

Date: 12 - 14 June 2012  
(Tuesday - Thursday)  
Time: 8.30 am - 5.30 pm  
Venue: IMU Bukit Jalil,  
Kuala Lumpur, Malaysia







## COMPUTATIONAL CHEMISTRY TECHNIQUES IN DRUG DESIGN

Limited to 25  
participants  
per day

A three-day workshop on contemporary trends in research into drug discovery with topics ranging from homology modelling to structure- and ligand-based drug design. Participants can select any workshop or any combination of 2 or all 3 workshops.

### Highlights

- Lectures by renowned scientists
- One-on-one attention & hands-on training by highly skilled, experienced and qualified trainers
- Docking and QSAR studies by participants on their own data set
- Complimentary evaluation version of the software with 90-day licence key

PROGRAMME					
Core topics	12-6-2012 WORKSHOP ON LIGAND BASED DRUG DESIGN	13-6-2012 WORKSHOP ON HOMOLOGY MODELLING	14-6-2012 WORKSHOP ON STRUCTURE BASED DRUG DESIGN		
	<b>Objectives</b> Be able to:- <ul style="list-style-type: none"> <li>• Perform pharmacophore models development</li> <li>• Give a pharmacophore search query</li> <li>• Explain the quantitative structure activity relationship(QSAR)</li> <li>• Build the predictive QSAR models</li> </ul>	<b>Objectives</b> Be able to:- <ul style="list-style-type: none"> <li>• Understand approaches on how to determine protein structures</li> <li>• Predict protein structure using homology modelling method</li> <li>• Do the model optimisation</li> </ul>	<b>Objectives</b> Be able to:- <ul style="list-style-type: none"> <li>• Carry out molecular docking</li> <li>• Understand advances and challenges of protein-ligand and protein-protein docking</li> <li>• Prepare protein and ligand for docking studies</li> <li>• Differentiate the scoring methods</li> </ul>		
8.30 – 9.00am	REGISTRATION				
9.00 – 10.30am	 Lecture 1: QSAR and molecular modelling in drug discovery research Speaker: Dr A.K. Saxena <ul style="list-style-type: none"> <li>• Research papers: 157</li> <li>• Patents: 70</li> <li>• Awards: 8 awards (Best: Ranbaxy award)</li> </ul>	 Lecture 1: Comparative modelling of protein structures and protein-protein complexes Speaker: Prof N. Srinivasan <ul style="list-style-type: none"> <li>• Research papers: 191</li> <li>• Awards: 3 awards (Best: Shanti Swarup Bhatnagar award)</li> </ul>	 Lecture 1: Scoring function for Molecular docking Speaker: Prof R. Sowdhamini <ul style="list-style-type: none"> <li>• Research papers: 133</li> <li>• Awards: 2</li> </ul>		
10.30 – 11.00am	TEA BREAK				
11.00 – 12.30am	 Lecture 2: Quantitative structure-activity relationships and its application for lead optimisation Speaker: Prof Sudhir A. Kulkarni <ul style="list-style-type: none"> <li>• Research papers: 48</li> <li>• Patents: 5</li> </ul>	 Lecture 2: Homology modelling and protein analysis Speaker: Dr Kundan Ingale <ul style="list-style-type: none"> <li>• Research papers: 18</li> <li>• Patent: 1</li> </ul>	 Lecture 2: Protein-ligand docking and its application in novel lead optimisation technique Speaker: Prof Sami Mukhopadhyay <ul style="list-style-type: none"> <li>• Research papers: 30</li> <li>• Awards: 2</li> </ul>		
12.30 – 1.30pm	LUNCH BREAK				
1.30 – 5.30pm	Hands-on training: Quantitative structure-activity relationship & Pharmacophore modelling	Hands-on training : Homology modelling	Hands-on training : Protein-ligand docking prediction		

### Who should attend?

Researchers having background in chemistry, biology, biophysics, bioinformatics, cheminformatics, crystallography, biochemistry, life science, pharmacology fields.

### Registration Fee

	Early Bird (Before 30/04/2012)		Regular	
	Malaysian	International	Malaysian	International
1 Workshop	RM800	USD250	RM1000	USD300
2 Workshops	RM1500	USD450	RM1750	USD550
3 Workshops	RM2000	USD600	RM2250	USD750

Supported by



### Contact Person

Ms Liong Siao Lin / Dr M. Arockia Babu  
Tel : +60 3 2731 7669 / 2757  
Fax : +60 3 8656 7299  
Email : siaolin\_liong@imu.edu.my /  
arockia\_babu@imu.edu.my

### Computational Chemistry Techniques In Drug Design

International Medical University  
126, Jalan Jalil Perkasa 19, Bukit Jalil,  
57000 Kuala Lumpur, Malaysia

Navigate your future



**REGISTRATION FORM**

Name: \_\_\_\_\_ Nationality: \_\_\_\_\_  
 Gender: Male  Female  Title: Mr  Mrs  Ms  Prof  Dr  Other: \_\_\_\_\_  
 Organisation: \_\_\_\_\_  
 Department: \_\_\_\_\_ Position: \_\_\_\_\_  
 Tel No: ( ) \_\_\_\_\_ Fax No: ( ) \_\_\_\_\_ Mobile Phone No: \_\_\_\_\_  
 Address: \_\_\_\_\_  
 \_\_\_\_\_  
 Postcode: \_\_\_\_\_ City: \_\_\_\_\_ State: \_\_\_\_\_  
 Please indicate whether this is your office or home address: Organisation  Home   
 Email: \_\_\_\_\_  
 Organisation's Website (if any): \_\_\_\_\_  
 Dietary Needs/Preference: Vegetarian  Non-Vegetarian   
 Are you an IMU Alumni member? Yes  No

**REGISTRATION FEE****PLEASE SELECT DATE**

<b>1 Workshop</b> Regular: Malaysian <input type="checkbox"/> RM1000 International <input type="checkbox"/> USD300	Early Bird: Malaysian <input type="checkbox"/> RM800 International <input type="checkbox"/> USD250	<input type="checkbox"/> 12 June 2012
<b>2 Workshops</b> Regular: Malaysian <input type="checkbox"/> RM1750 International <input type="checkbox"/> USD550	Early Bird: Malaysian <input type="checkbox"/> RM1500 International <input type="checkbox"/> USD450	<input type="checkbox"/> 13 June 2012
<b>3 Workshops</b> Regular: Malaysian <input type="checkbox"/> RM2250 International <input type="checkbox"/> USD750	Early Bird: Malaysian <input type="checkbox"/> RM2000 International <input type="checkbox"/> USD600	<input type="checkbox"/> 14 June 2012

**MODE OF PAYMENT**

Please tick your option:

- Cash  
 Cheque\* (for Malaysian Banks only)  
 Credit Card

I hereby authorise the processing of my card for the sum of (USD/RM): \_\_\_\_\_

Please complete the following sections. These details are required for security purposes.

Type of Card:  VISA  MASTERCARD Issuing Bank: \_\_\_\_\_

Cardholder's name (as it appears on the card): \_\_\_\_\_

Card Number:               Card Expiry Date:   /   (MM/YY)Card Security Code (3 digits found on reverse VISA / MASTERCARD)    Bank Draft\* Bank of Issue: \_\_\_\_\_ Date: \_\_\_\_\_ Total Amount (USD/RM): \_\_\_\_\_ Telegraphic Transfer (T.T.)\*

Account Name: IMU Education Sdn Bhd Account No. 1

Account No: **5-14187-427448** Bank: Malayan Banking Berhad\*Made payable to: **IMU Education Sdn Bhd**

\*Reference No: \_\_\_\_\_

Please send/fax registration form together with cheque/bank draft/copy of T.T. slip.

**CANCELLATION POLICY**

- Any cancellation of registration must be made in writing to the Secretariat of Computational Chemistry Techniques in Drug Design.
- There will be a 50% refund of registration fee for cancellation made before 1 May 2012.
- There will be a 30% refund of registration fee made before 15 May 2012.
- There will be no refund of registration fee for cancellations made after 1 June 2012, however a substitute participant will be welcomed.
- The Organiser reserves the right to cancel or change the topic of the workshop, if for whatever reasons beyond its control, the workshop cannot be held as scheduled or the topics need to be altered.

Signature

Date

**DISCLAIMER:**

The organiser reserves the right to make such alterations to the programmes as circumstances dictate and will not accept responsibility for any errors, omissions or changes made to the speakers' information. The views and opinions expressed by the speakers at this workshop are not necessarily the views and opinions of the organiser.

**FOR MORE INFORMATION, KINDLY CONTACT:**

Ms Liong Siao Lin / Dr M. Arockia Babu  
 126, Jalan Jalil Perkasa 19, Bukit Jalil, 57000 Kuala Lumpur, Malaysia  
 Tel: +60 3 2731 7669 / 2757 Fax: +60 3 8656 7299  
 Email: siaolin\_liong@imu.edu.my / arockia\_babu@imu.edu.my

**www.imu.edu.my**