Contribution ID: **44** Type: **Poster**

Enhancement of methane catalysis rates in Methylosinus trichosporium OB3b

Wednesday, May 11, 2022 4:00 PM (1 minute)

The particulate methane monooxygenase (pMMO), a membrane-bound enzyme having three-subunits (α, β, and γ) and copper-containing centers, is found in most of the methanotrophs that selectively catalyze the oxidation of methane into methanol. Active sites in pMMO of Methylosinus trichosporium OB3b were determined by docking the modeled structure with ethylbenzene, toluene, 1,3-dibutadiene, and trichloroethylene. The docking energies between the modeled pMMO structure and ethylbenzene, toluene, 1,3-dibutadiene, and trichloroethylene were -5.2, -5.7, -4.2, and -3.8 kcal/mol, respectively, suggesting the existence of more than one active site within the monomeric subunits due to the presence of multiple binding sites within the pMMO monomer. The evaluation of tunnels and cavities of the active sites and the docking results showed that each active site is specific to the radius of the substrate. To increase the catalysis rates of methane in pMMO of M. trichosporium OB3b, selected amino acid residues interacting at the binding site of ethylbenzene, toluene, 1,3-dibutadiene, and trichloroethylene were mutated. Based on screening the strain energy, docking energy, and physiochemical properties, five mutants were down selected, B:Leu31Ser, B:Phe96Gly, B:Phe92Thr, B:Trp106Ala and B:Tyr110Phe, which showed docking energies of -6.3, -6.7, -6.3, -6.5 and -6.5 kcal/mol, respectively as compared to the wild type (-5.2 kcal/mol) with ethylbenzene. These results suggest that these five mutants would likely increase methane oxidation rates compared to the wild-type pMMO.

Primary author: Mr SAMANTA, Dipayan (South Dakota School of Mines and Technology)

Co-author: Prof. SANI, Rajesh K. (South Dakota School of Mines and Technology)

Presenter: Mr SAMANTA, Dipayan (South Dakota School of Mines and Technology)

Session Classification: Poster Session

Track Classification: Biology