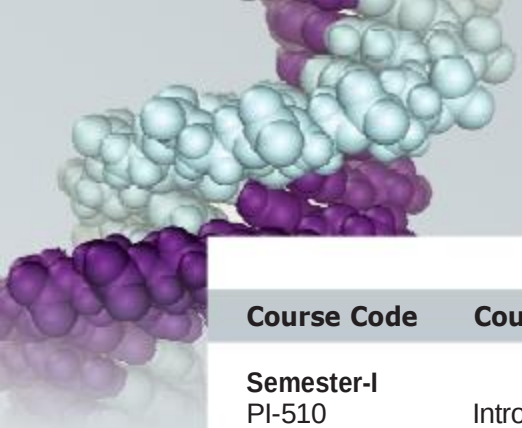
COURSES OF STUDY

Ph.D.; M.S. (Pharm.); M.Pharm.; M.Tech. (Pharm.);
M.B.A. (Pharm.)

JULY 2018

S.A.S. Nagar

National Institute of
Pharmaceutical Education and Research,
S.A.S. Nagar, Mohali



PHARMACOINFORMATICS

M.S. (Pharm.)

Course Code	Course Name	Credits
Semester-I		
PI-510	Introduction to Pharmacoinformatics	1
PI-520	Pharmacoinformatics – C++ Programming	2
PI-540	Pharmacogenamics	1
MC-510	Basics of Drug Action	2
GE-510	Biostatistics	2
GE-520	Fundamentals of Intellectual Property (IP) and Technology Management	1
GE-511	Seminar	1
LS-510	General Lab experience	3
	Total Credits	**13**
Semester-II		
PI-610	Pharmacoinformatics-Bioinformatics	2
PI-620	Pharmacoinformatics -Chemoinformatics	2
PI-630	Metabolomics and Toxicoinformatics	2
PI-650	Pharmacoinformatics Database Management	1
PI-660	Data Analytics	2`
PI-670	Pharmacoinformatics - Perl Programming	1
MC-610	Drug Design	2
BT-610	Molecular Biology	2
GE-611	Seminar	1
LS-610	General Lab Experience in the Area of Specialization	2
	Total Credits	**17**
Semester-III		
TH-598	Synopsis	5
TH-599	Presentation	3
	Total Credits	**8**
Semester-IV		
TH-698	Thesis	9
TH-699	Defence of Thesis	3
	Total Credits	**12**
	Grand Total (I to IV semesters)	**50**

Courses of Study 2018
Semester-I

Pharmacoinformatics

PI-510

Introduction to Pharmacoinformatics (1 credit)

1. Introduction of bioinformatics: Different sub domains of bioinformatics, Applications; Amino acid and nucleic acid structure; Properties.
2. Protein folding: Concept, Theoretical and experimental techniques to identify the molecular structure; Principles of protein structure; Structural bioinformatics in drug discovery, Metric system.
3. Structural genomics: Approaches, Structural genomics effort, Protein structural initiative, structural genomics consortium, Impact of structural genomics.
4. Introduction to chemoinformatics: Chemoinformatics and drug discovery, Simulation methods and their importance, Representation of molecules, Visualization and generation of 2D and 3D molecular structures; Molecular modeling, Data analysis, Chemical information.
5. Databases and its importance: 2D and 3D databases, Structural and chemical databases, Implications.
6. Energy of molecules: Bioactive conformation of the molecules, Crystallography, energy minimized and bioactive conformation, Conformational search approaches, Force field, Potential energy surface, Different conformations, examples.
7. Ligand based drug design: Overview, Similarity methods, Superimposition methods, Pharmacophore, QSAR methods.
8. Structure based methods: Overview, Introduction to molecular docking methods, scoring function, synergy between ligand and structure based methods.
9. ADME/T predictive methods: Overview of methods, *in silico* approaches to ADME/T models, pharmaceutical issues; software tools in ADME/T prediction, limitations of *in silico* approaches.
10. Applications: Application of bioinformatics, chemoinformatics, ADME/T in drug discovery and development.

Recommended books:

1. Molecular Modeling: Basic Principles and Applications by Holtje, Hans-Dieter, Wiley-VCH
2. Molecular Modelling for Beginners by Hinchliffe, Alan John, Wiley-VCH
3. Computer-Aided Drug Design by Perun, Thomas J. , B. I. Waverly, Taylor & Francis
4. An Introduction to Chemoinformatics by Leach, Andrew R, Kluwer Academic Publisher
5. Modern Methods of Drug Discovery by Hillisch, Alexander, Springer Basel AG
6. Drug Discovery Strategies and Methods by Makriyannis, Alexandros, Wiley-VCH
7. Evaluation of Drug Candidates for Preclinical Development: Pharmacokinetics, Metabolism, Pharmaceutics, and Toxicology by Han, Chao, John Wiley & Sons

PI-520

Pharmacoinformatics – C++ Programming (2 credits)

1. Problem Solving, Introduction to programming languages, C++ development environment, program structure and main function, header files
2. Input and output statements, comments, data types, variable declarations, dynamic initializations of variables, scope of variables, constants, operators and scope of operators, statements, block of codes
3. Iteration: while loops, do-while loops, for loops, nesting of loops
4. Selection: Switch statement, if-then-else statement, terminating a program
5. Functions: Definition, declaration, prototypes, return type, arguments, inline functions, recursive functions, overloaded functions
6. Arrays: Dimension, initialization, arrays as arguments to functions, strings: arrays of characters, string manipulation
7. Files: File stream objects, open and close files, input and output file streams, stream's states, file member functions
8. Pointers: Defining pointer variables, pointers and arrays, pointers as arguments to functions, arithmetic and logical operations on pointers
9. Class: Objects, object oriented design, data abstraction, class access specifiers, members, inline; static and friend functions, constructor and destructor, overloading constructor, inheritance and its types, order of invocation, virtual inheritance, polymorphism, virtual functions, operator overloading, and exception handling
10. Data structures: Arrays, Stacks, Queues, List: Link List; Two way lists; Circular link list; Insert; Delete; Searching and Sorting of data in List; Linked stack and queues; Graphs: Depth first search; Breadth first search, Trees: Binary Trees; Height balance Tree.

Note: All above concepts of C++ programming will be taught with reference to pharmaceutical sciences

Recommended books:

1. Object Oriented Programming with C++ by Balaguruswamy, McGraw-Hill Education
2. Thinking in C++ by Bruce Eckel, Prentice Hall
3. The C++ Programming Language by BjarneStroutstrup, Addison-Wesley
4. The Complete Reference to C++ by Herbert Schildt, McGraw-Hill Education
5. Data Structure Using C and C++ by A. Tanenbaum, Y. Langsam, M. J. Augenstein, Prentice Hall
6. Theory and problems of Data Structures by Seymour Lipschutz, McGraw-Hill Education
7. Data Structures & Program Design, Robert L. Kruse, Prentice Hall

PI-540

Pharmacogenomics (1 credit)

1. Pharmacogenomics: Inter individual differences in therapeutic response to drugs, susceptibility to adverse effects, polymorphism of drug metabolizing enzymes, sub-therapeutic and supra-therapeutic concentration of drugs.
2. Pharmacogenomics in PK and PD: Species difference, extrapolation to humans, selection of animal models.
3. Pharmacogenomics of Phase I metabolism: CYP 450 enzyme polymorphism, poor/rapid/ultrarapidmetabolisers, case study of CYP2D6, CYP3A3 and CYP3A4 polymorphism.
4. Pharmacogenomics of Phase II metabolism: Expression of different UGT isoforms, change in drug glucuronidation parameters, polymorphism of UGTs, atypical kinetics exhibited by UGTs, IVIVC/*in silico* modeling.
5. Pharmacogenomics of Phase III metabolism: Expression of efflux/influx transporters, drug resistance due to over expression of efflux transporters, substrate/inhibitor selectivity for efflux transporters.
6. Toxicity profiles of PPAR agonists: PPAR mediated adverse events, different isoforms of PPAR, development of dual PPAR α/γ agonists, case study.
7. Toxicity profiles of PXR agonists: PXR mediated expression of P-gp and CYP3A4, enhanced metabolism and efflux of drugs, PXR in drug development, neurological disorders and PXR.
8. Toxicity profiles of CAR agonists: Target genes, expression of CYPs and UGTs due to induction of CAR, case study.
9. Toxicity profiles of AhR agonists: Target genes, expression of CYPs and UGTs due to induction of CAR, case study.
10. Immunoinformatics: Immunoinformatics and system biology integration for personalized medicine.

Recommended books:

1. Immunoinformatics: Bioinformatics Strategies for better understanding of Immune Function Vol. 254, by Gregory Bock, Jenie Goode, John Wiley & Sons
2. Immunoinformatics: Predicting Immunogenicity *in silico* by Darres R Flower, Humana Press
3. Immunoinformatics by ShobhaRanganathan, Vladimir Brusic, Springer
4. Chemical Genomics and Proteomics by Zanders Edward D., Humana Press

LS-510

General Laboratory Experience with Computer Lab. (3 credits)

All the programming exercises will be related to Pharmaceutical Sciences

A) Computer programming (140 hours)

Write programs in C++:

a) To calculate the amount of CFC left after specific time by using half life of decay reaction.
b) To find out the prime numbers.
c) To find the roots of quadratic equation.
d) To find square root of a number by Newton Raphson method.

e) To design a calculator that simulate the workings of a basic four operation.
f) To construct a Fibonacci series by using first two value of series.
g) To calculate the sum of n terms of given series.
h) To calculate value of mathematical functions like tan, sin, cos etc.
i) To convert decimal number into hexadecimal or octal form.
j) To find the factorial of a number.
k) To find the factorial of a number using the recursive function.
l) To arrange numbers in ascending and descending order.
m) For addition and multiplication of matrices.
n) To generate distance matrix for molecule using coordinates of its atoms. Read the coordinates from mol2 file
o) To assign a value to variable using * pointer (dereferencing operator) and & (address operator).
p) To swap value of two variable using functions and pointers.
q) For appending and comparing two string.
r) To find out whether a string is palindrome or not.
s) To reverse a string.
t) To find the torsion angle using Cartesian coordinates of atoms.
u) To find the RMSD of different structure of protein by using the information given in their PDB
v) To calculate tanimoto coefficient from bitmap
w) To calculate total no of residue, no of same type of residue, no of het atom, avg of beta factor by analysis of PDB file of protein.
x) To extract coordinate of ligand from PDB of Co crystal protein-drug complex into a small file and convert it into a mol2 file.
y) Calculate the RMSD of ligand take from PDB by using the coordinate before and after energy minimization.
z) Write a program extracts the coordinate of final conformation ligand from Gaussian output file with energy.
aa) To calculate the molecular weight using smile notation of molecule.
bb) To find out the linear equation between two variable, also calculate the coefficient of correlation, standard deviation and F-value.
cc) To calculate the wiener index of compound by using its mol2 file.
dd) To calculate charge on protein and generate file without hydrogen by using PDB of protein.

B) Chem 3D (30 hours)
a) Sketching molecules in 3D space, Single point energy, energy components, energy minimization using different methods, application of charges, force fields, chiral molecules and geometry, atom types, IUPAC and smile notation, different file formats, examples.
b) Superposition of molecules and similarity, physicochemical parameters of molecules, Lipinski rule, applications.
c) Rigid and flexible molecules and their conformational search.

C) Computer and application in pharmaceutical sciences (100 hours)
a) Microsoft Office
b) Chemdraw
c) Molecular Modeling
d) Endnote
e) Statistical Software: SPSS/SAS

Courses of Study 2018
Semester-II

Pharmacoinformatics

PI-610

Pharmacoinformatics-Bioinformatics (2 credits)

1. Bioinformatics basics: Computers in biology and medicine, Information Chaos, Challenges in post genomic era, Database concept, Protein and nucleic acid databases.
2. Databases and search tools: Structural databases, Gene databases, Protein databases, Searching databases, The NCBI; Publicly available tools, Resources at EBI, Resources on the web; Database mining tools.
3. Protein folding: Diversity in proteins function and protein structure, Link between sequence, structure and function, Misfolding problem, Anfinsen's dogma, Lavinthal's paradox, Challenges in understanding structure, Methods for determining 3D structure, Protein data bank, Visualization of macromolecules.
4. Protein Flexibility: Dynamic motion in biological processes, Motion and function, Examples, Types of molecular motions, Time scale of protein motion, Methods to study protein motion, Data base of macromolecules, Online servers and software tools.
5. Molecular recognition: Process of recognition, Complementary features upon binding, Tolerance upon binding, Induced fit theory, Adaptation of enzyme and ligand, Domino effect, Ensemble of conformations, Forces involved in recognition, Solvent effect, Hydrophobic effect.
6. Secondary and tertiary structure of proteins: Protein architecture, Conformation, Ramachandran plot, Characteristics of secondary structural elements, Alpha helices, Beta sheet and reverse turns, Super secondary structure, Domains, New levels of protein architecture.
7. Classification of protein folds and topology: All alpha topology, All beta topology, Alpha-beta topology, Alpha + beta topology, Classification of proteins, CATH, SCOP.
8. Sequence Alignment: DNA/protein sequences analysis, Alignment, pairwise and global alignment, Multiple alignment, structure based alignment, software tools, BLAST, FASTA, CLUSTAL, Scoring matrices, Algorithms, Needleman-Wunsch and Smith-Waterman algorithms, Dynamics programming.
9. Structure prediction of proteins: Homology modeling, Template selection, Sequence alignment, Secondary structure prediction methods, Online servers and software, Protein main chain and side chain modeling, Loop modeling, Refinement and evaluation of models, Structure prediction of GPCRs.
10. Applications of bioinformatics: Proteins history, Proteins and pharmaceutical industries, Disease areas, Complex proteins, Applications, structure based drug design.

Recommended books:

1. Essentials of Genomics and Bioinformatics by Sensen, Christoph W. D., Wiley-VCH
2. Essential Bioinformatics by Xiong, Jin, Cambridge University Press
3. Sequence Analysis in a Nutshell: A Guide to Common Tools and Databases by Markel, Scott, O'Reilly
4. Structural Bioinformatics by Bourne, Philip E., Wiley-Blackwell
5. Computational Biology and Genome Informatics by Wang, Jason T. L., World Scientific
6. Computational Molecular Biology: An Introduction by Clote, Peter, John-Wiley
7. Introduction to Bioinformatics by Lesk, Arthur M., Oxford University Press
8. Bioinformatics: A Primer by Narayanan, P., New Age International Publishers
9. Bioinformatics: Concepts, Skills & Applications by Rastogi, S. C., Cbs Publishers & Distributors
10. Discovering Genomics, Proteomics and Bioinformatics by Campbell, A. Malcolm, Pearson

PI-620

Pharmacoinformatics-Chemoinformatics (2 credits)

1. Structure prediction methods: 2D, 3D, representing chemical structures in 1D notations searching analyzing. 4D-7D definition of structure. Morgan algorithm. Similarity searching: Tanimoto coefficient, Sorensen coefficient, Carbo coefficient, Euclidean distance, power distance, Soergel distance, Hamming distance. Full structure search and partial structure search.
2. Matrices of chemical structures: Adjacency matrix, bond matrix, distance matrix, etc., Hash codes, bitmap generation, fragment based methods. Coordinate matrix, z-matrix; their interconversion. Descriptor generation: Molecular graphs and molecular trees, 2D QSAR: structure-activity relationships; Weiner index, Hosaya index, Randic index, Balaban index, etc. topological descriptor generation.
3. Chemoinformatic tools: CDK tools, CCSD tools; Scifinder tools and algorithms associates with these tools, algorithms associated with search tools. Web based applications in chemoinformatics: MolEngine, ChemAxon, sysment reaction tool. Combinatorial library: design and molecular diversity; Applications in structure-based drug design, enumeration techniques.
4. Algorithms in chemoinformatics: C++ code generation for smiles notation, matrices, linear regression, Newton-Raphson method, conformational search. Genetic algorithms. Chemoinformatics databases: Creation, analysis of chemoinformatics databases. Generate reports from the chemical databases.
5. Pharmacoinformatics: Integration of Bioinformatics, Chemoinformatics, genomics and proteomics. *In silico* identification and validation of novel therapeutic targets: Bioinformatics followed by computational biology, Homology modeling. Pattern searching methods in drug identification. Ab initio gene prediction techniques to predict novel gene targets. Case studies.
6. Databases in pharmacoinformatics: Evaluation of diverse compound subsets from chemical structure databases. Recognition of hypotheses, validation of hypotheses using pharmacophore pattern searching methods in chemoinformatics. Spectral and Crystallographic databases. 3D database search methods: Artificial neural network methods, Genetic algorithm methods in chemoinformatics.
7. Virtual screening: Lead compound selection and lead optimization using virtual screening. Filtering methods. Rapid QSAR methods for virtual screening, Rapid molecular docking methods for virtual screening.
8. Receptor selectivity mapping. Testing the lead drug candidates (from chemoinformatics methods) for their selectivity across a broad panel of targets (from bioinformatics methods). Scoring functions and their importance in virtual screening. Case studies. Internet computing in drug discovery.
9. Algorithms in pharmacoinformatics: Development of small packages for Pharmacoinformatics analysis. Advanced algorithms in descriptor development. Algorithms for QSAR.
10. Case studies: Pharmacoinformatics in anti-diabetic drug design, Pharmacoinformatics in anti-malarial drug design. Quantum chemical methods in troglitazone toxicity, metabolism of omeprazole, proguanil, mechanism based inhibition.

Recommended books:

1. Chemoinformatics by J. Gasteiger, Wiley-VCH
2. Introduction to Chemoinformatics by A.R. Leach, Springer
3. Chemoinformatics: Concepts, Methods, and Tools for Drug Discovery by J. Bajorath, Humana Press
4. Chemoinformatics and Computational Chemical Biology by J. Bajorath, Humana Press
5. Textbook of Drug Design and Discovery by Ulf Madsen, T. Liljefors, PovlKrogsgaard, CRC Press

PI-630

Metabolomics and Toxicoinformatics (2 credits)

1. Metabolomics: Definition, metabolomics vsmetabonomics, identification of target organ, severity, onset, duration and reversal effects.
2. Optimizing drug candidates-Phase I metabolism: Reaction phenotyping of CYPs (*in silico*/*in vitro*/*in vivo*), identification of site of metabolism (SoM), structure metabolism relationships, nucleophilicity, hardness and quantum chemical parameters in determining SoM, case studies.
3. Optimizing drug candidates-Phase II metabolism: Reaction phenotyping of UGTs (*in silico*/*in vitro*/*in vivo*), identification of site of metabolism (SoM), structure metabolism relationships, nucleophilicity, hardness and quantum chemical parameters in determining SoM, case studies.
4. Optimizing drug candidates-Phase III metabolism: Substrate identification by transporters (influx and efflux) (*in silico*/*in vitro*/*in vivo*), structure transporter relationships, case studies
5. Optimizing drug candidates- Non CYP metabolism: aldehyde oxidase as drug metabolising enzyme, prediction of SoM, case studies.
6. Techniques of metabolite elucidation: LCMS/HRMS/ NMR.
7. Mechanism of drug induced toxicity: Metabolic activation and idiosyncratic drug reactions.
8. Reactive metabolites and drug safety: Adverse drug reaction (ADR), drug attrition, bioactivation/reactive metabolite formation, metabolites in safety testing (MIST), structural alerts, experimental techniques to detect reactive metabolites, strategies to avoid reactive metabolites, human hepatocytes in evaluation of adverse drug properties.
9. Pharmcokinetic DDI: Mechanisms of drug interaction, CYP inhibition/induction, UGT inhibition/induction, nuclear receptors in DDI.
10. Drug metabolism and disposition profile of drugs: Non clinical and clinical aspects, integrating *in silico* models for disposition profile of drugs.

Recommended books:

1. Drug Metabolism in Drug Design and Development, edited by Donglu Zhang, Mingshe Zhu, W. Griffith Humphreys, Wiley
2. Evaluation of Drug Candidates for Preclinical Development. Pharmacokinetics, Metabolism, Pharmaceutics and Toxicology, edited by Chao Han, Charles B. Davis, Bringhe Wang, Wiley
3. Early Drug Development: Strategies and Routes to First-in-Human Trials, edited by Mitchell N Cayes, Wiley
4. Handbook of Drug Metabolism, edited by Paul Gerard Pearson, Larry C Wienkers, CRC Press

PI-650

Pharmacoinformatics - Database Management (1 credit)

1. Database Management: Data, database, database vs file oriented approach, database management system, types of databases, databases models, three-schema architecture, data independence,data dictionary, general architecture of a database management software, components of DBMS, derived databases, data mining.
2. Relational Database Design: Basic DBMS terminology, Entities, Attributes, Relationships, ER-Diagram, Dependencies, Normalization forms, data integrity

3. SQL: Introduction to SQL, Fundamentals of SQL, SQL data types, types of statements, create and drop database
4. Data Definition Language (DDL): creating tables, constraints, alter table, add and drop columns, create view, truncate table, rename table and column, drop table and view
5. Data Manipulation Language (DML): Inserting records, deleting records, modifying records, retrieving and manipulating data: where, order by, group by; operators: arithmetic, logical, comparison; SQL functions; aggregate functions: maximum, minimum, counting records, average, sum; joins:types of join, having clause; inline views, subqueries, wildcards, distinct
6. Database Security and Privileges, GRANT Command, REVOKE Command, COMMIT and ROLLBACK, Backup and Recovery
7. PHP Programming: Data types and variables, constants, operators, statements, strings, selections, loops, comments, functions, arrays.
8. Database Connectivity: Connect to mysql: create database and table, insert records, delete records, update records, retrieve data.
9. File Organization: Heap, Sequential, Indexing and Hashing.
10. System Development Life Cycle: System Analysis and Design, Development, Testing, Implementation, Maintenance, SDLC Models.

Recommended books:

1. Learning SQL by Alan Beaulieu, O'Reilly
2. Database Systems By Rob Coronel, Thomson/Course Technology
3. Principles of Databases by JD Ullman, Galgotia Publications
4. Learning PHP, MySQL & JavaScript: With JQuery, CSS & HTML5 by Robin Nixon, O'Reilly
5. File Organization and Processing by Alan L. Tharp, Wiley-India
6. Analysis and Design of Information Systems by Arthur M. Langer, Springer

PI-660

Data Analytics (2 credits)

1. Pattern recognition: Introduction to pattern recognition and data mining, clustering vs. classification; applications; data handling and preprocessing, feature selection, normalization, dataset preparation: training, test, external; training of model; validation of model: internal validation, k-fold cross validation, external validation, y-randomization; applicability domain analysis, learning paradigms: supervised and unsupervised.
2. Machine learning algorithms for classification: k-NN, PNN, SVM
3. Machine learning algorithms for clustering: Different distance functions and similarity measures, K-means clustering, single linkage and complete linkage clustering, hierarchical clustering, logic behind these algorithms.
4. Artificial intelligence: Overview on basic concepts and its application in Pharmacoinformatics.

5. Artificial neural network: Overview of biological neuro-system, mathematical models of neurons, ANN architecture, learning rules, ANN training algorithms-perceptions, training rules, delta, back propagation algorithm, multilayer perceptron model, applications of ANNs.
6. Genetic algorithms: An overview, GA in problem solving, implementation of GA, selection, mutations, crossover.
7. Fuzzy logic: Introduction to fuzzy logic, classical and fuzzy sets: overview of classical sets, membership function, fuzzy rule generation, operations on fuzzy sets: compliment, intersections, unions, combinations of operations, aggregation operations; application of fuzzy logic in medicine.
8. Expert systems: Expert systems (knowledge based systems), expert system examples, expert system architectures, rule based expert systems, statistical systems, hybrid systems, non-monotonic expert systems, decision tree based expert systems.
9. R language: Introduction to R programming, functions, variables, data types, operators, data structures in R, objects, classes
10. Application of machine learning algorithms using R

Recommended books:

1. Pattern Recognition and Machine Learning by Bishop, Christopher, Springer
2. Pattern Recognition by SergiosTheodoridis and KonstantinosKoutroumbas, Academic Press
3. Data Mining and Analysis Fundamental Concepts and Algorithms by Mohammed J. Zaki and Wagner Meira, Jr, Cambridge University Press
4. Data Mining: Practical Machine Learning Tools and Techniques by Ian H. Witten, Eibe Frank, Mark A. Hall and Christopher J. Pal, Morgan Kaufmann
5. Neural Networks for Chemists: An Introduction by Johann Gasteiger, Wiley
6. Artificial Intelligence and Molecular Biology by Lawrence E. Hunter, AAAI Press
7. A Handbook of Statistical Analyses Using R by TorstenHothorn, Brian S. Everitt, CRC Press

PI-670

Pharmacoinformatics – Perl Programming (1 credit)

1. Introduction to Perl: History, Built in functions
2. Data types and operator: scalar data type, array data types, hash data types, subroutines, array and hash operators, Perl data structures
3. Perl operators: Arithmetic operators, Relational operators, Logical operators, assignment, Bitwise operators
4. Control structures: statement blocks, branching structures, loops, for loop, foreach loop, do… until etc.
5. Subroutines: Subroutine data types, Writing subroutine, Return function, Calling subroutine, Global and lexical variable
6. File handles: STDIN, STDOUT, Formatted output, Here strings, File tests, handling file opening errors
7. Pattern matching: Writing regular expressions, Simple meta characters, Special variable, Wild cards quantifiers, Flags, Sub expressions
8. Biocomputing: Introduction to Bioperl, Retrieval and alignment of sequences using applications.

Recommended Books:

1. Programming Perl by Larry Wall, O'Reilly
2. Beginning Perl for Bioinformatics by James Tisdall, O'Reilly
3. Effective Perl Programming by Joseph N. Hall, Addison Wesley
4. Perl from the Ground Up By Michael Mcmillan, Osborne McGraw-Hill
5. The Complete Reference Perl by Martin C. Brown, Tata McGraw-Hill

LS-610

General Laboratory Experience-10 hours/week (2 credits)

Total 180 hours:

1. Bioinformatics basics (40 hours)
    a. Analyses of protein structure complexes
    b. Energy minimization of macromolecules
    c. Sequence alignment
    d. Homology modeling
    e. Usage of online servers and applications
2. Database design and development in mysql (40 hours)
    a. Insertion of data
    b. Updation of data
    c. Deletion of data
    d. Retrieval of data
3. PHP Programming (40 hours)
    a. Connecting mysql
    b. Creating web server for developed database
4. ADME/ Tox. Informatics (20 hours)
5. Discovery Studio/TOPKAT/DEREK
6. Molecular modeling / drug design (40 hours)
    a. Conformational analyses of small molecules
    b. Molecular Docking

Courses of Study 2018
Semester-III

Pharmacoinformatics

TH-598 Synopsis	**(5 credits)**
TH-599 Presentation	**(3 credits)**

Courses of Study 2018
Semester-IV

Pharmacoinformatics

Semester-IV

TH-698 Thesis **(9 credits)**

TH-699 Defence of Thesis **(3 credits)**