2 DAY WORKSHOP | DRUG DISCOVERY TECHNOLOGY
18-19 JANUARY, 2018

BIODISCOVERY GROUP INDIA

SHAHEED RAJGURU COLLEGE OF APPLIED SCIENCES FOR WOMEN

COMPUTATIONAL APPROACHES IN DRUG DISCOVERY & DESIGN

INTRODUCTION

The simple answer to whats holding the industry back in terms of adoption of latest drug discovery techniques is Education. There simply arent enough individuals trained on the use of Proteomics, Virtual Screening, Molecular Docking, Simulations, Dynamics and ADMET-multidisciplinary approaches, which is why we continue to offer courses, for both novice and experienced users, on the use of this technology as it applies to their research functions.

BioDiscovery Group, India in collaboration with Department of Biomedical Science, Shaheed Rajguru College of Applied Sciences for Women, University of Delhi will conduct 2 day training cum workshop on Drug Discovery Technology entitled "DRUG DISCOVERY TECHNOLOGY | COMPUTATIONAL APPROACHES IN DRUG DISCOVERY & DESIGN"

This 2 day training is unique as participants perform on their laptop hence learn in a better way. The 2 day, hands-on training course will focus on the use of efficient technologies used in Drug Discovery & Designing. The course will be of great help to students/ researchers/ scientists in learning this latest science and technology.

TOPICS

- Introduction of Drug Designing
- Science involved in disease target identification
- Virtual screening

Practical application will be done on 5-10 molecules and the software on which DEMONSTRATION & TRAINING will be given

- In-silico generation of ligands by ChemSketch
- Conversion of Mol files to Pdb files by Open Babel
- Protein optimization & Energy Minimization by SPDBV
- Molecular Docking by MGL Tools | Creation of Grid Parameter & Dock Parameter files by AutoDock Software
- Running the Docking Algorithm by Cygwin
- Selection of potent inhibitors on the basis of binding energies(delta G) and Lipinski's Rule of 5
- Creating docking complex
- Structure Analysis- Protein & ligand complex & H-bond interaction by UCSF Chimera
- Prediction of Molecular Properties- Molinspiration
- Prediction of Bioactivity- Molinspiration & ACD iLabs
- Drug Likeness- Mol Soft
- Bioavailability & ADME- ACD iLabs
- Toxicity- OSIRIS Property Explorer & ACD iLabs

FEE-

Student- 1500 INR

PhD/Research Scholar- 2200 INR

Teacher/ Faculty/ Professor- 3000 INR

Scientist/Industry Delegate- 5000 INR

BRING YOUR LAPTOPS HAVING WINDOWS OS FOR SOFTWARE & TRAINING

REGISTRATION QUERIES

Dr. Manisha Khatri
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Dr. Indu Arora
Assistant Professor
aroraindu2004@gmail.com

WHO SHOULD ATTEND

With basic knowledge in Life Science and Drug Design that would like to receive a comprehensive overview or refresher on the Drug Discovery Technology the target audience comprises

Student & Faculty: Bachelor, Masters, PhD, students as well as Faculty and Professors from Microbiology, Biochemistry, Biotechnology, Immunology, Pharmacy, Pharmaceutical Chemistry, Biomedical Technology, Genetics, Bioinformatics, Plant Science and Life Sciences.

Professionals: Biotechnology, Bioinformatics and Pharmaceutical scientists from industry, academia and regulatory agencies.

Hands-on exercises will be performed individually using software tools (no prior experience required).

OUTCOME

Participants will

- be able to understand the science behind the disease condition
- Learn how to identify the biological target critical to the disease
- Learn Molecular Editing
- Learn docking molecules computationally.
- Learn how to create docking complex and visualize the 3D structure which is difficult to envision in any other way.
- Learn about the intricate atomic scale properties critical for drug design.
- Learn about the standard parameters of Structure based Drug Design.

2 DAYS WORKSHOP ON DRUG DISCOVERY TECHNOLOGY

COMPUTATIONAL APPROACHES IN DRUG DISCOVERY & DESIGN

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Department of Biomedical Science, Shaheed Rajguru College of Applied Sciences for Women, University of Delhi, Vasundhara Enclave, East Delhi, New Delhi- 110096

BRING YOUR LAPTOP WITH WINDOWS OS FOR SOFTWARE INSTALLATION & TRAINING

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