World Academy of Science, Engineering and Technology
International Journal of Biotechnology and Bioengineering
Vol:9, No:06, 2015

Conformation Prediction of Human Plasmin and Docking on Gold Nanoparticle

Authors : Wen-Shyong Tzou, Chih-Ching Huang, Chin-Hwa Hu, Ying-Tsang Lo, Tun-Wen Pai, Chia-Yin Chiang, Chung-Hao Li, Hong-Jyuan Jian

Abstract : Plasmin plays an important role in the human circulatory system owing to its catalytic ability of fibrinolysis. The immediate injection of plasmin in patients of strokes has intrigued many scientists to design vectors that can transport plasmin to the desired location in human body. Here we predict the structure of human plasmin and investigate the interaction of plasmin with the gold-nanoparticle. Because the crystal structure of plasminogen has been solved, we deleted N-terminal domain (Pan-apple domain) of plasminogen and generate a mimic of the active form of this enzyme (plasmin). We conducted a simulated annealing process on plasmin and discovered a very large conformation occurs. Kringle domains 1, 4 and 5 had been observed to leave its original location relative to the main body of the enzyme and the original doughnut shape of this enzyme has been transformed to a V-shaped by opening its two arms. This observation of conformational change is consistent with the experimental results of neutron scattering and centrifugation. We subsequently docked the plasmin on the simulated gold surface to predict their interaction. The V-shaped plasmin could utilize its Kringle domain and catalytic domain to contact the gold surface. Our findings not only reveal the flexibility of plasmin structure but also provide a guide for the design of a plasmin-gold nanoparticle.

Keywords : docking, gold nanoparticle, molecular simulation, plasmin
Conference Title : ICBN 2015 : International Conference on Biotechnology and Nanotechnology
Conference Location : New York, United States
Conference Dates : June 04-05, 2015