

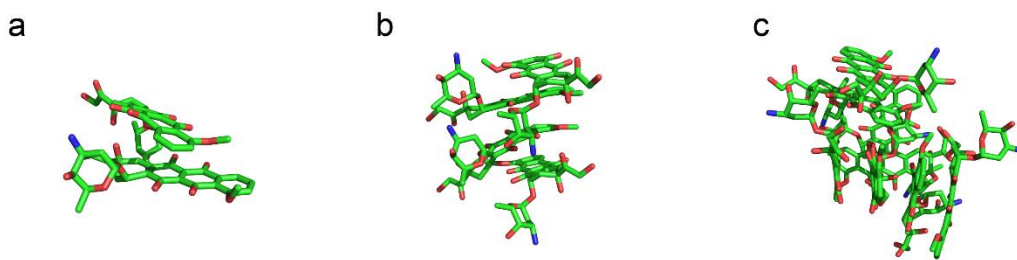
**Supporting Information for**  
**Loading of DOX into a tetrahedron DNA nanostructure:**  
**The corner does matter**

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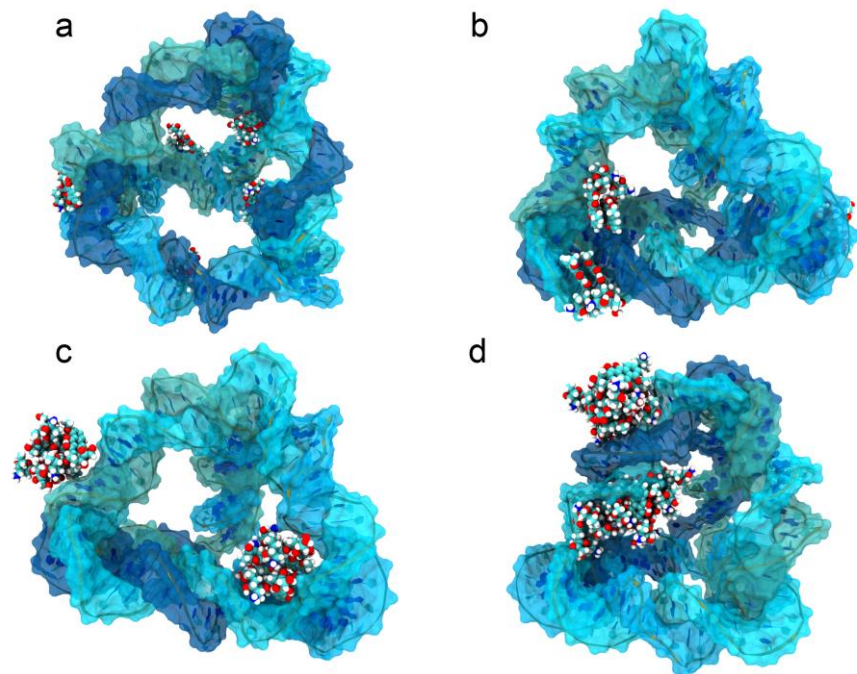
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**Figure S1.** Final snapshots for the DOX (a) dimer, (b) tetramer, (c) octamer in the water.



**Figure S2.** Final snapshots illustrating the typical modes in the ionized DOX-TDN-17 interaction: (a) DOX monomer, (b) DOX dimer, (c) DOX tetramer, and (d) DOX octamer.