Conformational variability in proteins bound to single-stranded DNA: a new benchmark for new docking perspectives

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Abstract

We explored the Protein Data-Bank (PDB) to collect protein-ssDNA structures and create a multi-conformational docking benchmark including both bound and unbound protein structures. Due to ssDNA high flexibility when not bound, no ssDNA unbound structure is included. For the 143 groups identified as bound-unbound structures of the same protein , we studied the conformational changes in the protein induced by the ssDNA binding. Moreover, based on several bound or unbound protein structures in some groups, we also assessed the intrinsic conformational variability in either bound or unbound conditions, and compared it to the supposedly binding-induced modifications. This benchmark is, to our knowledge, the first attempt made to peruse available structures of protein – ssDNA interactions to such an extent, aiming to improve computational docking tools dedicated to this kind of molecular interactions.

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`p_bench.mk2.Proof.odt` available at https://authorea.com/users/412462/articles/521169-conformational-variability-in-proteins-bound-to-single-stranded-dna-a-new-benchmark-for-new-docking-perspectives