Short course on Molecular Docking: Structure-based virtual screening for Drug Discovery 2020.

UTM UNIVERSITI TEKNOLOGI MALAYSIA

INTERNATIONAL ISLAMIC UNIVERSITY MALAYSIA
Garden of Knowledge and Virtue

Bioinformatics & Computational Biology is crucial to better prepare Scientists especially Biotechnologists, Chemists and Pharmacists to tackle the challenges in modern science. In relation to this, Biosciences Department (UTM) and Biotechnology Department (IIUM) in collaboration with Malaysian Society of Bioinformatics and Computational Biology (MaSBIC), are pleased to invite academics & research students to attend the Short Course on Structure based-Drug Discovery 2020. The audience is aimed at advanced PhD students and post-doctoral researchers who are doing or planning to start research in Computational aided-drug design.

Date:
17 & 18 February 2020

Time:
9am to 5pm

Venue:
Bioinformatic Lab, Level 5, T02 Building, Biosciences Department, Faculty of Science, UTM Johor Bahru Malaysia.

Course Synopsis

Computational techniques such as molecular docking is a valuable tool to predict the binding sites as well as the binding mode of small molecules into binding sites, to search ligand database for candidate drugs as a part of drug discovery process. The protein-ligand complex generated by the protein-ligand docking simulation can be further investigated through molecular dynamics simulation approach. These methods have been increasingly used together to investigate the specificity, selectivity and stability in molecular interactions. This information can be used for designing better drug, protein engineering, and biotechnology. This workshop will provide the fundamental theory and technicalities on setting up docking simulation using Autodock Vina and MD simulation using GROMACS program. In the workshop, participants will also learn how to perform virtual screening, analyse molecular docking outputs and MD results including MMPBSA calculation using GROMACS utility.

Registration Fee Early Bird before 31st January 2020:
RM500.00 (or USD 120) only
Normal RM600
Limited seats: available for maximum of 20 participants only

REGISTRATION FORM

To confirm your registration, please complete this form including payment.

No.	Name of Participant	Mobile No.	Email	NRIC (for HRDF claim)	Fee (RM)

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Cancellations received in writing 30 days prior to the programme are eligible for a refund, subject to a 15% cancellation fee. Cancellations received less than 14 days from the date of the programme are not eligible for a refund. However, substitute attendees are welcome. Please note that the speakers and topics are confirmed at the time of printing. However, circumstances beyond the control of the organisers may necessitate substitutions or cancellations of speakers and/or topics. As such UTMSPACE reserves the right to alter or modify the advertised speakers and/or topics.

Trainers

Dr. Azzmer Azzar Abdul Hamid
International Islamic University Malaysia
(IIUM), Kuantan

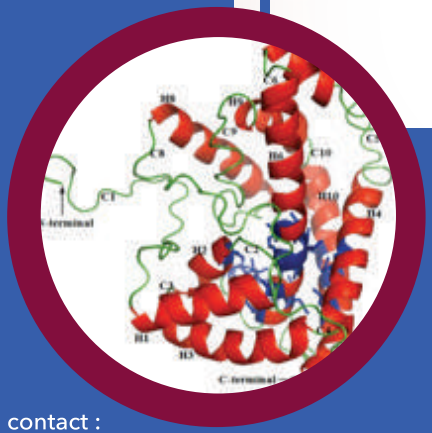
Azzmer Azzar Abdul Hamid obtained his Ph.D from IIUM in the field of Biotechnology. Upon completion of his study, he was appointed as a lecturer at the Department of Biotechnology, Kulliyyah of Science, IIUM, Kuantan Campus. He had gained research experience since he was a Research officer at the Faculty of Biosciences and Medical Engineering (FBME), UTM, Johor under supervision of Professor Fahrul Huyop. Presently, Dr. Azzmer is an active researcher in the area of enzymatic dehalogenation of toxic compounds. Dr. Azzmer has published a number of articles in high impact journal related to protein modelling and molecular recognition. At national level, Dr. Azzmer is an Exco for Malaysia Society for Bioinformatics & Computational Biology (MaSBIC).

Dr. Khairul Bariyyah Abd Halim
International Islamic University Malaysia
(IIUM), Kuantan

Following her graduation in Bioinformatics at the University of Malaya in 2005, she worked at the same university for one year as a tutor in the Department of Bioinformatics and Computational Biology. Then, she went to the University of East Anglia to do her MSc degree in Bioinformatics in September 2006. During her three-month MSc dessertation, she worked at the Genome Institute of John Innes Centre, Norwich. In 2008, she returned to Malaysia and worked as a researcher at the Centre of Research in Computational Sciences and Informatics for Biology/Bioindustry/Environment/Agriculture and Healthcare (CRYSTAL), University of Malaya, Kuala Lumpur. She was a recipient of an outstanding scholarship from Yayasan Khazanah to read Doctor of Philosophy (D.Phil.) in Biochemistry under supervision of Prof Mark Sansom, the leader of the Structural Biology and Computational Biochemistry (SBCB) group in the Department of Biochemistry, University of Oxford, United Kingdom for three years. She completed her D.Phil. in 2014 and joined IIUM as a lecturer at the Department of Biotechnology, Kulliyyah of Science, IIUM Kuantan Campus.

First Day

7.30	Registration
8.30	Opening Ceremony
8.45	Keynote-lecture: Profesor Shahir Shamsir (MaSBIC)/Dr. Syazwani Itri Amran
10.00	Tea Break
10.30	Workshop – Molecular Docking/Principles virtual screening and molecular docking simulations
	Hands-on Virtual Screening
13.00	Lunch and prayer
14.00	Molecular Docking Simulations
	Hands-on Practical 1: Protein and Ligand preparation for docking simulation using Autodock Vina
	Hands-on Practical 2 - Docking simulation and Analysis
	Hands-on Practical 3 – Visualization and H-bond analysis using Ligplot
16.00	Continue
17.00	Tea break



Second Day

8.30	Breakfast
9.00	Workshop – Molecular Dynamics (MD)
	Principles of MD simulations using GROMACS
	Hands-on Practical 4 : System preparation and Setting up Molecular Dynamics simulation
10.00	Tea break
10:30	Workshop – Molecular Dynamics (MD) simulation
	Hands-on Practical 5: Introduction to analysis tools for MD simulations and analysis of MD trajectory
	Hands-on Practical 6 : Molecular visualization using PyMol and VMD
12.00	Lunch and Prayer
14.00	Hands-on Practical 6: Analysis of MD trajectory using GROMACS tools
16.00	Wrap up and discussion
17.00	Tea break and Certificate Awards

Please contact :
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