Professional Postgraduate Program in Chemoinformatics (PPGP-CI)

(Autonomous, full-time, 11 months, residential Program
in association with **vLife Sciences**)

Technological innovations in life sciences in the last decade have cast profound impact on modern day drug discovery processes. Advances in genomics, proteomics, comparative genomics, structural bioinformatics and allied disciplines have surfaced opportunities to reveal new targets for the drug discovery and to screen millions of compound against these targets to find out the new drug leads. Chemoinformatics is a generic term in drug lifecycle that encompasses the design, creation, organization, storage, management, retrieval, analysis, dissemination, visualization and use of chemical information. Mixing of information resources to transform data into information and information into knowledge, for the intended purpose of making better and faster decisions in the arena of drug lead identification and optimization. The development of high-throughput screening and combinatorial chemistry techniques has led to a huge increase in the volumes of data about structures and their bioactivities. The explosion of data has increased the need for integration of chemical information (archival functions) with molecular modeling techniques. Chemoinformatics contributes significantly in reducing the time factor in designing new drugs as it is employed not only in forming the new structure and screen of millions of compounds but also for screening of the toxicity of lead compounds which reduces chances of failure of the compounds due to unusual toxicities in the clinical phase. There is a growing demand of chemists with expertise in chemoinformatics tools in the pharma industry world over.

This Professional Postgraduate Program in Chemoinformatics offers an attractive alternative to the chemists who can use tools of information technology to discover innovations in finding the new drugs.

Distinctive Features

☐Theory and laboratory sessions to gain practical experience of generating information based hypothesis

☐Working with in-house developed and industry standard Chemoinformatics tools

☐Collaboration with the Chemoinformatics / Bioinformatics companies at National and International levels (CLC bio, ATG Biosystems, vLife Science etc.)

☐Expert lectures, seminars and case studies by leading experts from industries

☐Twelve weeks, full time project to enhance the understanding of translational research in integrative chemoinformatics and drug design

Eligibility

Postgraduates with MSc degree in Chemistry / any other subject with Chemistry as one of the main subjects at the graduate level (with minimum 50 percent marks or equivalent grades).

Curriculum

Basic Courses:

CS001 / CS002 / CS003 Life Skills Development – I / II / III (Each 20 Hours): The Life Skills Development Program prepares the participants for communication and interaction in an organizational set-up. The focus would be on grammar, vocabulary, spoken English, remedial English, presentation skills, debates, group discussions, team building, time management, cross-cultural communication, creative and business writing. The objective of this course is to develop individuals with high intelligence and emotional quotients and will be competent in spoken English. At the end of the Life Skills Development Program the participant will be well equipped with language skills, soft skills to enter the challenging corporate world.

Core Courses:

CI601 Fundamental Computer Concepts for Informatics (60 Hours): Fundamental Principles of Computer Concepts. An Overview of Computer Architecture. Computer Algorithms. Introduction to Computers. The CPU. RAM and ROM memories. The BUS. Input and Output Devices. Controllers and Mass Storage Devices. Programming Languages. Machine Languages. Assembler. High Level Languages. Compiled Languages. Interpreted Languages. Operating Systems. Networking Applications. Internet. Computer Clusters. Supercomputers.

CI602 Introduction to Informatics (60 Hours): Basic Information Representation and Processing. Searching and Organization. Evaluation and Analysis of Information. Internet-based Information Access Tools. Ethics and Economics of Information Sharing. Survey of Data Management Issues in Medical, Health, Chemical, and Biology. Database Structures and Models. Data Access Strategies, Management and Indexing.

CI603 Informatics in Chemistry (60 Hours): Fundamental Notions in Genome and Proteome Informatics and Chemical Informatics. Design and Organizing Issues in Information Systems. Overview of Chemical Informatics Techniques. Chemical Structure Coding. Chemical Data Representation. Chemical Database and Search Systems. Molecular Visualization and Modeling Techniques. Development of Chemical Informatics Software.

CI604 Introduction to Bioinformatics (60 Hours): Introduction. Text-based and functional databases. Sequence databases. Structure Databases. Genomics Databases. Transcriptomics. Proteomics Databases. Biological Data Integration. Literature Analysis. Text analysis. Information Retrieval. Information Extraction. Applications. Sequence and Structure Analysis.

CI605 Statistics for Drug Design (50 Hours): The Role of Statistics in Chemistry and Computational Chemistry. Random Sampling and Data Description. Point Estimation of Parameters. Statistical Intervals. Single Sample. Tests of Hypotheses. Statistical Inference. Simple Linear Regression and Correlation. Multiple Linear Regressions. Design and Analysis of Single-Factor Experiments: Analysis of Variance. Design of Experiments. Nonparametric Statistics. Multivariate Analysis. Bayesian Networks. Neural Networks. Classification and Clustering.

CI606 Introduction to Advanced Cell Biology (60 Hours): Levels of Organization in Biology. Prokaryotic and Eukaryotic Cells. Viruses. Growing Cells and Viruses. Control of Microorganisms. Organelles of the Eukaryotic Cells. Structure and Function. The Cell Cycle. Mendelian Genetics. Genetics of Bacteria and Phages. Development and Cell Differentiation. Population Genetics and Evolution. DNA and Genetic Information. Genome Structure. DNA Replication. DNA Transcription. Gene Expression Regulation. Messenger RNA Translation. Biomolecules. Protein Synthesis. Protein Structure. Metabolism. Signal Transduction Pathways. Second Messenger Molecules. Cell Adhesion. Extracellular Matrix. Cell Cycle. Programmed Cell Death. Methylation of DNA and Modification of Chromatic Structure. Abnormalities in Signal Transduction Pathways to Oncogenesis and Other Disease States.

Advanced Courses:

CI701 Programming for Chemical Informatics (60 Hours): Software Development for Chem- and Bioinformatics. Programming for the Web, Depiction of Chemical and Biological Structures in 2D and 3D. Science Informatics Tool Kits. Software APIS. AI and Machine-Learning Algorithm Development. High Performance Computing. Database Management. Design and Usability of Science Informatics Software. Perl/JAVA Programming Skills.

CI702 Chemical Genomics (60 Hours): Introduction to Biology of Drugs. Introduction to Chemical Genomics. Forward Chemical Genetic Screens. Reverse Chemical Genetic Screens. Microarrays. Small Molecule Arrays. Chemical Genetics by Design. Whole Genome Approaches to Drug Mechanism of Action Profiling. Xenobiotic Metabolism Induction by Drugs. NCGC Assay.

CI703 Proteomics in Drug Research (60 Hours): Proteomics and Function. Proteomic Data Standardization, Deposition and Exchange. Proteomic Technologies. Biological Mass Spectrometry: Basics and Drug Discovery Related Approaches. Multidimensional Column Liquid Chromatography (LC) in Proteomics. Peptidomics Technologies and Applications in Drug Research. Applications.

CI704 System and Integrative Physiology (50 Hours): Structure and Function of the Cardiovascular, Respiratory, Digestive, Renal, and Reproductive Systems, as well as Pathophysiology During Disease Processes. Metabolic Physiology. Drug Intervention in Above Systems.

CI705 Molecular Modelling & Docking (60 Hours): Computer Models of Molecules and their Behavior in Gas and Condensed Phases. Implicit and Explicit Salvation Models. Quantum and Molecular Mechanics. Conformational Analysis. Geometry Optimization Methods. Information Content from Monte Carlo and Molecular Dynamics Simulations. QSAR. COMFA. Docking.

CI706 Structural Bioinformatics (60 Hours): Sequence and 3D Structure of Biological Macromolecules (DNA, RNA, Protein). Function Biomolecules. Molecular Visualization. Structure Determination. Alignment and Databases; Prediction of Protein Structure. Protein-Protein Interactions and Function.

CI707 Industry Perspective Seminar (40 Hours): In the initial part of this module, Industry experts will be invited to deliver talks on state-of-the-art technologies and happenings in the Industry to enable students to know industry requirements. In the later part, the students have to present seminars on the latest topics in their domain.

Project:

CI801 Project (400 Hours): Students can take up an industry-sponsored project or in-house project as one of the requirements of this program. For industry-sponsored projects, the Career Management Cell facilitates interaction between students and the industry. The students can also take-up the in-house projects under the guidance of the faculty and/or industry experts in their area of expertise. Students are encouraged to work on projects that will enhance their understanding in certain technology domains in real-life scenario. The project report has to be submitted to the Institute in the prescribed format, and which will be examined by experts nominated by the Institute. The project is the culmination of the student's learning in the Institute and is expected to be of high standards as demanded by the industry from time to time.

Program Structure			
Level	**Subject Code**	**Subject Name**	**Hours**
Basic			
	CS001	Life Skills Development - I	20
	CS002	Life Skills Development - II	20
	CS003	Life Skills Development - III	20
Core			
	CI601	Fundamental Computer Concepts for Informatics	60
	CI602	Introduction to Informatics	60
	CI603	Informatics in Chemistry	60
	CI604	Introduction to Bioinformatics	60
	CI605	Statistics for Drug Design	50
	Ci606	Advanced Cell Biology	60
Advanced			
	CI701	Programming for Chemical Informatics	60
	CI702	Chemical Genomics	60
	CI703	Proteomics in Drug Research	60
	CI704	System and Integrative Physiology	50
	CI705	Molecular Modelling & Docking	60
	CI706	Structural Bioinformatics	60
	CI707	Industry Perspective Seminar	40
Project			
	CI801	Project	400
			Total Hours: 1200