In (yet another scientific artificial reality application) and

Business, Industries

In anotherstudies of the lipase B interfacial activation that shows the interfacialactivation of PAL B happens in a highly hydrophobic surface and it favor large, bulky substrates (Zisis et al.

, 2015). From their studies, they concludethat the interfacial activation of lipase B happened in highly hydrophobicsurface but the conformational change only happen to the large, bulky substrates. Due to this reason, Zisis et al. (2015) write that lipase B acts like anesterase for small substrates and acts as lipase for substrates with largealcohol substituent.

In their studies that combine both experimental andcomputer simulation shows that ? helix 5 plays a crucial role on the substratebinding to the lipase B. Where they have confirmed that ? helix 5 are the mostmobile part of the enzyme structure and they also add that it can adopt a largerange of different conformation, including transient folding. I. Studies of structure-function relationships usingcomputational molecular simulation approachesThe advancement of the technology have developed aplatform for scientist and research to further study the complexity of thestructure – function relationship of proteins. A molecular dynamic simulationgive more information for detailed microscopic modelling on the molecular scaleand the method follows the constructive approach by mimicking the behaviour ofmolecules with the use of model systems (Ali et al., 2013). Ramakrishnan et al. (2008) in their review paper writethat molecular dynamic simulation is a powerful tool to study the structure –function relationship of proteins.

The most widely use software to perform molecularmodelling and molecular dynamic (MD) simulation are YASARA (Yet AnotherScientific Artificial Reality

Application) and GROMACS. Molecular dynamic simulation can be performed in different temperature, pH, and solvent to study the structural adaptation of the enzyme at differentcondition. The result form the simulation is analyzed through the computed rootmean square deviation (RMSd) and root mean square fluctuation (RMSf). The RMSdand RMSf are computed for the protein backbone and residues to check thestability and to study the flexibility of the enzyme.

Besides RMSD and RMSf, further analysis can be done to study the radius of gyration (Rgyration) andsolvent accessible surface area (SASA) (Ali etal., 2013). Ramakrishnan et al. (2008) in their review paper haslist out a few studies on the structural adaptation of lipase from variousmicroorganisms in different condition. The molecular dynamic simulations thatwere perform on the Candida rugosalipase shows an increase in the flap movement with the increasing of thesolvent hydrophobicity. In another molecular dynamic simulation that wereperform on Pseudomonas aeruginosa lipaserevealed the presence of a double lid and the result from molecular dynamicsimulation on Rhizomucor mieheilipase has bring out a new founding, where Rhizomucormiehei lipase were be able to retain its active site even though its globalconformation is changing due to the presence of cyclohexane (Ramakrishnan et al., 2008). A molecular dynamic simulation were previouslyperform using YASARA software on cold – active lipase from Pseudomonas sp.

strain AMS8 in water at different temperature (0°C, 5°C, 25°C, 37°C, 50°C and 100°C) to study the structural adaptation of theenzyme at low

temperature and result from the simulation shows that thecatalytic domain of the enzyme (LipAMS8) is more stable at 0°C and 5°C, whilethe non catalytic domain is not stable at the same temperature (Ali et al., 2013). Previously a moleculardynamic simulation was performed using GROMACS in water at differenttemperature on the Antarctic yeast Glaciozymaantarctica ?-mannanase and the result from the analysis shows that it hasoptimum stability at 15°C Parvizpour et al., 2014). The modelled structure of cold – active esterasefrom psychrophilic marine bacterium Rhodococcussp.

were simulated at different pH with constant temperature for 10 ns usingGROMACS software (Santi et al., 2013). Result from the simulation shows that the enzyme is seems to be quitestable at neutral pH and alkaline pH that make Santi et al. (2013) concludethat the cold – active esterase are extremely alkaliphilic. The stability and movement of the lid of lipase indifferent types of solvent has also been studied.

Tejo et al. (2004) in theirstudies conclude that the study of the lipase stability and lid movement indifferent solvents will help to improve the understanding of the lipase in organicsolvent so later it can be manipulated in the industry. In their studies of theeffect of the organic solvent to the structure and dynamics of Candida rugosa lipase has revealed thatthe movement of the lid was highly constrained in the organic solvent. Themolecular dynamic simulation that were perform on the Pseudomonas fluorescens strain AMS8 lipase in different solvent; methanol, ethanol, 2 – propanol, DMSDO, toluene and hexane shows thathydrophobic solvent (toluene) activate the opening of the lipase lid (Yaacob et al.

, 2016). It is due to the stronginteraction between the non – polar organic solvent with the AMS8 lipase.