J Proteomics Bioinform 2016, 9:10(Suppl)
http://dx.doi.org/10.4172/0974-276X.C1.089

6th International Conference on
Structural Biology
August 22-23, 2016 New Orleans, USA

Rationalization of protein side chain flexibility and ligand binding based on cooperative interaction networks

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Network concepts have been widely applied in structure biology research to help the understanding of protein structure and function. Our research approach is based on applying small world network concepts to ligand-protein complexes, using atomic level representation of favorable close contacts, focusing on local cooperativity. Specifically, we believe that there are patterns of networked interactions, currently overlooked using traditional additive methods that play important roles in ligand-protein binding. We believe small world network concepts are keys in identifying these patterns because although they may involve weakly favorable contacts, they can be highly stabilizing. To demonstrate the effectiveness of these novel small world network concepts we show complexes involving Aurora A kinase, and how the visualization of key interaction networks supports the rationalization of binding site hot-spots and residue mobility. To further explore the local cooperativity of interacting residues in protein crystal structure data, we introduce new and novel methods for the fast searching of networked interactions.

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Three dimensional dynamic structures of DNA-nanogold conjugate by individual-particle electron tomography

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DNA base-pairing has been used for many years to direct the arrangement of inorganic nano-crystals into small groupings and arrays with tailored optical and electrical properties. The control of DNA-mediated assembly depends crucially on a better understanding of the three-dimensional (3D) structure of the DNA-nanocrystal hybridized building blocks. Existing techniques do not allow for the structural determination of these flexible and heterogeneous samples. Here, we employed electron tomography and negative-staining techniques to investigate the 3D structure of DNA-nanogold conjugates that were self-assembled from a mixture of an 84-base-pair double-stranded DNA (dsDNA) conjugated with two 5-nm nanogold particles for potential substrates in Plasmon coupling experiments. We reconstructed 14 electron density maps at a resolution of ~2 nm from each individual dsDNA-nanogold particle using the individual-particle electron tomography (IPET) reconstruction method. Using these 3D density maps as a constraint, we projected a standard flexible DNA model onto the observed EM density maps and derived 14 conformations of dsDNA by molecular dynamics simulations. The variation of the conformations was consistent with the variation from liquid solution, but the IPET approach provides the most complete experimental determination of the flexibility and fluctuation range of these directed nanocrystal assemblies to date. The general features revealed by these experiments can be expected to occur in a broad range of DNA-assembled nanostructures.

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