DNA origami-protein interactions and steric hindrance control

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Here, we characterize the structure and dynamics of a triangular-shape DNA origami with the use of Langevin-type molecular dynamics simulations, using the coarse-grained OxDNA model. In particular, we focus on two different network geometries and analyse the different fluctuations properties to characterize the digital behaviour of restriction enzymes over sites contained in the folded M13 sequence, which we recently reported [1]. We link the local and global conformational changes, and the local DNA network properties, to the binding propensity of restriction enzyme HinP1I. Finally, we will attempt to use the Michaelis-Menten model to connect the prediction of molecular dynamics simulations with gel electrophoresis experiments.

References

[1] A Stopar, L. Coral, S. Di Giacomo, A.F. Adedeji, M. Castronovo, Nucl. Ac. Res. 2018, **46**, 995–1006.