Comparative modeling of DszC, an enzyme in biodesulfurization, and performing in silico point mutation for increasing tendency to oil

Abstract:
Desulfurization protein named DszC from Rhodococcus erythropolis is the key enzyme for biodesulfurization of dibenzothiophene (DBT) in 4S pathway, which is a pathway with four enzymes. DszC enzyme biodesulfurizes DBT and its derivatives in oil components and biphasic systems. It functions well at the oil-water interface. In this study point mutation performed in DszC enzyme regarding to increase protein hydrophobicity and stability for application in immobilized form. 3D model of DszC predicted using Phyre2, SAM-T08 and M4t servers. I-Mutant 2 server used to determine potential spots for point mutation, and Molegro Virtual Docker (MVD) used for performing point mutation on 3D model. Hydrophobicity plots generated by Bioedit version 7.0.8.0 in Kyte-Doolittle scale indicated that protein hydrophobicity is increased after mutation. Also protein stability increased 26.11 units in scale of DDC2.

Authors: Ibrahim Torktaz1, Zahra Etemadifar2* & Peyman Derikvand
Year: 2012

Journal reference: http://bioinformation.net/

Source URL: http://tintin.science.uu.nl/wenmr/market/article/comparative-modeling-dszc-enzyme-biodesulfurization-and-performing-silico-point-mutation