Molecular Dynamics Simulation of Rem GTPase Obtained from Homology Modeling (Poster Presentation) - Bandung International Conference on Medicinal Chemistry, 6-8 August 2010

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Rem GTPase is a member ofRGK subfamily (Rad, Rem, Rem2, Gem and Kir) found recently. Rem is highly expressed at cardiac muscle.[l] Crystal structure of Rem (2NZJ) unveiled disordered structures of switch I (residue 102-110) and switch II (residue 135-145). These both regions have been acknowledged to be involved in nucleotide binding and GTP hydrolysis . The purpose of this study is to construct Rem GTPase model by using homology modeling method and to analyze the movements of Rem by performing molecular dynamics (MD) simulation. The selected Rem model, model_Rem_6.pdb, was constructed from multiple templates composed of 421P _A (Ras), 2A78_A (RalA), and 2NZJ_A. Furthermore Rem model was used for ten nanoseconds MD simulation provided for GDP, GTP and without ligand system by using GROMACS 3.3.2. The result was observed from visualization point of view, potential energy, RMSD and RMSF factors. MD simulation revealed that switch regions moved more flexible than other regions in the structure and tended to move away from nucleotide binding site, distinct from the movements of Ras switches which had shown interactions occurred within y-phosphate and both switches.