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氯化血红素分子对牛血清白蛋白电子传输能级的调控

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Regulating Electron Transport Band Gaps of Bovine Serum Albumin by Binding Hemin

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Details of the molecular docking

We performed the molecular docking for intermolecular interactions between hemin and BSA. The molecular docking was performed using the Discovery Studio 2.5 (DS 2.5) software package (Accelrys) (Discovery Studio, version 2.1, Accelrys Inc., San Diego, CA, 2008). The crystal structure of the three-dimensional structure of BSA used in the calculations was obtained from the protein data bank (PDB, code: 4F5S). For docking study, the DFT/B3LYP method with the 6-31G(*d*,*p*) basis set was employed to perform the geometry optimization and vibration analysis of hemin. The quantum chemistry calculations were carried out with the use of the Gaussian 03 program package with the default convergence criteria. The flexible docking between hemin and BSA molecules was carried out with hemin (with optimized structure) as a ligand and BSA molecule as a receptor to obtain the ligand (hemin)-protein (BSA) energy minimized docked conformation. During the docking study, all crystallographic water molecules and heteroatoms were removed from BSA and hydrogen atoms were added. The potential of the 3D structure of the protein was assigned according to the CHARMM force field. The minimum binding energy conformer was searched out of 10 different conformers for the docking simulation by considering the values of Libdockscore, Cdocker energy, Cdocker interaction energy, and hydrogen bonds and the resultant one was used for further analysis.

The preparation of the EGaIn tip

We followed a published procedure (Whiteside *et al*. Eutectic gallium-indium (EGaIn): A moldable liquid metal for electrical characterization of self-assembled monolayers, Angew. *Chem. Int. Ed*. **2008,** *47*, 142–144) to form EGaIn tip. The EGaIn electrode was formed by suspending a drop of EGaIn (consist of 75.5% Ga and 24.5% In, 5 g, Sigma-Aldrich) from a metal syringe, bring the drop into contact with the bare surface of a sacrificial hemin-BSA layer of Au under manual operation. As the needle slowly retracts, the EGaIn adhered to both the needle and the Au. The EGaIn drop contracted into an hourglass shape until it divided into two structures, one attached to the Au surface and other one attached to the syringe. The EGaIn tip diameters is 1–5 μm and its protruding from the needle did not retract into a semispherical droplet.