Registration Form

International Hands on Workshop

on

"Molecular Modelling For Drug and Materials Design" 18 -21 June 2019

Name	:
Designation	:
Organization	:
Mailing Address	:
Email	:
Phone	:
Payment Details	
D.D. No	:
Date and Amount	:
Bank Name	:
Filled in registration	form is to be sent to the Convener, Office of the
Dean, Faculty of	Science, Annamalai University along with the
appropriate Demand	d Draft in favour of The Registrar, Annamalai
University payable a	t Annamalainagar.
Place:	
Date:	Signature



(Accredited with "A" Grade by NAAC)

Celebrating the 90th Anniversary

International Hands on Workshop

"Molecular Modelling for Drug and Materials Design"

18th – 21st June 2019



Organized by

Faculty of Science

Department of Chemistry

(Under the aegis of IQAC, Annamalai University)
Annamalai University
Annamalai Nagar – 608 002
Tamil Nadu, INDIA.

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Schrodinger Inc, U.S.A.

About the Annamalai University

In the early 1920s Rajah Sir S.R.M. Annamalai Chettiar founded Sri Meenakshi College, Sri Meenakshi Tamil College and Sri Meenakshi Sanskrit College at Chidambaram. In1928, Rajah Sir S.R.M. Annamalai Chettiar agreed with the local Government to handover the above said institution for establishing a University. Thus, on 01.01.1929 Annamalai University was established as per Annamalai University Act 1928 (Tamil Nadu Act 1 of 1929). One of the most significant developments is the enactment of the Annamalai University Act, 2013 (Tamil Nadu Act 20 of 2013), which has come into force from September 25, 2013. Annamalai University is accredited with 'A' Grade by NAAC in 2014. It is ranked 4th in Tamil Nadu and 20th among the top 100 institutions for Higher Education in India by "SCImago Institutional Ranking". Annamalai University is rated as the top Indian Institute in Pharmacology with highest Subject area Publication Count in Pharmacology.

Annamalai University is one of the largest unitary, teaching and residential Universities in Southern Asia comprising of 10 Faculties and 49 departments of study. This University has played a pivotal role in providing access to higher education to thousands of youth cutting across the social spectrum, especially from economically and socially disadvantaged classes. In this respect, this University's service to the nation is tremendous.

About the Department of Chemistry

The Department of Chemistry, established in 1929, has attained excellence in research under the headship of Professor V. Baliah. Since its inception, the Department has been one of the premier centers of excellence and continues to be recognized as one of the major post-graduate and research centers in Chemistry. Now with 32 dedicated team of teachers, it offers M.Sc, 5-year integrated M.Sc, in addition to M.Phil and Ph.D programmes. The department has produced more than 350 doctorates and nearly 1050 research papers have been published in national and international journals of repute in the past 7 years. In addition, the department has been actively conducting seminars, workshops, special lectures, etc., every year. The members of the teaching faculty have earned academic distinctions and awards besides receiving research grants from UGC, DST, BRNS, DBT(NEC), DRDO, CSIR and MOE&F. The Department of Chemistry is DST-FIST and UGC- SAP sponsored department.



4-Day International Hands-on Workshop on "Molecular Modeling for Drug and Materials Design"

About the Training Course:

This workshop has been designed to provide the theoretical background as well as a hands-on approach to molecular modeling in the context drug and materials design. It will cover the use of different simulation techniques such as docking, molecular dynamics, quantum mechanics, etc., and will also focus on chem-informatics methods such as QSAR and QSPR.

Workshop Topics include:

- > Catalysis Homogeneous and Heterogeneous
- Polymer Thermophysical, Mechanical and diffusion properties
- Nanomaterial Shape formation, interactions and collapse
- Optoelectronic properties OLED materials, absorption and emission spectra
- > Coating materials binding energy and surface interactions
- Pharmaceutical formulation studies understanding drug-drug carrier interactions
- Membrane modeling Solubility and diffusivity studies
- Reaction mechanisms transition state calculations
- NMR, IR, absorption, emission, VCD, Fluorescence, Phosphorescence spectra
- Solubility, diffusivity, permeability studies
- Methods and Advances in computer aided drug design
- Approaches in Target selection and refinement for docking studies
- Identification and evaluation of Binding Pocket / Active site
- > Docking approaches in virtual screening and Lead identification
- Modeling the unknown proteins for docking studies
- Pharmacophore modeling and virtual screening of novel compounds
- Refinement of novel leads using ADME prediction
- Similarity and dis-similarity based methods in lead identification
- 3D-QSAR Modeling and Lead optimization
- Biologics Design and Protein engineering

Date: 18-21 June 2019 Venue: KRM Building (Tech Park) A.U.

Level of Participants: Academicians /Scientists / Research Scholars

Registration Fee: Rs. 250/-

Number of Participants: 60 (Limited seats since workstation based)

Last date for Registration: 15.06.2019
For the receipt of filled in Registration form

Organizing Committee

Patron

Prof. V. Murugesan

Vice-Chancellor

Annamalai University

Vice-Patron

Dr. N. Krishna Mohan

Registrar i/c

Annamalai University

Convener

Dr. S. Kabilan

Professor of Chemistry & Dean, Faculty of Science

Co-Conveners

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Prof & HOD of Chemistry Faculty of Science

Dr. A. Raiasekaran

Director,

Academic Affairs

Dr. A. Murugappan

Prof. of Civil Engineering & Co-ordinator, IQAC

Organizing Secretaries

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Professor

Department of Chemistry

Dr. B. Karthikeyan

Associate Professor Department of Chemistry

Dr. R. Elancheran

Research Associate

Department of Chemistry