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

(Syllabus for the session 2014-15 onwards)

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

Time: 3 Hours

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

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

(Syllabus for the session 2014-15 onwards)

CPI 102: Chemoinformatics and Drug Design MM: Th 80 + IA:20

Time: 3 Hours

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

CPI 103: Predictive Pharmacology MM: Th 80 + IA:20

Time: 3 Hours

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).

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

(Syllabus for the session 2014-15 onwards)

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

Time: 3 Hours

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.