Employability

Pending
Value Added
Basics of Clinical Research

BI. SCT-1.7.1 Biostatistics and R-Programming

Total: 60 hrs

Unit I

Introduction and scope of statistics-Role of statistics in Bio-informatics, scientific method, experiment and observational, population statistics, protocol writing, Aims and objectives. Organization an collection of data - Data units population vs sample-Standardization of terms variables-Levels measurement –Dealing with response and non response

8 h

Unit II

Classification (Objectives and Methods-Quantitative and qualitative) Tabulation-Graphical a Diagrammatical representation-Spatial Data Analysis-summarization.
Measures of central tendencies-Arithmetic mean, Median, Mode, Percentages, Proportion, Harmon mean, Geometric mean, Rates, Ratios, Percentiles, Indicators and Indices.

8 h

Unit III

Measures of Dispersion-Range, Standard deviation, standard errors and co-efficient of variation and us normal distributions, skewness and kurtosis.

6 h

Unit IV

Bivariate statistical methods-Pearson's correlation coefficient-specific measures-Measures of associati Spearmen rank correlation coefficient-contingency coefficient.
Regression-Linear regression-Logistic regression-Prediction-Applications in Bioinformatics-validity Reliability.

8

Unit V

Time variable-Survival Analysis-Life table-Life expectancy measures-Time series Data analysis- square test, t-test, F-test and Z-test, ANOVA and its types.

8

Unit VI

Concept of probability-A priori & posterior Probabilities - Laws of probability-Additive multiplica and complementary probabilities conditional probability.

6

R-language

Unit VII

Introduction to R, R as statistical software and language, R as calculator, graphics with R. Getting into R and R objectives, extracting subsets of data-frames by value, sorting data, merging data, expo data, simple functions (t-apply, s-apply, summary and table).

Unit VIII

Basic plotting tools, revisiting the plot functions, loops, functions and if statements. ANOVA and t significances. Management of biological data with R.

Common Sequencing File Formats- GenBank flatfile format, Fasta file format, NBRF/PIR, GDE; Multiple Sequence Format (MSA), ALN Format, Files from Structural Data –PDB flatfile format,

Unit VIII 4 hrs

Data: Access, retrieval and submission of sequences to GenBank and structures to PDB.
Standard Search Engines Data Retrieval Tools- ENTREZ, DBGET and SRS. 4 hrs

BI. HCP-1.6 Lab based on BI. HCT-1.5

Biological databases

1. Entrez and Literature Searches.
   a. Pubmed
   b. Pubmed Central
   c. OMIM/OMIA
   d. Citation Matcher.
2. SRS of Biological Databases.
   a. Nucleotide/ Genome Databases
   b. Protein Sequence Database.
   c. Structure Database
   d. Protein Pattern Databases.
3. Sequence Analysis
   a. Dotplot
   b. Pairwise Alignment
   c. Multiple Sequence Alignment
4. Softwares.
   a. Bioedit
   b. Clustalw/X, MEGA, MEME
5. Visualization Tools.
   a. Rasmol
   b. Cn3D
   c. Molmol

References:

1. Balaguruswamy, E. (1985) "Computer Fundamentals And Applications ", Second Edition, Tata Mcgraw Hill Publishing Co Ltd., India.
2. Baxevanis, A.D. and Ouellette, B.F.F. 2001. Bioinformatics, A Practical Guide to the Analysis of Genes and Proteins, 2nd ed. Wiley Inter-science, New York.
3. Pennington, S.R. and Dunn, M.J. 2002. Proteomics, from Protein Sequence to Functions. Viva Books Pvt Lrt., New Delhi.
4. Rastogi, S. C, Mendiratta, N & Rastogi, P. 2004. Bioinformatics Methods and Applications, Genomics, Proteomics and Drug Discovery. PHI private limited, NewDelhi.
5. Rajan, S.S. and Balaji R. 2002. Introduction to Bioinformatics. Himalaya Publishing House, Mumbai.
6. Rastogi, S. C., Mendiratta, N. and Rastogi, P. 2003. Bioinformatics: Concept Skill and Applications. CBS Publisher and distributors, New Delhi.
7. Baxevanis, A.D. and Ouellette, B.F.F. 2001. Bioinformatics, A Practical Guide to the Analysis of Genes and Proteins, 2nd ed. Wiley Inter-science, New York.
8. Attwood and Parry-Smith, D.J. 1999. Introduction of Bioinformatics. Pearson Eduaction Ltd, Delhi

Semester IV

BI. HCT-4.1 Chemo–informatics and Drug Designing

Total: 60 hrs

Chemoinformatics

Unit I

Introduction and evolution of chemoinformatics, medicinal chemistry, high throughput synthesis and screening of compounds, prospects of chemoinformatics, chemical structure design (2D and 3D structure), physiochemical properties of compounds, chemical databases. Computational chemistry, classical, potential energy methods, quantum chemistry, geometry optimization, molecular mechanics and force fields, primary, secondary and tertiary chemical information, chemical indexing.

10 hrs

Unit II

Functional Groups and their biological properties of drugs

Alkylene groups, alkylating and acylating groups, sulfonic acids and derivatives, aldehyde and ketone groups, hydroxy groups, nitroso and nitro compounds, amines, effect of methyl groups on bioactivity and biotransformation.

8 hrs

Unit III

Action, Administration, Toxicity and Efficacy of drugs, pharmacodynamics and pharmacokinetics, drug action, drug interactions, Adverse drug reactions and remedial measures, effectiveness and safety, drug abuse.

Routs of drug administration, merits & demerits, distributions, Toxicity: acute, sub-acute and chronic toxicity. Management of acute toxicity and excretion, ADMET property prediction, selectivity of drug action, receptors potency and efficacy, tolerance & intolerance.

8 hrs

Drug Designing

Unit IV

Drug Discovery: Basics, technologies and strategies.

Historical perspective, objectives and strategies of dug discovery, animal models in drug discovery, management and regulatory issues, important parameters in drug discovery, process of drug discovery, computational techniques, areas influencing drug discovery, modeling, simulation and algorithms in drug discovery.

8 hrs

Unit V

Peptide combinatorial library technology, use of chemical databases in identifying drug targets, G-protein coupled receptors as drug targets, structure of GPCRs, GPCR modeling and screening, Orphan GPCRs (OGPCRs).

4 hrs

Unit VI

Drug Designing techniques and approaches. Preclinical Pharmacology, Pharmacological screening of Candidate molecules, Clinical trials.

Unit VIII

Gene structure prediction tools – GenScan, Genome Scan, GRAIL, GLIMMER, ORF finder.

Drug designing softwares: ArgusLab, Hex, Autodock, GOLD, Schrodinger, Molegro, Discovery Studio, Hyperchem, Dragon, Avegadro.

10 hrs

References:

9. Balaguruswamy, E. (1985) "Computer Fundamentals And Applications ", Second Edition, Tata Mcgraw Hill Publishing Co Ltd., India.
10. Baxevanis, A.D. and Ouellette, B.F.F. 2001. Bioinformatics, A Practical Guide to the Analysis of Genes and Proteins, 2nd ed. Wiley Inter-science, New York.
11. Pennington, S.R. and Dunn, M.J. 2002. Proteomics, from Protein Sequence to Functions. Viva Books Pvt Lrt., New Delhi.
12. Rastogi, S. C, Mendiratta, N & Rastogi, P. 2004. Bioinformatics Methods and Applications, Genomics, Proteomics and Drug Discovery. PHI private limited, NewDelhi.
13. Rajan, S.S. and Balaji R. 2002. Introduction to Bioinformatics. Himalaya Publishing House, Mumbai.
14. Rastogi, S. C., Mendiratta, N. and Rastogi, P. 2003. Bioinformatics: Concept Skill and Applications. CBS Publisher and distributors, New Delhi.
15. Baxevanis, A.D. and Ouellette, B.F.F. 2001. Bioinformatics, A Practical Guide to the Analysis of Genes and Proteins, 2nd ed. Wiley Inter-science, New York.
16. Attwood and Parry-Smith, D.J. 1999. Introduction of Bioinformatics. Pearson Eduaction Ltd, Delhi.

BI. HCP-3.6.3 Lab based on BI. HCT-3.5.3

Practicals are designed based on the BI.HCT-3.5.3 syllabus

Practicals:

1. Problem based exercise
2. Process of patenting
3. Preparing Business Plan
4. Case based study on patent and its violation
5. Clinical Trials

#BI-ESS-3.7 Entrepreneurship and Start up Studies

#ESS- Entrepreneurship and Start-up Studies * Entrepreneurship and Startup Studies Report is mandatory in 3rd Semester, **In C3 evaluation 70 marks is been distributed as 50 marks for report submission and 20 marks for presentation and Viva-Voce

BI. OET-3.8 Biological databases and Tools

Total: 60 hrs

Unit I

Bioinformatics: An Overview- Introduction to Computational Biology and Bioinformatics, scope and applications; Emergence of Bioinformatics as a Separate Discipline; Some of the biological problems that require computational methods.

6 hrs

Unit II

Biologically Data Acquisition- DNA Sequencing Methods- Basics of DNA Sequencing, Automated DNA Sequencing, DNA Sequencing by Capillary Array and Electrophoresis; Types Of DNA Sequences- Genomic DNA, cDNA, Recombinant DNA, Expressed Sequence Tags(ESTS), Genomic Survey Sequences(GSS); RNA Sequencing Methods; Protein Structure Determination Methods; Gene Expression Data.

12 hrs

Unit III

Biological databases – types of databases, literature databases, sequence databases, structure database, functional databases and chemical databases.

Nucleotide Sequence Database – GenBank, EMBL-EBI, DDBJ and INSDC.

Protein sequence data – Swiss-Prot, TrEMBL, Uniprot KB, PIR, CDD.

Structure Databases (PDB, MMDB)

8 hrs

Unit IV

Genome databases – Bacterial genome database – GOLD, MBGD, Viral genome databases – ICTVDB, VirGen, Human genome databases – MapViewer, Ensembl, UCSC, Vista-genome Browser, OMIM/OMIA.

Organisms Specific Databases (Wormbase, Ecogene, SGD, TAIR, Flybase etc).

8 hrs

Unit V

Common Sequencing File Formats- GenBank flatfile format, Fasta file format, NBRF/PIR, GDE; Multiple Sequence Format (MSA), ALN Format, Files from Structural Data –PDB flatfile format,

4 hrs

Unit VI

Data: Access, retrieval and submission of sequences to GenBank and structures to PDB.

Standard Search Engines Data Retrieval Tools- ENTREZ, DBGET and SRS.

4 hrs

Unit VII

Design of Circuits and Databases: Introduction- databases KEGG, EcoCyc, MetaCyc and BioCyc, PantherDB, Reactome, Biocarta, StringDB, Expression databases and various databases related to systems biology.

8 hrs

PGDBI-T2.4 Biological data Analytics

Total: 60 hrs

Unit I

Introduction to Bioinformatics : History of Bioinformatics, Role of Bioinformatics in biological sciences, scope of bioinformatics. Introduction to internet: WWW, network basics, LAN & WAN standards. Network topologies and protocols: ftp, http.

6 hrs

Unit II

Introduction to Database: Types of database. Biological Database: Need of biological database, Sequence and Structure database – (NCBI, EMBL, DDBJ, and PDB), other databases - KEGG, PubMed, OMIM, PubChem, NCI, ZINC, Drug Bank, Ligand. Format of Databases: GenBank and PDB flat file. Protein Structure Visualization: RasMol, PyMol, Jmol, CN3D, Swiss PDB viewer, Chimera and Discovery Studio visualizer. Protein Structure Comparison: Intra-molecular Method, Intermolecular method, combined method. Protein Structure Comparison: SCOP and CATH.

8 hrs

Unit III

Sequence Alignment and Motif, Domain Prediction Pairwise Alignment: Dot Matrix Method, Dynamic programming - (Local and Global Alignment) Gap Penalties, POA Alignment. Scoring Matrices: Amino acid scoring matrices, PAM, BLOSUM. Database Similarity Searching: BLAST. BLAST variants. BLAST output format. FASTA. Multiple Sequence Alignment: Scoring function, exhaustive algorithms, and Heuristic algorithms. PSSM, Markov Model and Hidden Markov Model. Protein Motif and Domain Prediction: Motif and Domain Databases PROSITE. Sequence Logos and Web-logo.

10 hrs

Unit IV

Gene and Promoter Prediction and Phylogenetic Gene Perdition in Prokaryotes: Conventional determination of Open Reading Frames (ORF), Markov model and HMM. Gene Prediction in Eukaryotes: An Initio based program, Neural Networks. Promoter and Regulatory Element Prediction: Prokaryotes and Eukaryotes. Introduction to Phylogenetic: Phylogenetic Basics, Terminologies. Phylogenetic Tree construction Methods: Distant based method - (UPGMA, NJ) Character Based Method – (MP and ML), Phylogenetic Tree Evaluation: Bootstrapping.

10 hrs

Unit V

Protein Structure Prediction and Molecular Dynamics Globular Proteins: Ab-Inition, Homology Based, Neural networks method. Transmembrane Proteins: Prediction of Helical membrane, β-barrel membrane proteins. RNA Structure Prediction: Ab Initio approach, dot matrices. Introduction to Homology modeling: Model refinement, model evaluation, homology model databases. Threading and fold recognition, CASP.

8 hrs

Unit VI

Introduction of Molecular Modeling: Coordinate system, potential energy. Steps in Molecular Modeling: introduction to Quantum Mechanics, introduction to Molecular mechanics. Force Filed: Types of force fields: Amber force field, CHARMM force field. Introduction about molecular dynamics (GROMACS).

8 hrs

Unit VII

Drug Discovery ...duction: Drug Discovery Process, Molecular Modeling in Drug Discovery, Molecular Doc... ...ntitative Structure-Activity Relationship (QSAR). Chemoinformatics: Introduction, st... ...er, origin of stereospecificity in molecular recognition, importance of stereochemistry i... ...design. Docking and Virtual Screening: Using different docking algorithms, Optimization of ... ...algorithms based on different target, Ligand - Receptor Interactions: Docking software's (AUT... ...K, LEAD IT), Post docking analysis. Pharmacokinetics: Absorption, Distribution, Meta... ...Excretion and Toxicity of drugs.

10 hrs

PGDBI-P2.4 Lab based on PGDBI-T2.4

1. Entrez an... ...ure Searches. a. Pubmed
   b. Pubmed ...
   c. OMIM/G...
   d. Citation ...

2. SRS of B... ...Databases. a. Nucleotide/ Genome Databases
   b. Protein S... ...Database.
   c. Structure ...
   d. Protein P... ...tabases.

3. Sequence ...is a. Dotplot
   b. Pairwise ...nt
   c. Multiple ... Alignment

4. Software... ...dit
   b. Clustalw/... ...A, MEME

5. Visualiza... ...ols. a. Rasmol
   b. Cn3D
   c. Molmol ...

Note: Including th... ...ve experiment, teachers can design additional experiment if needed.

References

1. David W Mou... ...oinformatics sequence and Genome analysis", Second Edition, Cold Spring Harbor Laboratory ..., 2013.

2. Attwood T K, P... ...y-Smith, "Introduction to Bioinformatics", Pearson Education, 2005.

3. Neil C. Jones a... Pavel A. Pevzner, "An Introduction to Bioinformatics Algorithms", MIT Press, 2005. 2. Steffen S... ...ze-Kremer, "Molecular Bioinformatics: Algorithms and Applications", Walter de Gruyter, 1996.

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PGDBI-T2.3 Molecular Modeling and Drug Discovery

Unit I **Total: 60 hrs**

Force field parameters and models: Introduction:- Hooks law, Harmonic Oscillator Model for Molecules, Morse Potential and comparison with Harmonic Potential, Intra- and Inter- molecular forces and energies, Potentials: Lennard-Jones, Truncated Lennard-jones, Exponential-6, Ionic and Polar potentials. Types of Force Fields: Biomolecular force fields (AMBER, GROMOS, etc.), Molecular Mechanics potentials for small organic molecules (MM series), second generation force fields (UFF, CFF and MMFF)

Unit II **8 hrs**

Potential Energy Surface and Energy Minimization: PES and features, Convergence Criteria and Characterization. Minimization:- multivariable minimization Algorithms, level Sets and Curves, Gradients, Minimization Criteria, Unidirectional Search, Finding Minimum Point, First order methods:- Steepest Descent and Conjugate Gradient Methods.

Unit III **8 hrs**

Molecular Dynamics Simulation: Introduction, Newtonian dynamics, Integrators- Leapfrog and Verlet algorithm, Radial distribution functions, Pair Correlation function, Potential truncation and shifted-force potentials, solvation and models, Periodic boundary conditions, Temperature and pressure control in molecular dynamics simulations.

Unit IV **8 hrs**

Basis of drug action: How drugs work - Pharmacokinetics (ADME) and pharmacodynamics basis of drug action.

Unit V **4 hrs**

New drug discovery process - Target identification and validation, lead identification and optimization. Pre-clinical and clinical testing of new drugs.

Unit VI **4 hrs**

Drug Design approaches:- Structure based drug design: Prediction and validation of 3D structure of proteins using homology modeling for docking. Basis of Docking (pose prediction and scoring algorithms) and its application in lead identification and optimization, De Novo Drug Design (Fragment Placements, Connection Methods, Sequential Grow), Virtual screening strategies for lead identification.

Unit VII **8 hrs**

Ligand based drug design - Pharmacophore generation (3D database searching, conformation searches, deriving and using 3D Pharmacophore, constrained systematic search, Genetic Algorithm, clique detection techniques, maximum likelihood method) and application for virtual screening. Introduction to QSAR, descriptors used in QSAR study, model building (regression Analysis, Partial Least Squares (PLS), Principle Components Analysis (PCA)), model validation methods and applications of QSAR.

12 hrs

PGDBI-P2.3 Lab based on PGDBI 2.3

1. Chemical databases
2. Pharmacophore identification
3. Protein structure database
4. Homology modelling
5. Binding site/active site identification
6. Computational Toxicity and druggability studies
7. Computational pharmacokinetics studies
8. Computed atlas of surface topography of protein (cast p).
9. Software - V-Life, Marvin sketch, Chemsketch, etc
10. Molecular Docking studies (Autodock)
11. QSAR studies
12. *In silico* Protein-protein interaction studies

Note: Including the above experiment, teachers can design additional experiment if needed.

Reference:

1. Computational Chemistry and Molecular Modeling-Principles and Applications by Ramachandran, Deepa and Namboori., 2008, Springer-Verlag.

2. Molecular Modeling Principles and Applications (2nd Ed.) by Andrew R. Leach., Prentice Hall, USA. 2001 46

3. Computational Drug Design: A Guide for Computational and Medicinal Chemists, by David C. Young, Wiley, 2009.

4. Molecular Modelling for Beginners, (2nd Edition) by Alan Hinchliffe., John Wiley & Sons Ltd.2008

5. Molecular Modeling and Simulation – An Interdisciplinary Guide by Tamar Schlick., Springer-Verlag 2000

6. Computational Medicinal Chemistry for Drug Discovery, edited by Patrick Bultinck., Hans De Winter, Wilfried Langenaeker, Jan P. Tollenare, CRC press, 2003.

7. The art of molecular dynamics simulation, second edition by D. C. Rapaport, Cambridge University Press, 2004

8. Homology Modeling Methods and Protocols by Andrew J.W. Orry.,University of California,USA.2012.