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Predicting the most stable EpB/target molecule complex by stochastic tunneling-basin Hopping-Discrete Molecular Dynamics method

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The global minimum search method (STUN-BH-DMD method for abbreviation) combining the strengths of the Stochastic Tunneling, Basin Hopping and Discrete Molecular Dynamics method was used to predict the most stable AptEpB/EpCAM complex. The epithelial cell adhesion molecule (EpCAM, PDB code: 4MZV) was used as a target molecule for the EpCAM aptamer EpA (AptEpB). For the most stable AptEpB/EpCAM complex predicted by the STUN-BH-DMD method, the AptEpB is attached to the entangling loop fragments of two EpCAM molecules with most AptEpB residues. After the AptEpB/EpCAM complex equilibrated with the water environment by the MD simulation at 300 K for 10 ns, the stable hydrogen bonds formed between the bases of AptEpB and EpCAM residues of the secondary structures including the alpha helix and beta sheet become less stable in the water environment.

Biography

Yu Sheng Lin is currently pursuing Master's degree from National Sun Yat-sen University in Taiwan. He has focused on the molecular dynamics simulation during his period of study, mainly analyzing the structure types of molecular adsorption between the aptamer and target molecules.

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