PRO-Media Coordinator's Office
Jamia Millia Islamia

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Press Release

JMI researchers develops InstaDock, easiest and fastest molecular docking tool to be used in the drug discovery pipeline

A team of researchers led by Dr. Md. Imtaiyaz Hassan at the Centre for Interdisciplinary Research in Basic Sciences, Jamia Millia Islamia(JMI) developed a molecular docking-based high-throughput virtual screening tool as freeware named InstaDock.

Molecular docking is an in-silico method used for exploring protein-ligand interactions of therapeutic interest and is one of the most widely used approaches in drug development and discovery. Drug discovery is a complex and long-drawn process that requires an interdisciplinary approach to discover new drug-like molecules called leads.

In-silico approaches such as molecular docking are used in "virtual high-throughput screening" of chemical libraries containing millions of compounds to find potential leads in drug design and discovery.

Dr. Hassan and his students Taj Mohammad and Yash Mathur developed InstaDock, a free and open access Graphical User Interface program that uses standard tools to perform molecular docking and virtual high-throughput screening efficiently.

InstaDock suite is a single-click executable, made especially for the convenience of non-bioinformatician and for people who are not experts in using computers. It is the easiest and more interactive interface than ever existing software that facilitates on-board visualization and docking analysis in just a single click.

InstaDock has been accepted for publication by the Briefings in Bioinformatics, a reputed journal of the Oxford University Press with an Impact Factor of 9.1. InstaDock is freely available for academic and industrial research purposes at www.hassanlab.org/instadock.

"It is quite challenging for non-expert users to perform molecular docking and high- throughput virtual screening directly at a universal platform, as the process involves a large number of steps. We have presented InstaDock in such a way that it can be used by even non-bioinformaticians and people with very little knowledge of computers, which greatly enhances its scope of usefulness", Taj Mohammad, Senior Research Fellow at Dr. Hassan's Lab said.

Yash Mathur said "we developed InstaDock with an aim to provide a simple and interactive drug-discovery platform to help curious minds and professionals alike, experiment and understand proteins in-silico with just a single click"

"The fields of molecular docking and high-throughput virtual screening are the much-needed areas of drug discovery and thus deployment of InstaDock is bound to greatly enhance the pre-

existing procedures. It is a novel method that gives non-expert users the freedom and efficiency that is not provided by existing programs", said Dr. Hassan.

Dr. Hassan quoted this work is a great effort of his students Mr. Taj Mohammad and Mr. Yash Mathur who worked constantly for a long time even in the lockdown situation. They are dedicatedly working in the field of structural biology, machine learning, drug discovery, and NGS analytics to contribute towards modern medical science.

Dr. Hassan's lab is running several research projects related to drug design and discovery which can be accessed via www.hassanlab.org.

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