Performance Analysis of Curcumin Molecular Dynamics Simulation using GROMACS on Cluster Computing Environment (Proceedings of the International Conference on Advanced Computer Science and Information Systems, ICACSIS 2010)

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Abstrak

Molecular dynamic simulation is one field of science that uses computer as a resource for computational methods to calculate the number of forces acting within a molecular system and analyzing its movement. This simulation is useful for the discovery of drug compounds from an illness. This study uses Gromacs as molecular dynamics application which is running on cluster computing environment. A significant speed up is obtained during the experiments.