MOSAIC

MOlecular Structure generAtor In the Cloud

Introduction

MOSAIC is a cloud based conformational search tool, in which semi-empirical method will be used to explore the potential energy surface of biomolecule of interest in parallel mode. The tool also will be useful to screen millions of small drug like molecules databases to understand their energetics, electrostatic using semi-empirical method. This torsion angle driven conformational search method will be useful in a range of chemical design applications, including drug discovery and design of targeted chemical hosts. The tool is useful for finding the target drug ligands by calculating the energy of all the conformers. We have developed the cloud based tool which provides Software as a Service (SaaS) for trajectories from all simulation package. Multiple instances are created for energy calculations of small molecules.

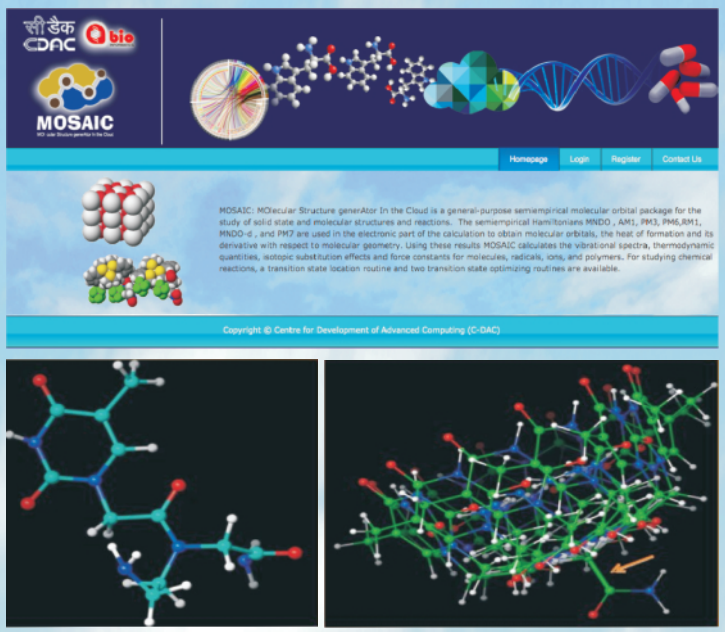
MOSAIC on Cloud

- MOSAIC has been deployed on OpenStack based Cloud
- MOSAIC interface has the capability of configuring any OpenStack based cloud by dynamically creating Cloud VM in distributed manner
- The interface is developed using LAMP (Linux, Apache, MySQL and PHP) framework
- MOSAIC uses the advantages of Cloud Computing like dynamic scaling and on-demand computing
- Configurable orchestration mechanism for virtual hardware configuration

MOSAIC Method

Input	Drug database in sdf format (same molecule with different conformation)
Parsing	Parsing of sdf format to .mop format
Optimization	.mop to mopac for semi-empirical optimization
Selection	Output files parsing based on energy value
Output	A few best optimized ligand molecules for docking

MOSAIC User Interface



MOSAIC Features

- Cloud based High-Throughput Optimization of Ligand database in parallel using distributed environment
- Easy to use interface for bioinformatics community which abstracts the complexity of Cloud based job execution
- OpenStack based Cloud environment to facilitate users with on-demand scalable virtualized resources
- User specific secured private work area to store and retrieve results
- Integrated browser based visualization of the optimized ligand molecules
- Configurable for any OpenStack based Cloud based on OpenRC script

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प्रगत संगणन विकास केंद्र
CENTRE FOR DEVELOPMENT OF ADVANCED COMPUTING
एस. पी. पुणे विश्वविद्यालय परिसर, गणेशखिंड, पुणे - 411 007, भारत
S. P. Pune University Campus, Ganeshkhind, Pune 411 007, India.
फ़ोन / Tel: +91-20- 2569 4084, फैक्स / Fax : +91-20 -2569 4084
Website: www.cdac.in email : braf-help@cdac.in