POST GRADUATE (P.G.) CERTIFICATE COURSE IN PHARMACO-INFORMATICS

(Syllabus for the session 2014-15 onwards)

Duration: 1 Year (Weekend) - 10 credits

Intake: 20 Seats

Course fee: Rs. 15,000/-

About Pharmaco-informatics

Target specific drug discovery is the need of the hour. Techniques evolved in the post genomic era have given us an opportunity to accelerate discovery process by looking at many cellular processes simultaneously. Advances in combinatorial chemistry, molecular modelling, computational algorithms, and modern database mining techniques are accelerating the discovery science even more.

New strategies and disciplines are emerging to identify the role of specific molecules in causing and counteracting diseases. Pharmacoinformatics, a new emerging field integrates Bioinformatics and Chemoinformatics along with pharmaceutics, pharmacology (ADME/toxicity) Pharmacy-informatics, Medical-informatics and IPR issues relevant to drug discovery.

Career prospects

The course gives an added value to the professionals of biological sciences particularly, pharmaceutical sciences. The jobs are available at scientist level in pharma industries, vaccine development, clinical research projects, academic research, etc.

Eligibility

Any of the following (minimum 50% marks required in qualifying examination):

MBBS / B.D.S. / BAMS / B.H.M.S / B.Pharmacy / B.Tech-Biotech / BVSC / B.Sc. (Nursing) / M.Sc./ M.Pharm/ B.Sc (with minimum one year relevant industry/ academic research work experience).

Note: Any candidate pursuing post-graduate course in M.D. University, Rohtak, may also co-opt for this course along with their regular course.

Course Duration

Post Graduate Certificate course in Pharmaco-informatics will be covered within six months beginning with a foundation in bioinformatics and computational biology, followed by modules on drug designing. Medium of instruction will be English. The course is designed for postgraduates and those working in industry/academics and is scheduled on weekends only.

Teaching Methodology

- Theory and practical lectures will be conducted over weekends at the venue by faculty approved by Centre for Bioinformatics, M.D. University, Rohtak.
- Projects: Each student will select the topic for his/her project within eight weeks of joining the course. Thus the projects can be taken by a group of students (not more than 5). Students will send their proposal to the Course Coordinator, who will help to nominate the guides. The project should involve about 10 days of research work.
- Note: This being a post graduate certificate course the students are expected to gain knowledge through interaction with the faculty, use of library /internet and self-study of course material.
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Evaluation and Examination

Students will be evaluated through periodic internal examination, evaluation of assignment and project work. At the end of the course students will appear for final examination conducted by Centre for Bioinformatics, M.D. University, Rohtak.

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Program Specific Outcomes

The students completing this Certificate course will be able to:

PSO1 Apply the concepts of pharmacoinformatic technologies in improving the efficiency of the medication use process.

PSO2 Address IPR issues relevant to drug discovery.

PSO3 Serve the global scientific society to accelerate *in-silico* drug discovery process.

PSO4 Emerge new strategies and disciplines to identify the role of specific molecule in causing and counteracting diseases.

PSO5 integrate the Bioinformatics and Chemoinformatics along with pharmaceutics, pharmacology (ADME/toxicity) Pharmacy-informatics, Medical-informatics and IPR issues relevant to drug discovery.

The students will be awarded as per absolute grading system, detailed below:

Interval of Marks	**Grade**	**Grade Points**
> or = 80 but <or =100	O (Outstanding)	10
> or = 70 but <80	A+(Excellent)	9
> or = 65 but <70	A (Very Good)	8
> or = 55 but <60	B+ (Good)	7
> or = 50 but <55	B (Above Average)	6
> or = 45 but <50	C (Average)	5
> or = 40 but <45	P (Pass)	4
Less than 40	F (Fail)	0
	Ab (Absent)	0

Note:A student obtaining Grade F shall be considered failed and will be required to reappear in the examination.

Course syllabus outline & Scheme of examination

S.No.	**Paper code**	**Paper title**	**Internal evaluation**	**End term evaluation**	**Credits**	**Total marks**
1.	CPI 101	Basic bioinformatics & Biostatistics	10	40	2	50
2	CPI 102	Chemo-informatics & Drug Design	10	40	2	50
3	CPI 103	Predictive Pharmacology	10	40	2	50
4	CPI 104	Medico-informatics & Pharmaco-genomics	10	40	2	50
5	CPI 105	Lab-course	-	50	-	50
6	CPI 106	Project work	-	50	2	50
Total			**40**	**260**	**10**	**300**

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CPI 101: Basic Bioinformatics and Biostatistics MM: Th 80 + IA:20

Time: 3 Hours

Students completing this course will be able to:

- **CO1** Access the world of Bioinformatics, different types of biological data and databases.
- **CO2** Access and explain the tools and techniques of analyzing DNA and protein sequences.
- **CO3** Describe & solve questions based on hidden markov model, monto carlo method.
- **CO4** Analyze in detail with reference to genetics following techniques & solve questions based on them: X2 -test, t-test.

Note: Nine questions are to be set in all and the candidates are required to attempt five questions including compulsory question. Question no. I is compulsory covering the whole syllabus. Out of remaining eight questions, two questions are to be set from each unit. Candidate is required to attempt four questions, selecting one question from each unit.

UNIT I

Bioinformatics resources

Biological databases, Basic classification – Sequence & Structure; Generalized & Specialized; Primary & Secondary, with example databases (Genbank, EMBL, DDBJ, INSDC, Swiss Prot, PIR, PDB, NDB, BLOCKS, Pfam, ProSITE, etc.); Literature databases.

UNIT II

Bioinformatics tools

Information retrieval system (Entrez, SRS); Sequence alignment tools (BLAST, FASTA, CLUSTAL-W/X, MUSCLE, TCOFFEE), Variants of BLAST (BLASTn, BLASTp, PSI-BLAST, PHI-BLAST, etc)

UNIT III

Biostatistics

Clustering: Unsupervised Learning In Large Biological Data, Measures of Similarity, Clustering, Assessment of Cluster Quality, Statistical Network Analysis For Biological Systems And Pathways, Boolean Network Modeling, Bayesian Belief Network, Modeling of Metabolic Networks , Hidden Markov Model, Monte Carlo Method.

UNIT IV

Statistical Bioinformatics

Samples and Sampling Distribution, Standard Error, significance level, Degrees of freedom, Tests of significance, tests for proportion, t and F tests Confidence Intervals, Contingency tables of χ^2 (Chi square) tests of goodness of fit and homogeneity.

Correlation: Simple, Partial and Multiple Correlation, Methods of averages and least squares, polynomial fitting, Regression Analysis. Analysis of variance for one and two way classification

Suggested Readings:

- Essential Bioinformatics by Jin Xiong.
- Bioinformatics : Sequence and Genome Analysis by David W. Mount.
- Bionformatics: Concepts, Skills and applications by R. C. Rastogi.
- Introduction to Bioinformatics by Singhal and Singhal.
- Bionformatics: A Practical Guide to analysis of Genes and Genomes by Andreas D. Baxevanis and b. F. Francis Ouellette.
- Bioinformatics Basics by Hooman H. Rashidi, Lukas K Buehler.
- Bioinformatics: A modern approach by Vittal R. Srinivas.
- Bioinformatics: Database and Systems by Stanley Latovsky.

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CPI 102: Chemoinformatics and Drug Design

MM: Th 80 + IA:20

Time: 3 Hours

Students completing this course will be able to:

- **CO1** Explain CANGEN algorithms, internal co-ordinates and caculation of Z matrix of simple organic molecule.
- **CO2** Describe the concept of QSAR,ADMET,Lipinski rule of five and their applications in drug design.
- **CO3** Explain distance matrix for calculating Weiner Index, Hosoya Index, Balban Index, Randic Index.
- **CO4** Discuss ligand and structure based design of compound and tools for drug discovery.

Note: Nine questions are to be set in all and the candidates are required to attempt five questions including compulsory question. Question no. I is compulsory covering the whole syllabus. Out of remaining eight questions, two questions are to be set from each unit. Candidate is required to attempt four questions, selecting one question from each unit.

UNIT I

Structure representation systems, 2D and 3D structures; General introduction to chemical structure-hybridization, tetrahedron geometry etc.; The degeneracy of isomeric SMILES and introduction to unique SMILES; Reaction transformations notation like SMIRKS, Introduction to graph theory, vertex partitioning algorithms- CANGEN algorithm, Internal co-ordinates and introduction to calculation of Z matrix of simple small organic molecules.

UNIT II

Chemical Databases – Design, Storage and Retrieval methods; Introduction to database filters, property based & (drug-like)-Lipinski Rule of Five, *In silico* ADMET; QSAR approach, Knowledge-based approach**.**

UNIT III

Modeling of small molecules and methods for interaction mapping; Chemical properties 2D and 3D; Introduction to adjacency, distance matrix and use of these matrices for calculating Weiner Index, Hosoya Index, Balban Index, Shultz Index, Randic Index. Introduction to shape indices- Kappa Shape index and calculation of molecular shape.

UNIT IV

Role of Chemoinformatics in pharmaceutical/chemical research; Integrated databases; HTS analysis; Ligand based design of compounds; Structure based design of compounds, Chemoinformatics tools for drug discovery; Integration of active drugs; Optimization techniques; Filtering chemicals

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Suggested Readings:

- Chemoinformatics: A Textbook edited by Johann Gasteiger, Thomas Engel
- Chemoinformatics for Drug Discovery By Jürgen Bajorath
- Chemoinformatics Approaches to Virtual Screening edited by Alexandre Varnek, Alex Tropsha
- Chemoinformatics: Concepts, Methods, and Tools for Drug Discovery edited by Jürgen Bajorath
- An Introduction to Chemoinformatics By Andrew R. Leach, V.J. Gillet
- Chemoinformatics in Drug Discovery edited by Tudor I. Oprea

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(Syllabus for the session 2014-15 onwards)

CPI 103: Predictive Pharmacology

MM: Th 80 + IA:20

Time: 3 Hours

Students completing this course will be able to:

- **CO1** Describe drug receptor interaction theories, SAR, pharmcodynamic and pharmacokinetic aspects of chiral drugs.
- **CO2** Discuss Virtual Screening, molecular Docking, ligand and structure based design of compound and several tools for drug discovery.
- **CO3** Explain Pharmacophore, pharmacophore features and pharmacophore hypothesis.
- **CO4** Describe chemical database, drug database and resources (pubchem, drug bank, super drug) and chemical sketching (ISIS Draw, Chemsketch).

Note: Nine questions are to be set in all and the candidates are required to attempt five questions including compulsory question. Question no. I is compulsory covering the whole syllabus. Out of remaining eight questions, two questions are to be set from each unit. Candidate is required to attempt four questions, selecting one question from each unit.

UNIT I

General Pharmacology

Drug receptor interaction theories, Structure activity relationships, pharmacodynamic and pharmacokinetic aspects of chiral drugs, allosteric binding, thermodynamics of drug interactions with the receptors.

UNIT II

Drug Discovery and Development

The Lead compound, Drug Discovery Cycle, Bioinformatics in drug discovery and development, chemical databases, ADME and Toxicity , Virtual Screening, Molecular Docking, Structure and Ligand Based Drug Designing, Case studies.

UNIT III

Pharmacophore Kinetics

Characterization of chemicals by Class & by Pharmacophore. Introduction to pharmocophore Identification of pharmacophore features. Building pharmacophore hypothesis; Searching databases using pharmocophores. Design & Analysis of combinatorial libraries; Reagent and product base combinatorial library generation; Focus library and HTS library.

UNIT IV

Bioinformatics in Pharmacology

Chemical Databases – Design, Storage and Retrieval methods. Introduction to database filters, property based & (drug-like)-Lipinski Rule of Five. Chemical file formats. Drug databases and Resources (Pubchem, Drug Bank, Super Drug, Chemfinder).Chemical sketching (ISIS Draw, Chemsketch).

Suggested Readings:

- Pharmacology By Gary C. Rosenfeld, David S. Loose
- Pharmacology edited by Michelle A. Clark, Richard A. Harvey, Richard Finkel, Jose A. Rey, Karen Whalen
- Chemoinformatics Approaches to Virtual Screening edited by Alexandre Varnek, Alex Tropsha
- An Introduction to Chemoinformatics By Andrew R. Leach, V.J. Gillet
- Structure-based Drug Discovery: An Overviewedited by R. E. Hubbard

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CPI 104: Medico-informatics and Pharmaco-genomics **MM: Th 80 + IA:20**

Time: 3 Hours

Students completing this course will be able to:

CO1 Explain ADMET, QSAR and discuss docking methods to generate new struture.

CO2 Describe ligand and structure based design of compound and several tools for drug discovery.

CO3 Introduction of pharmacogenomics, TagSNPs, pfSNPs and other web tools and databases.

CO4 Describe GWAS in pharmacogenomics, molecular genetics, transcriptomics, metabolomics.

Note: Nine questions are to be set in all and the candidates are required to attempt five questions including compulsory question. Question no. I is compulsory covering the whole syllabus. Out of remaining eight questions, two questions are to be set from each unit. Candidate is required to attempt four questions, selecting one question from each unit.

UNIT I

Tools for drug discovery

Integration of active drugs, Optimization techniques, Filtering chemicals, In silico ADMET; QSAR approach, Knowledge-based approach. Introduction to docking methods to generate new structure

UNIT II

Structure and Ligand-based drug designing

Introduction, Structure and Ligand based drug designing approaches: Target Identification and Validation, homology modeling and protein folding, receptor mapping, active site analysis and pharmacophore mapping, Grid maps. Lead Designing, combinatorial chemistry, High Throughput Screening (HTS), QSAR, Database generation and Chemical libraries, ADME property

UNIT III

Pharmacogenomics

Overview of pharmacogenetics and pharmacogenomics. Study designs in pharmacogenetics and phenotype selection. Identifying biological candidate genes. Linkage disequilibrium, HapMap and 1000 Genomes. TagSNPs, pfSNPs and other web tools and databases.

UNIT IV

GWAS

Genome-wide association studies in pharmacogenomics, Association analyses, After GWAS: Next-gen sequencing, Defining function: Molecular genetics; Transcriptomics; Metabolomics. Regulatory issues in pharmacogenomics.

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Suggested Readings:

- Structure-based Drug Discovery: An Overview edited by R. E. Hubbard
- Drug Design: Structure- and Ligand-Based Approaches edited by Kenneth M. Merz, Jr, Dagmar Ringe, Charles H. Reynolds
- Structure-based Drug Design: Thermodynamics, Modeling and StrategyJohn E. Ladbury, Patrick R. Connelly
- Pharmacogenomics: Methods and Applications edited by Federico Innocenti
- Concepts in Pharmacogenomics edited by Martin M. Zdanowicz
- Pharmacogenomics edited by Werner Kalow, Urs B. Meyer, Rachel F. Tyndale
- Principles of Pharmacogenetics and Pharmacogenomics edited by Russ B. Altman, David Flockhart, David B. Goldstein
- Chemoinformatics: Concepts, Methods, and Tools for Drug Discovery edited by Jürgen Bajorath