

About the Workshop

The two day workshop on “**Computational Tools for Drug Design (Hands on training)**” aims to integrate biological approaches with computational methods for effective drug discovery. It is designed with the help of senior scientists from Schrodinger to provide deeper insight to various tools involved in molecular modeling, drug design, cheminformatics and bioinformatics. Advances in computational techniques and in parallel hardware support have enabled *in silico* methods becoming inevitable tools for the discovery of small drug molecules in various stages of drug discovery, including new target selection, identification of hit of optimizing affinity, reducing off-targets and improving pharmacokinetic properties. This workshop provides theoretical as well as hands-on experience on the application of various computational tools for molecular modeling like

- Computational methods for small drug designing**
- Target refinement for SBDD**
- Maestro GUI**
- Structure based lead identification and optimization**
- Docking Scoring Functions**
- Homology modeling of unknown targets**
- Pharmacophore modeling**

- Protein Ligand Complex Molecular Dynamics**
- ADMET modeling**
- Protein-Protein Docking**
- 3D QSAR on chemical derivatives**

About the Department

Department of Chemistry, Gujarat University is one of the oldest departments in the state of Gujarat. It was established in 1958 and since its inception the department has earned reputation both on the area of post-graduate teaching and research. The department has been recognized as a Centre of Excellence in Supramolecules and Nanomaterials by Gujarat Council of Science and Technology, Gujarat. It is covered under UGC Special Assistance Programme (DRS III) in the thrust area of Supramolecules and Nanomaterials and also under DST-FIST, Phase I, New Delhi. The department offers post-graduation in analytical, inorganic, organic and physical chemistry along with M.Phil. and Ph.D. programs. The department is well-known for its research activities and has very well equipped research laboratories and library facilities. The main areas of research include: Supramolecular Chemistry, Medicinal Chemistry, Bioanalysis, Heterocyclic Chemistry,

Nanochemistry, Corrosion Science, Liquid Crystals and Co-ordination Chemistry.

Who can Register

Research scholars (M. Phil. and Ph. D.), faculty from academia and scientists from industries can register. Registration is restricted to limited number of participants (100) on first come first basis and having relevant research interest. Registered participants will be provided with study material, lunch and tea. Participants are required to register online https://docs.google.com/forms/d/13g9jk1w3Y8pStw3EzEjZ4S39yi1dqHXJpUeVb_dtdxI/viewform?edit_requested=true. Registration fees can be paid through NEFT/ RTGS, Name: Gujarat University Chemistry Conference; Account number: 919020016286299; IFSC Code: UTIB0000058, MICR: 3802110 60; Axis Bank, Corporate Road Branch, Ahmedabad.

Important Information

Date: 6th and 7th March 2019,

Time: 9.30 am to 5.00 pm

Place: Department of Chemistry, Gujarat University, Ahmedabad

Registration Fees: Research Scholars Rs 500/- and Academia/Industry Members Rs 700/-

Last date for registration: 3rd March 2019

No Spot Registration

NOTE: It is recommended to bring your laptop, preferably having Core i5 configuration.

3rd Workshop

On

Computational Tools for Drug Design (Hands on training)

6th and 7th March 2019

Organized

By



Department of Chemistry
School of Sciences
Gujarat University
Ahmedabad-380009

Venue: Department of Chemistry,
Gujarat University

About Schrodinger

Schrödinger, LLC is an American software company that develops chemical simulation software for use in pharmaceutical, biotechnology, and materials science research. Their mission is to improve human health and quality of life through development, distribution, and application of advanced computational methods that transform the way scientists design therapeutics and materials. To accelerate research and development activities, reduce costs, and make novel discoveries, they provide breakthrough scientific software solutions and services to clients, and also form collaborations and partnerships for research applications.

Patron : Prof. (Dr.) Himanshu A. Pandya

Honorable Vice-Chancellor
Gujarat University, Ahmedabad

Co-Patrons: Dr. Jagdish Bhavsar

Pro Vice-Chancellor
Gujarat University, Ahmedabad

And

Dr. Piyush M. Patel

I/C Registrar
Gujarat University, Ahmedabad

Chairperson: Prof. V.K. Jain

Department of Chemistry
Gujarat University

Convener: Prof. Hitesh D. Patel

Department of Chemistry
Gujarat University

Organizing Secretary: Dr. Dilip V. Vasava

Department of Chemistry
Gujarat University

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Prof. N. K. Jain (Gujarat University)
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Dr. D. R. Mishra (Gujarat University)

Catering Committee:

Prof. M. M. Maisuria (Gujarat University)
Dr. J. J. Maru (Gujarat University)

Arrangements Committee:

Dr. H. M. Parekh (Gujarat University)
Dr. V. D. Bhatt (Gujarat University)
Prof. P. S. Shrivastav (Gujarat University)

NB: All queries related to the workshop can be sent
to the Organizing Secretary,

Phone: +91-9913275906

Email: chemworkshopmarch19@gmail.com