

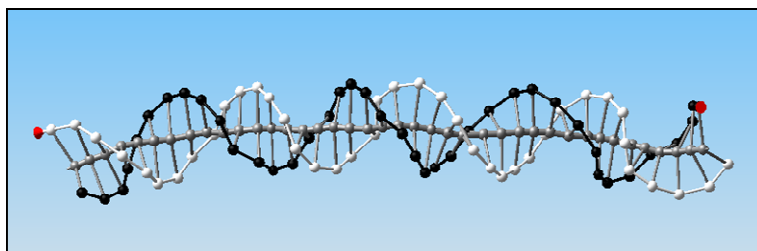
Supporting Material.

Quantum Dot DNA Bioconjugates: Attachment Chemistry

Strongly Influences the Resulting Composite Architecture

Boeneman *et al.*,

A.



B.

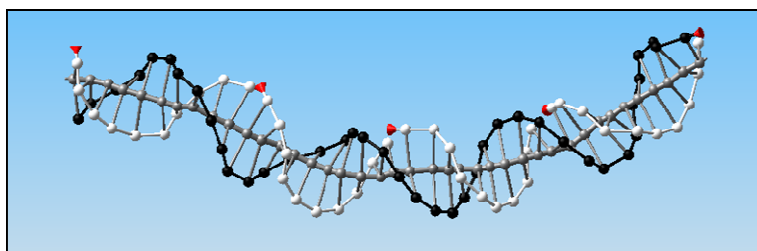


Figure S-1. Model of 40 bp dsDNA stability with (A) and without (B) nicks every 10 bases.

Nanoengineer-1 (from Nanorex, Inc.) was used to assess the flexibility of the short strands of duplex DNA with nicks. The program includes a capability to do simple molecular dynamics (MD) simulations using the GROMACS code with a reduced representation model for the DNA. The latter model simulates each base-pair by three particles and all base-pairs are treated the same, *ie* no sequence dependence. A Model was created for the 40 bp DNA strand both with and without three equi-spaced nicks in one strand. The time step was 0.1fs, the total simulation time was 36psec, and the flexibility of the strands was gauged by monitoring the molecular fluctuations. Images of the strands after the dynamic model are shown in Figure S-2.

While the model does not include sequence effects, work by Protozonova did investigate this by treating it as equilibrium between two states, stacked and unstacked, and measuring the associated free-energy. The latter measurement is done by comparing the mobility of 300bp DNAs with and without a single nick, while varying the bases at that nick. The mobility in both cases is almost identical, indicating that the nicked DNA remains rigid. Based on their work the free energy at the nicked regions would be; T-T: -1.11eV; T-A: -1.34eV; A-A: -1.11eV. The high values of these energies corroborates the assessment that this a rigid structure.

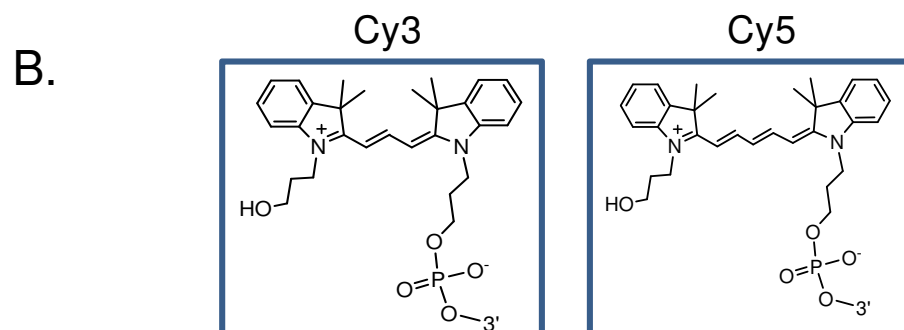
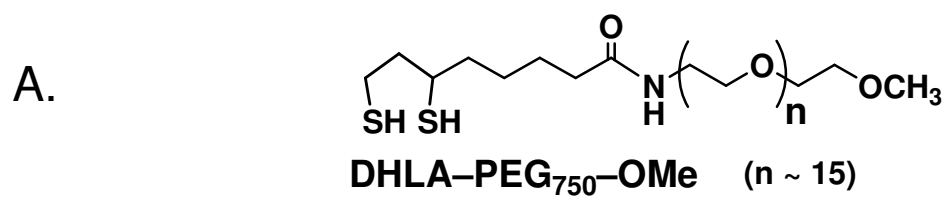


Figure S-2. Chemical structures of the DHLA-PEG-methoxy ligand used to make the QDs soluble (A) and the Cy3 and Cy5 dyes attached to the DNA termini via a phosphate bond.

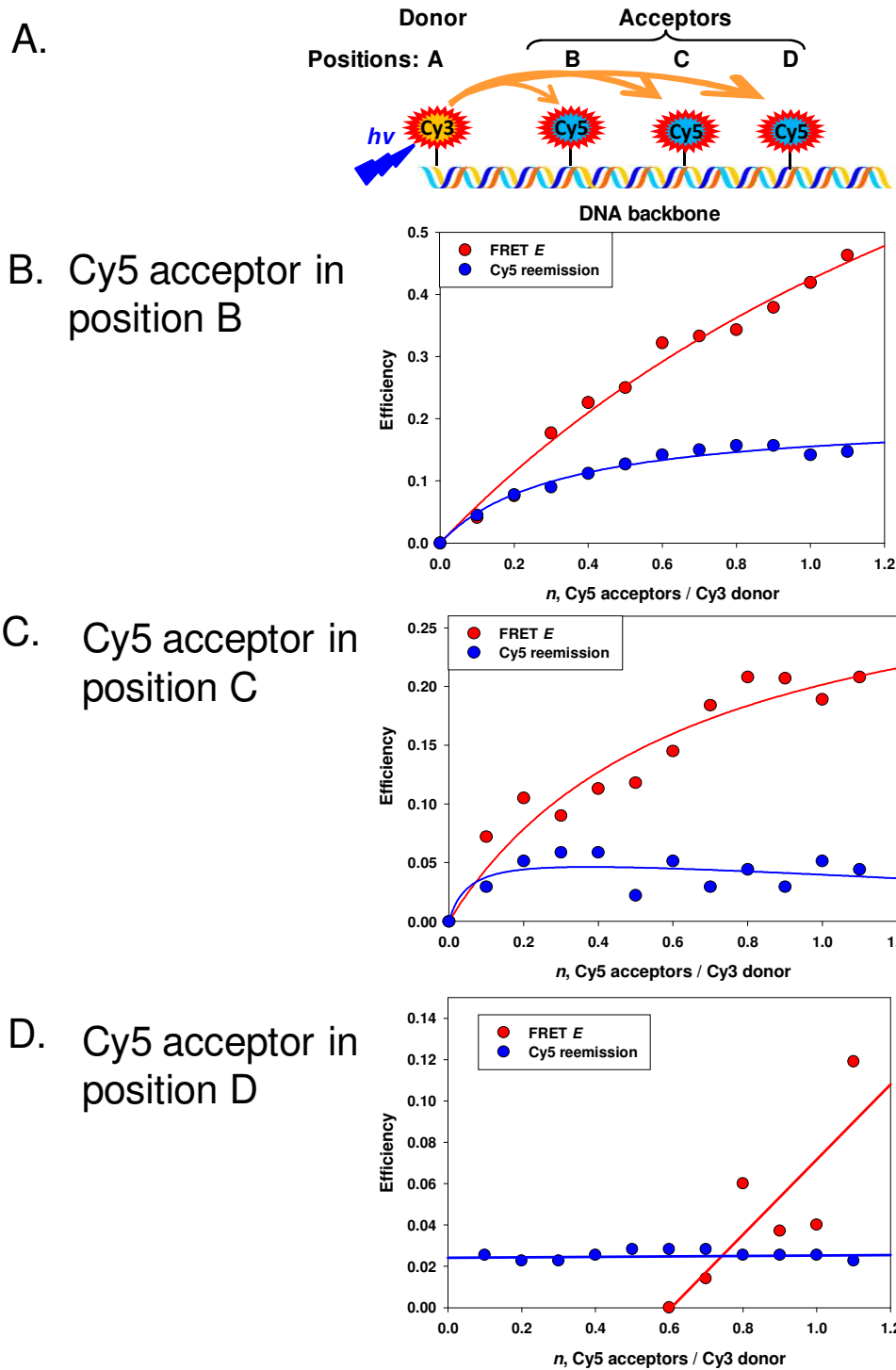


Figure S-3. Plots of FRET E and Cy5 acceptor reemission for all acceptor positions in construct 1.

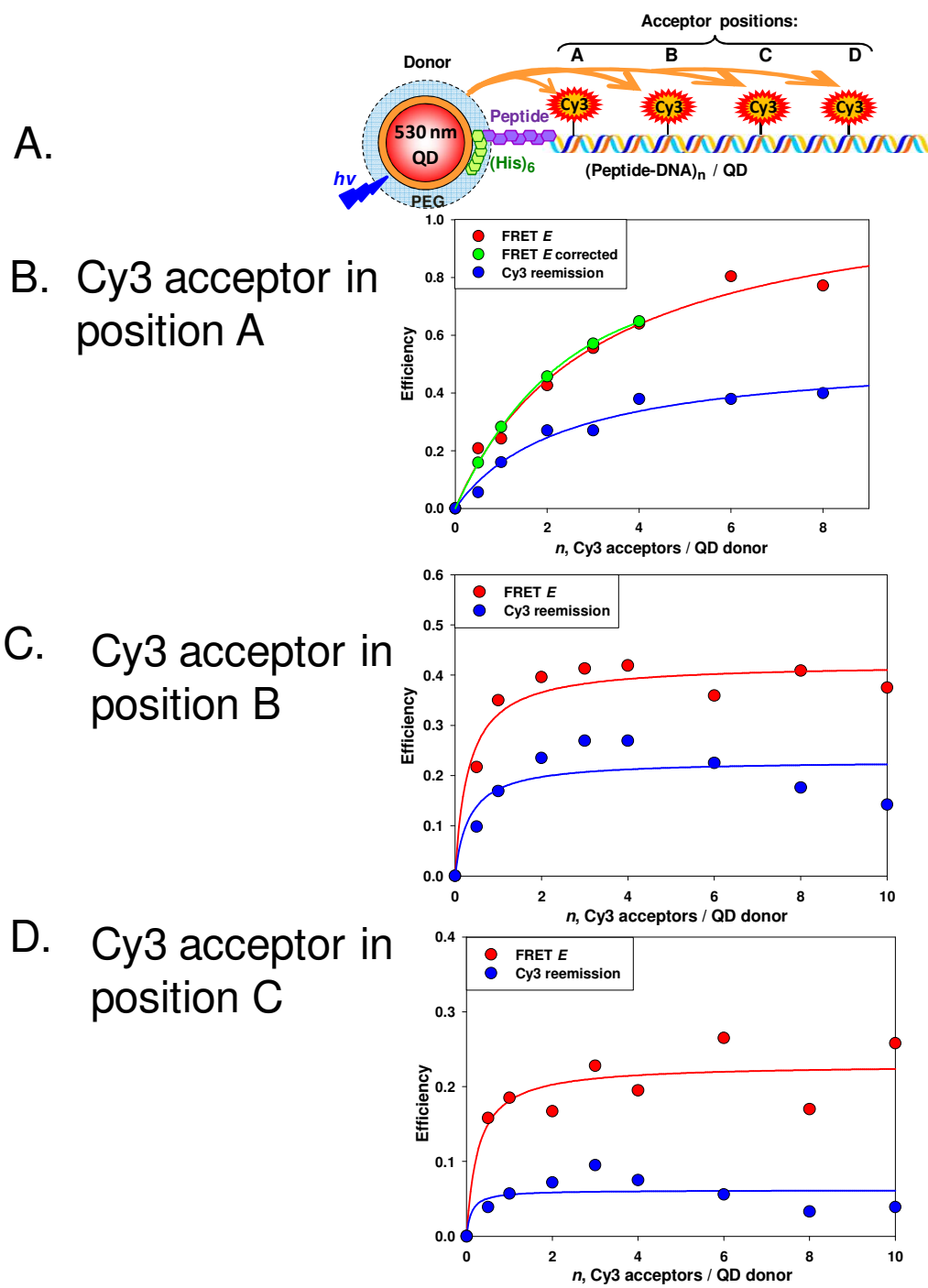


Figure S-4. Plots of FRET E vs. FRET E corrected for heterogeneity where appropriate and Cy3 acceptor reemission for selected acceptor positions in construct 2. Acceptor in position D had no significant sensitization.

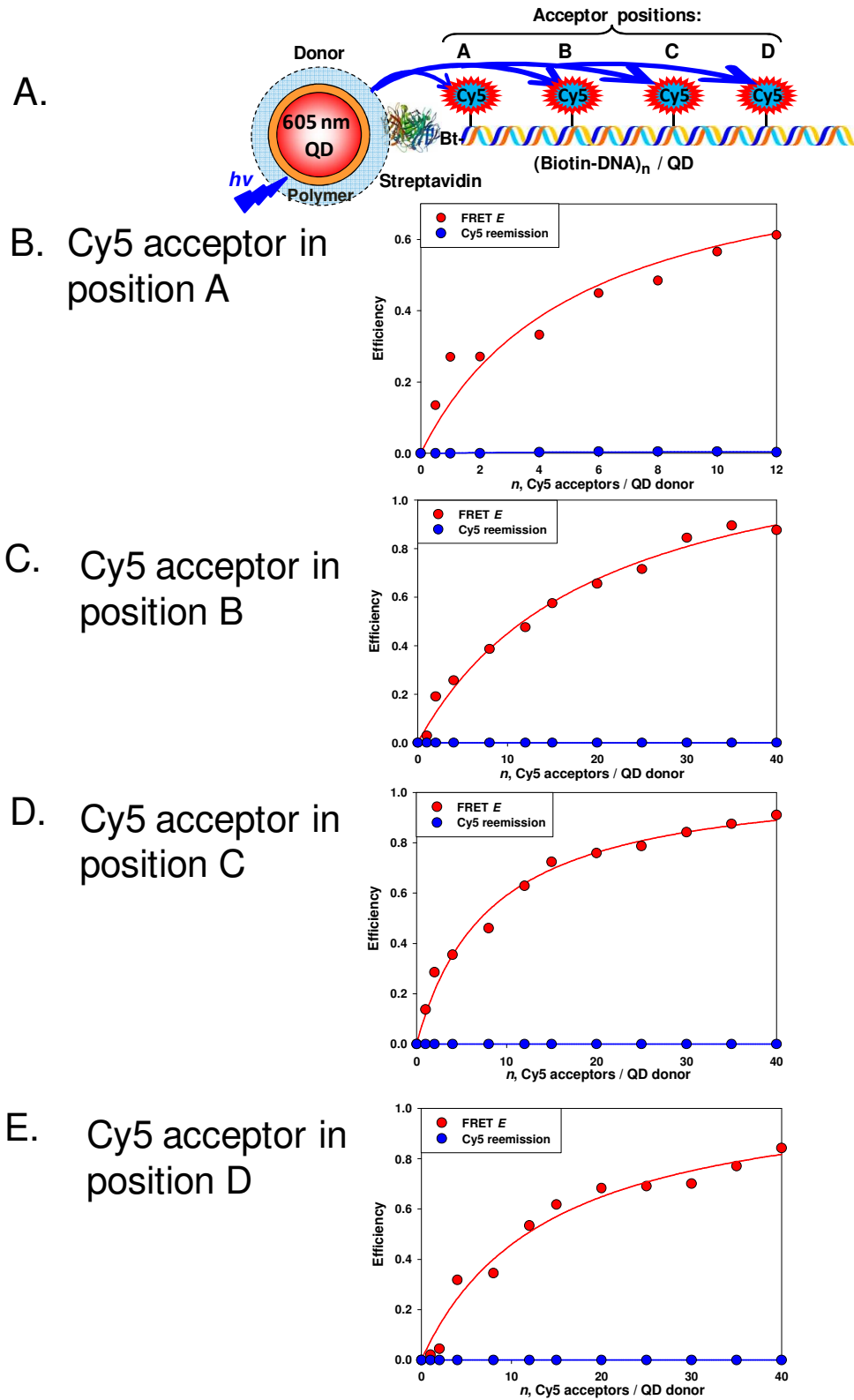


Figure S-5. Plots of FRET E and Cy5 acceptor reemission for all acceptor positions in construct 3.

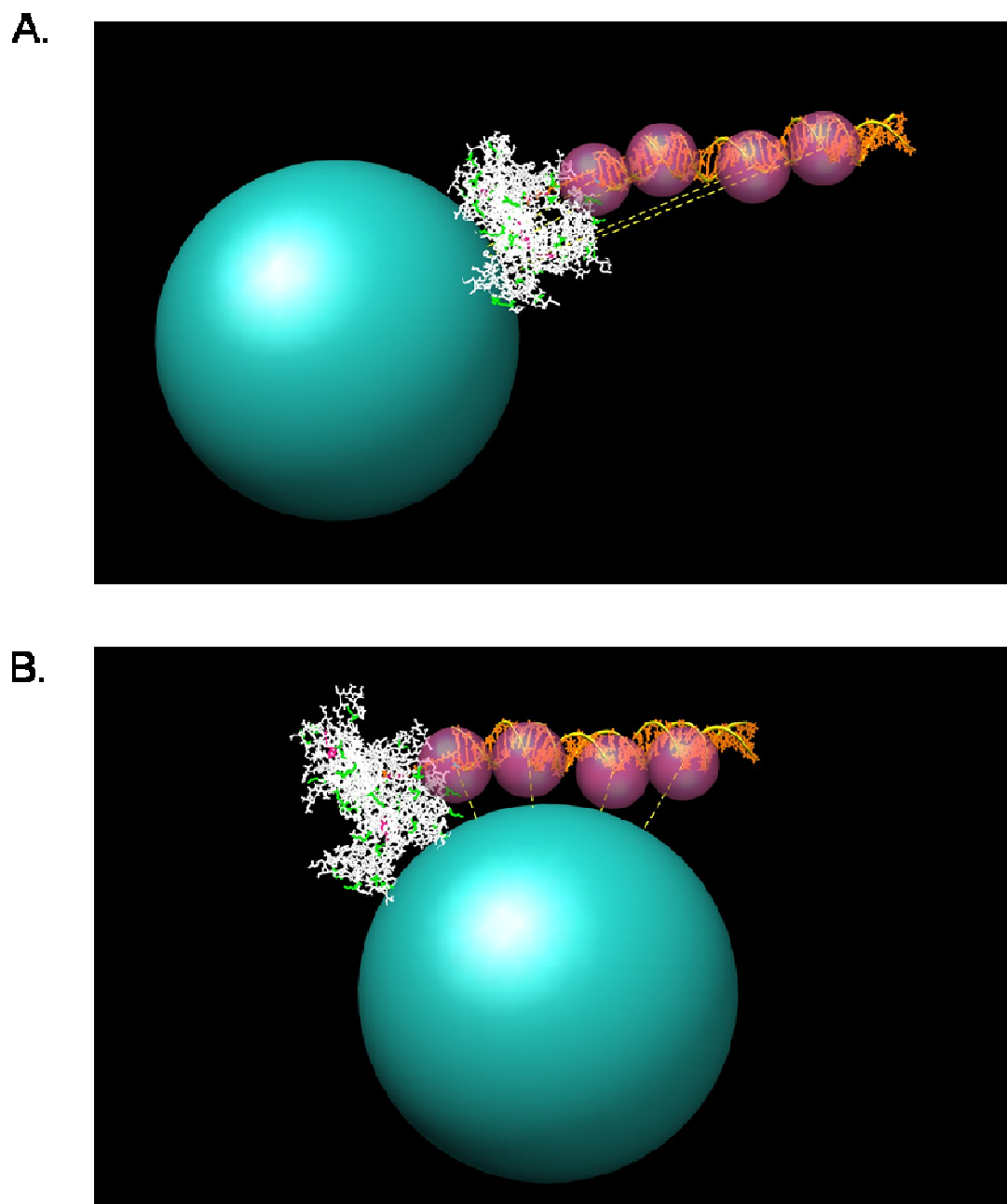


Figure S-6. Models of a single biotin labeled DNA docked to the streptavidin labeled QD in the extended (A) and tangential (B) positions.