

## About the Institute

Sardar Vallabhbhai National Institute of Technology previously by Sardar Vallabhbhai Regional engineering college, Surat is one of the 17 Regional Engineering Colleges that were set up as a joint venture of the Government of India and the Government of Gujarat. In September 2002 it is converted into the S.V. National Institute of Technology along with other REC's. The seven degree courses, fifteen M.Tech and six M.Tech research program which being offered by institute in addition of five years Integrated M.Sc. programme in chemistry, Mathematics and Physics with an intake of 30 in each through AIEEE/CATS examination, full time/ part time Ph.d. programme with scholarship is being offered by all the departments.

The Department of Applied Mathematics and Humanities, S.V. National Institute of Technology, Surat is organizing a National Workshop on Bioinformatics under Bioinformatics Infrastructure Facility of Department of Biotechnology, New Delhi and Special Interest Group on Bioinformatics of Computer Society of India. It may be mentioned here that a number of distinguished Applied Mathematicians from abroad visited the institution to participate in the International programme organized by the Deptt. Of Applied Mathematics and Humanities. This Department has supervised 20 M. Phil and 30 Ph.D. (Mathematics) candidates and successfully completed many scientific projects sponsored by National Scientific Agencies. The diamond and silk city Surat is one of the main nodes on the Bombay-Ahmedabad national highway no. 8 and is connected to the rest of the country by rail. The Institute is located in the outskirts of Surat city in an area known as Ichchhanath, at a distance of about 10 kms from the Surat Railway Station. The transportation like buses, auto and taxi are regularly available from railway/bus station from early morning till mid night. The buses heading Ichchhanath/ Piplod will be convenient to reach Institute.

### ADDRESS FOR CORRESPONDENCE

**Dr. Neeru Adlakha**

Associate Professor

Deptt. of Applied Mathematics & Humanities

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## Eligibility for Registration

Faculty, Students, Research Scholars, IT Professionals from academic institutions, research organizations, Engineers from Industries, Government / Semi-Government organization with specialization in Life Sciences / Computer Sciences / Engineering / Mathematics / Medical Sciences / Pharmacy / Chemistry/ Chemical Engineering. The number of seats are limited, preference will be given on first cum- first serve, basis.

### Registration Fee

(A) Academic & Research Institutions

(Without boarding and Lodging): **Rs. 2000/-**

(B) Industries, PSU & Govt. Department: **Rs. 5000/-**

**The boarding and lodging charges will be extra.** The boarding and lodging will be available in Institute on payment basis as per Institute norms.

The fee has to be paid in the form of **DD drawn in favour of "Director SVNIT" payable at Surat.**

Last date of receiving completed registration form is 01/03/2012. We also encourage sending a copy of registration through email at [bioinfo610@gmail.com](mailto:bioinfo610@gmail.com) to speed up the process. The participants sending the registration through email are requested to ensure that their DD and formal registration form should reach here not later than 01/03/2012 in any case. The registration process will be completed only if we received the DD and registration form.

We will confirm your selection through email latest by 05<sup>st</sup> Mar 2012 the candidates who are not selected will be intimated and their draft will be returned.

### Accommodation

Accommodation to outstation participants can be arranged at Institute Hostels or Guest House on request and on payment basis as per Institute norms. The request for the accommodation should be made well in advance.

### Note: Rates of rooms are

Non AC in Hostel guest house: Rs 200/- per day per person.

AC rooms in Hostel guest house: Rs 400/- per day per person.

# National Workshop

On

## *Molecular Modeling for Drug Designing*

March 13<sup>th</sup> -17<sup>th</sup>, 2012

Under

*Bioinformatics Infrastructure Facility*

*of*

*Department of Biotechnology, New Delhi*

*&*

*Special Interest Group on Bioinformatics of  
Computer Society of India*

**Organized by**



**Coordinator**

**Dr. Neeru Adlakha**

**Associate Professor**

**Department of Applied Mathematics &  
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**Sardar Vallabhbhai National Institute of  
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**Fax: 0261 – 2228394, 2227334**

**Website: [www.svnit.ac.in](http://www.svnit.ac.in)**

## Preamble

Computational tools have become increasingly important in the drug discovery and design processes. Methods from computational chemistry are used routinely to study drug-receptor complexes in atomic detail and to calculate properties of small molecule drug candidates. Tools from information sciences and statistics are increasingly essential to help in organizing and managing the huge chemical and biological activity databases. All pharmaceutical companies now possess, and to make optimal use of these databases. Today, the use of computational chemistry methods permeates all aspects of the drug discovery process. Some of these computational methodologies are able to model the physical details of biochemical systems, such as, protein-ligand molecular recognition and binding affinity. In this context, a great deal of excitement emerged in 90's when computational docking methods were first applied in the virtual screening of new drugs.

The workshop is so designed that the participants would spend about 50% of time in learning from lectures covering basic concepts of computational chemistry with emphasis on drug design and drug discovery. The other 50% of time they will acquire hands-on experience on useful computational chemistry tools applied to drug design and drug discovery, through elucidation of some case studies. A project will be assigned to each participant to work on problems. The workshop will cover the knowledge of computational chemistry, structural biology and molecular modeling, molecular designing and docking tools. This workshop will cover the hands-on sessions on various software such as, ChemsSketch, ChemDraw, JDraw, JMol, SPDBV, ArgusLab, AutoDock, FOLDIT, ROSETTA, Procheck and several other standalone and Web based tools.

## Significance

- One of the frontier and interdisciplinary area which involves applications of Mathematics, Computer Science, IT etc. in Biological Sciences.
- Large volume of data has resulted from Biological Experiments which need to be collected described and organized in the form of databases/data warehouses for analysis.
- The huge volume of biological data poses' new challenges and opportunities for the development of computational models, Algorithms, Tools and Software's for analysis and discovering new hidden patterns and relationships in data to predict the dynamics of biological processes.
- It creates new opportunities for Biomedical scientists

and Biotechnologists to use IT tools for design of new biotech products like drugs etc. to meet the new challenges of food, energy and health due to growth of population.

## Objectives

- To familiarize basic concepts of computational chemistry/biology for molecular structure and drug design.
- Hands on Practice in various computational chemistry/biology software tools.
- To provide practical knowledge of working with live problems on molecular modeling and drug designing through project works.

## Topics/Contents to be Covered

- System biology and its role in Drug Designing
- Molecule structure representation and visualization
- Structure databases: PDB, CATH, SCOP, FSSP, PubChem
- Molecule Drawing tools: ChemsSketch and JDraw
- Structure optimization: Molecular mechanics and dynamics. Force field
- Computational methods in protein folding study
- Protein structure prediction: Homology modeling and threading
- Computational methods in Molecular docking: Protein-protein, drug-protein, DNA-Protein
- Methods in drug designing
- QSAR study
- Case studies.

## Resource Persons From

**Institute of Liver and Billiay Science, New Delhi,  
Institute of Cancer and Preventive Oncology, Noida,  
Center for Interdisciplinary Research in Basic  
Science, New Delhi,  
Bioinformatics Center, University of Pune,  
MANIT, Bhopal and DBT center Barkatullah  
University, Bhopal.**

## Awards

**\* The participants will be given project to work upon and the best project will be awarded.**

\* Course material, lecture slides and other reference material will be provided on CDs.

(You can visit our website [www.svnit.ac.in](http://www.svnit.ac.in) for details)

**Sardar Vallabhbai National Institute of Technology**

**Surat (Gujarat) – 395 007**

**Registration Form**

**National Workshop**

**On**

***Molecular Modeling for Drug Designing***

**Under**

***Bioinformatics Infrastructure Facility of  
Department of Biotechnology, New Delhi  
&***

***Special Interest Group on Bioinformatics of  
Computer Society of India***

**March 13<sup>th</sup> -17<sup>th</sup>, 2012**

✓ Please check:  Academic  Industry/Govt.  Student

✓ Please check: Accommodation Required:  Yes  No

Name: \_\_\_\_\_

Designation: \_\_\_\_\_

Affiliation: \_\_\_\_\_

Mailing Address: \_\_\_\_\_

Telephone No. (With STD code): \_\_\_\_\_

Fax: \_\_\_\_\_

Email: \_\_\_\_\_

Specialization: \_\_\_\_\_

DD No. / Date: \_\_\_\_\_

Amount: \_\_\_\_\_

Bank: \_\_\_\_\_

(DD must be drawn in favour of "Director SVNIT" payable at Surat)

Date: \_\_\_\_\_ Signature of Applicant

Signature of Sponsoring

Authority with seal

(If required Xerox of registration form can be used)

(Deadline for Registration: 01/03/2012)