

Computational approaches to identify the putative hydrogen and oxygen channels in Fe⁻ only hydrogenase

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Fe-Fe hydrogenases are focus of research due to its involvement in energy metabolism in many micro-organisms. The current global energy crisis necessitates biological hydrogen production as an alternative source of energy. Biological hydrogen production is one of the most challenging area of biotechnology. The technological outcome of this depends on research advances focusing on engineering strains and enzymes to develop efficient hydrogen energy. Fe-only hydrogenases do have medical relevance as well since these enzymes are involved in energy metabolism in protozoa like *Trichomonas vaginalis*. Fe-only hydrogenase is a distinct class of hydrogen producing metalloenzyme, present in number of prokaryotes and eukaryotes (algae). Various studies on this enzyme in last two decades have led to considerable insights into the functional and structural aspects. The aim of the present

study is to use computational approaches to elucidate further the mechanism of catalysis and identify targets for engineering efficient Fe-hydrogenase. In the present study we selected the Fe-only hydrogenase from the *Clostridium pasteurianum* as a model to identify the putative channels for passage of hydrogen and oxygen. To identify the gas migration pathway in the enzyme the implicit ligand sampling (ILS) approach was used. The method provides complete three dimensional maps of the gas molecule placed in the protein solvate system which allows identification of the gas diffusion by docking gas molecules at the sites in protein and identify the migration pathway. The present study identifies four putative gas channels lined by hydrophobic aminoacids which will be investigated as biotechnological engineering targets.

Biography

Dr. Razia Kutty has done Ph.D in Biochemistry from National Environmental Engineering Research Institute, Nagpur, India (Indo-Swiss Collaborative Project with EAWAG, Switzerland) and Postdoctoral Research at Centre for Cellular and Molecular Biology, Hyderabad, India as well as at Rice University, Houston, Texas.