms for two simulations. Error bars represent the standard deviations between two runs.

