

## The Workshop

Target oriented drug designing has been the main stay in drug discovery. With advances in biological sciences several new targets have been discovered and designing a target specific drug has been a major challenge. Chemoinformatics and computational drug design has therefore assumed great significance in drug discovery process. Chemoinformatics and Computational Drug Design approaches are based on the identification and characterization of small molecules targeting a particular biological target. If a validated 3D structure of biological target is not available, it may be possible to design a homology model of the target molecule.

Chemoinformatics based drug designing helps in drug discovery by utilizing structural information to improve the lead optimization. Together chemoinformatics and computation drug design have assisted in virtual screening, lead optimization, fingerprinting, pharmacophore designing, target identification. Molecular modeling using 3D graphics and optimization techniques helps the scientists to understand how drugs bind to proteins in the body. Classically, protein structure has been exploited in lead optimization, a process that uses structure to guide the chemical modification of a lead molecule to give an optimized fit in terms of shape, hydrogen bonds and other non-covalent interactions with the target. Protein structure can also be used in target identification and selection. These approaches are being increasingly used by research scientists in academic institutions and pharma industries as they help to reduce the time and cost in drug discovery process. The workshop aims:

- i) To familiarize the participants with applications of bioinformatics in drug discovery.
- ii) To familiarize the participants with applications of chemoinformatics and computational biology in drug designing.
- iii) To acquaint participants with the current approaches of rational drug designing for specific,

and non-toxic small-molecules through guided practicals.

- iv) To acquaint participants with in silico chemical and structural fingerprinting, designing and preparation of lead molecules for drug designing and various tools and techniques of bioinformatics and molecular modeling, docking and dynamics methods.

The participants of the workshop will be accessing online resources of macromolecule libraries, sketching chemical compounds and building 3-D molecules and undertaking molecular docking. They would also learn about prediction and analysis of various properties of compounds, bimolecular and structure prediction and visualization and their interaction analysis. The knowledge gained through this hands on workshop will help them in enhancing their skills in utilizing bioinformatics tools for their application in basic and industrial research & employment potential in research institutions and industry engaged in drug discovery.

### Who should attend

Scientists / Research fellows (National Laboratories, Universities & other R&D institutions) and Graduate / Post graduate students in Engineering / Biological / Chemical sciences/ Medical discipline.

**Duration : February 27-29, 2012**

### Venue

Biotech Park, Sector-G, Jankipuram, Near Biotech Square, Kursi Road, Lucknow-226021.  
E-mail : [sna.biotech@gmail.com](mailto:sna.biotech@gmail.com), [aobiotechpark@gmail.com](mailto:aobiotechpark@gmail.com)  
[www.biotechpark.org.in](http://www.biotechpark.org.in)

**Number of Participants :** A total of 25 participants will be accepted on first come first serve basis

### Registration Fee

Rs 2,000/- per participant. The registration fee includes lectures/presentation handouts, stationary, local transportation, lunch and tea. Fee is to be paid through bank draft drawn in favour of "CEO, Biotech Park, Lucknow". Completed registration form along with the fee should reach, CEO, Biotech Park on or before **February 20, 2012**.

### Faculty

The faculty will consist of scientists and teachers from local institutions who have wide experience in bioinformatics, genomics & proteomics, drug development and biotechnology.

### Accommodation

Lucknow has different categories of Hotels. Person desiring hotel accommodation are advised to book their accommodation directly. For Guest House accommodation contact us by E-mail: [sna.biotech@gmail.com](mailto:sna.biotech@gmail.com) or by phone 0522-4053010 / 4053000. Hotel accommodation can be book directly:

- Taj Residency ([www.tajhotel.com](http://www.tajhotel.com))
- Gemini Continental ([www.geminicontinental.com](http://www.geminicontinental.com))
- Hotel Sagar International ([www.hotelsagar.com](http://www.hotelsagar.com))
- Hotel Clarks Avadh ([www.clarksavadh.com](http://www.clarksavadh.com))
- Deep Hotel (Phone 0522-2223670)
- City Hotel (Phone:0522-2202676)

## Registration Form

Name/Designation : .....

Address.....  
.....  
.....

Areas of interest: .....

E-mail : .....

Fax : ..... Phone : .....

Accommodation required YES/NO .....

(Accommodation charges are extra. Please tick the type of accommodation required.)

Guest House

Hotel

The Guest House / Hotel accommodation charges will have to be paid directly by the participants at the time of check-out.

### Payment Details:

Registration Fee : Rs .....

DD No ..... Dated.....

For further details please contact :

Chief Executive Officer  
Biotech Park  
Sector 'G' Jankipuram, Kursi Road,  
(Near Biotech Square) Lucknow-21 UP (INDIA)  
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Email: aobiotechpark@gmail.com, sna.biotech@gmail.com  
Website : <http://www.biotechpark.org.in>

## Theme of the Workshop

**Bioinformatics and its Application**

**Chemoinformatics**

**Structural Proteomics**

**Fingerprinting**

**Proteins 3-D Structure Prediction**

**Computational Drug Design**

**Science Involved in Disease  
Target Identification**

**Pocket/Active Site Identification**

**Lead Identification and Optimization**

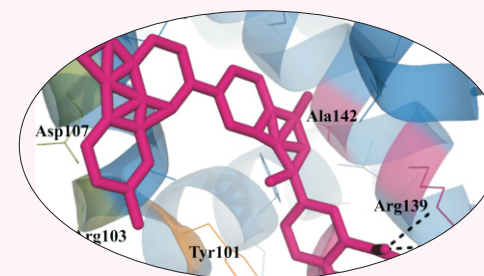
**Rational Drug Discovery**

**Biotech Park, Lucknow**  
*Where Cutting Edge Science Prospers*



## Workshop On Chemoinformatics and Computational Drug Design

**February 27-29, 2012**



**Sponsored By**

**Department of Biotechnology  
Govt. of India**

**Organised By**

**Biotech Park, Lucknow**

