(1) INNOVATIVE APPROACHES TO DRUG DESIGN

NSQF Level: 5

SECTOR: Life Sciences

ELIGIBILITY: Bachelor's degree in Chemical and Life Sciences, or B.Pharm.

FEES: Tuition Fees- Rs 3000/- (Rs 100/- per credit)-30 credits

Laboratory Fees- Rs 2000/-(Rs 2000/- per Semester)
Total Fees- Rs 5000/-

CERTIFICATE COURSE: 6 months (450 hours)

Credits: 30

KEY COMPETENCIES: The CADD Associate is responsible to propose and implement innovative chemo-informatics tools that are used by medicinal chemists and members of the CADD group to help with the design of optimized drug-like compounds. Data mining, analysis and predictive modelling for therapeutic project teams are also part of the job accountabilities

ASSESSMENT: Assessment include continuous assessments which will comprise of following:

- ✓ 20 marks of theory component
- ✓ 20 marks of internal assessments
- ✓ 60 marks of skill assessment conducted by assessors of SSC

Course Structure: The course can be run in any of the 2 semesters in a year.

Background

Currently, the drug discovery is facing severe innovation deficit. Number of new drugs approved has drastically reduced during last decades. Many drugs were withdrawn from market due to safety reasons. Clearly, present approaches to drug design need a fresh look. The 'lock and key' theory in which the drug key is acting on the single target lock was the basis of modern pharmacology. This led to the synthesis of one drug for one target for one disease. The major disadvantage of this approach was the side effects of drugs synthesized in that way. This guided the scientists to explore innovative approaches in drug design with multi targeted as well as multi compound drugs. This has led to a new branch in pharmaceutical science named as 'Network Pharmacology'. The Network pharmacology

utilizes the advancements in computational biology and systems biology to generate networks of interaction of drugs and their molecular targets.

Indian traditional system of medicine Ayurveda practices herbal formulations for thousands of years. But the exact mechanisms of action of these drugs are not explored much. In this scenario, the integration of drug discovery and bioinformatics with network pharmacology approach will give new perspective and larger acceptance to Ayurveda. These innovative approaches can also enrich modern pharmacology with new drug scaffolds, leads and methods for rational formulation design based on traditional knowledge systems like Ayurveda.

Objectives: The objectives of the course are –

- To make students learn the science and art of "Drug Designing"
- To make students learn to design and interpret the results of herbal formulations
- To have hands on experience with the advanced computational tools available for identifying drug-biomolecule interactions.
- To integrate diverse information into discovery knowledge by exploiting the advantages of integration of drug discovery and bioinformatics with network pharmacology approach

The course has been planned to have both theory and computational lab components. Theory modules of 150 hrs duration each will cover the lectures on Basics of Drug action mechanism, theories of drug-receptor interactions, introduction to fundamental concepts behind the molecular modeling software, structure activity relationship of drug & drug like molecules, molecular docking techniques and logic behind the Drug designing.

Structure: This course is designed for the students having Bachelor degree in any science streams like, biology, chemistry, biotechnology, microbiology, pharmacy, who aspire to make a career in the areas of Research and Development of pharmaceutical sciences with an aim to introduce them at an early stage to the modern concept of Drug Designing and the computational tools available. Students who have completed second year of Bachelor degree may be permitted to enroll as an 'add-on' course.

The course will also be suitable for entry level R&D scientists for training them to use computer based methods of research in Pharmaceutical and Agrochemical Industries.

Contents:

1. Introduction to pharmaceutical sciences
2. Introduction to Ayurveda and Herbal medicine
3. Introduction to safety pharmacology
4. Introduction to Drug Design, Discovery and Development
5. Current methods of drug design and their limitations
6. Computational biology and its applications in drug design
7. Network Pharmacology and its scope
8. Databases to identify bio actives of medicinal plants
9. Tools and software to identify known molecular targets
10. Tools and software to predict molecular targets
11. Tools and software to identify and predict diseases with molecular targets
12. Tools and software to generate networks
13. Tools and software to analyze the generated networks
14. Molecular docking studies
15. Exploring Network pharmacology to study Ayurveda
16. Network pharmacology to study Ayurvedic formulations
17. Innovative approach for multi targeted, multi compound formulation design
18. Seminar, Review and Analysis

Hands on Practical (300 hours)

Major equipment and facilities required:

1. Computer Lab with Networking
2. Multinode Cluster - parallel computing

3. Work stations - higher end Graphics

4. Software molecular modeling, chemo-informatics & compound library design

- SCHRODINGER
- GAUSSIAN
- GAUSS VIEW
- MOE
- CHEMAXON
- SCIGRESS
- DISCOVERY STUDIO
- VLIFE SCIENCES
- CHEMBIO OFFICE

Industry Collaboration:

- THINQ Discovery, Mumbai
- Centaur Pharmaceuticals, Hinjewadi Pune
- Serum Institute of India, Pune
- National Toxicology Institute, Pune
- Pharmanza Herbals, Dharmaj, Gujarath
- Natural Remedies, Bangalore
- Himalaya Healthcare, Bangalore