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# **SEMESTER I**

Course Code: CBB 411

**Course Name:** Introduction to PERL Programming

Course Instructor: Dr. Vikram Singh

**Credits Equivalent:** 2 Credits

(One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

**Course Objectives**: Programming skills constitute the core part of the MSc curriculum on Computational Biology and Bioinformatics.

#### This course is designed to

- 1. Help students in developing logical skills.
- 2. Introduce them the basic syntax of PERL programming.

Co-requisite: CBB 413–Practical Course on PERL

#### **Attendance Requirements:**

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student will not be permitted to appear in examination.

#### **Evaluation Criteria**:

- 1. Mid Term Examination: 25%
- 2. End Term Examination: 50%
- 3. Continuous Internal Assessment: 25%
  - a) Class participation 5%
  - b) Attendance 5%
  - c) Class test 10%
  - d) Assignment 5%

#### **Course Contents**

#### **Unit 1: Introduction to programming and PERL data types**

(5 hours)

Introduction to programming languages, Machine level v/s high level languages. Introduction to PERL, #!, Basic input/output variables. Usage of 'use strict' and 'use warning' pragma.

Scalar variables: Numeric and String operators.

Single and double quoted strings, backslash interpolation, substr function.

Lists and Arrays: Accessing elements of an array, Special array indices, Scalar and List context.

Array functions: push, pop, shift, unshift, join, split, splice, sort.

Hashes: Accessing elements of a hash.

Hash functions: keys, values, exists, defined, delete, each.

#### **Unit 2: Control structures**

(4 hours)

Decision Making (Branching) Structures – if and if-else statements, Nested if-else statement, else-if ladder.

Looping Structures – for, for each, while, do-while, until and do-until statements, next, last, continue, exit, redo statements.

#### **Unit 3: Input methods, File Operations and Randomization**

(3 hours)

Input from standard input, Input from the diamond operator. Chop and chomp operators.

To read, write, append, open and close files. Using pathnames and filenames. Usage of die function.

Generating random numbers and their applications in Biology.

# **Unit 4: Regular Expressions**

(4hours)

Matching with regular expressions. Matching with m//. Binding operator =~ Pattern matching, substitution operator, transliteration operator. Regexp basics, modifiers, quantifiers, metacharacters.

# **Unit 5: References, Subroutines and Introduction to BioPERL**

(4 hours)

References, Two dimensional arrays in PERL.

Global and local variables. Subroutines – (i) Pass by Value, (ii) Pass by reference. Writing modules, Creating and using BioPERL objects.

#### **Text Books:**

- 1. Schwartz et al.(2011), Learning PERL. O'Reilly
- 2. James Tisdall(2001), Beginning PERL for Bioinformatics. O'Reilly
- 3. James Tisdall(2007), Mastering PERL for Bioinformatics. O'Reilly

#### **Additional Readings:**

4. Christiansenet al.(2012), Programming PERL. O'Reilly

# Following is a tentative list of programs that students are supposed learn coding themselves

- 1 Learning mathematical operators
  - a. WAP to print the "hello world".
  - b. WAP for the addition of two numbers
  - c. WAP using other mathematical operators (-,\*,/,% etc.)
- 2. Learning string operators
  - a. WAP to describe the usage of  $\t$ ,  $\n$  etc.
  - b. WAP to illustrate the usage of a concatenation string operator
  - c. WAP to demonstrate the usage of repetition string operator
  - d. WAP to demonstrate the usage of length, reverse etc. operators
- 3. To calculate area and volume of basic objects
  - a. WAP to calculate area of circle
  - b. WAP to calculate volume of sphere
  - c. WAP to calculate area and volume of square
  - d. WAP to calculate area and volume of rectangle
  - e. WAP to calculate area and volume of cube
- 4. To transcribe DNA into RNA using substitution operator and transliteration operator
- 5. To calculate the reverse complement of DNA sequence
- 6. To calculate the values in a series in iterative manner

a. 
$$1^2, 2^2, 3^2, 4^2, 5^2$$
....

b. ..

7. To calculate the sum of first n-terms of a given algebraic series

a. 
$$(1+x^2+x^3+\cdots+x^n)$$

b. ..

- 8. To calculate the factorial of a given number
- 9. To generate first n terms of Fibonacci series
- 10. To find which term is greater using ASCII code
- 11. To find out triplets of given DNA sequence using substr
- 12. To count the percentage of nucleotides in a given DNA sequence
- 13. To translate a DNA sequence into an amino acid sequence in all six reading frames
- 14. To map genetic code using hash.
- 15. To translate a given RNA sequence into its corresponding peptide.
- 16 Programs to print various 2-dimensional patterns using "only one" for loop
  - a. for obtaining right triangle pattern
  - b. for obtaining inverted right triangle pattern

- c. for the matrix patterns 11111
  - 22222
  - 33333
  - 44444
  - 55555
- d. WAP to get the result  $1+1^2_2=2$ 
  - $2+2^2=6$  $3+3^2=12$
- 17. To check if the given number is prime or not.
- 18. To check if the given string is palindrome or not
- 19. To print 2-dimentionsional pattern using "nested" for loop
  - WAP to create a following matrix
    - i. 12345
      - 12345
      - 12345
    - ii. 1234
      - 2345
      - 3456
      - 4567
  - b. WAP to create following pattern
    - i.
- \*\*
- \*\*\*
- \*\*\*\*
- ii. \*\*\*\*
  - \*\*\*\*
  - \*\*\*\*
- iii. Equilateral triangle
- 20. To create a random DNA sequence using rand operator
- 21. To simulate DNA mutation i.e. insertion and deletion
  - WAP to randomly remove a nucleotide from a DNA sequence
  - b. WAP to randomly insert a nucleotide into a DNA sequence
- 22. To generate two random DNA sequences and find out the percentage identity between them
- 23. To read DNA sequence from a file and WAP to write DNA sequence into a file
- 24. Finding patterns in the DNA and protein sequences using various metacharacters (^,.,?,\*,+,{},(),\$,\,|)
- 25. Writing subroutines (Call by value)

- a. Addition
- b. Multiplication
- c. Subtraction etc.
- d. Factorial of given number
- e. Fibonacci series
- 26. Referencing and dereferencing of
  - a. Scalar
  - b. Array
- 27. Writing subroutine (Call by reference)
- 28. To construct and use a 2-D array
- 29. To design a simple module and use it in a program



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# **SEMESTER I**

Course Code: CBB 413

Course Name: Practical course on PERL

**Instructor:** Dr. Vikram Singh

**Credits Equivalent:** 2 Credits

(One credit is equivalent to 20 hours of lectures / organised classroom activity / contact hours; 10 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 30 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

**Course Objectives**: This course is designed to give students an opportunity for implementing the theoretical understanding of PERL programming (learned in the course CBB 411) into the PERL scripts.

Upon successful completion of this course students will be able to apply the knowledge of PERL programming to develop the applications in Computational Biology and Bioinformatics.

Pre-/Co-requisite: CBB 411 -- Introduction to PERL Programming

#### **Attendance Requirements:**

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student will not be permitted to appear in examination.

#### **Evaluation Criteria**:

Mid Term Examination: 25%
 End Term Examination: 50%

3. Continuous Internal Assessment: 25%

a) Class Test 10%

b) Assignments 5%

c) Home work 10%

#### **Course Contents**

# Unit 1: Understanding PERL data types (Scalar, Array, Hash) and usage of mathematical and string operators. (8 hours)

- Using Mathematical operators (Addition, Subtraction, Multiplication, Division, Modulus operators)
- Using String operators (Concatenation, Repetition operators)
- To calculate Area and Volume of basic objects (circle, sphere, parallelogram cube etc.).
- Finding reverse complement of a DNA sequence.
- Transcription, Reverse Transcription.

#### **Unit 2: Learning Control Structure**

(10hours)

- Counting nucleotides in the given DNA sequence.
- Translating a DNA sequence into an amino acid sequence in all six reading frames.
- To check if a given number is even, odd or prime. To generate first *n* terms of Fibonacci series.
- To calculate the factorial of a given number.
- Finding sum of first n terms of a given algebraic series.
- To check if the given number or string is palindrome.

#### **Unit 3: Input Methods, File Operations and Randomization(6hours)**

- Reading and writing DNA and/or protein data from/into a file.
- Generating random DNA, random protein sequence.
- Simulating DNA mutation.
- Finding % identity between two random DNA sequences.

#### **Unit 4: Regular Expressions(8 hours)**

- Finding simple motifs in DNA or protein sequences.
- Using regular expressions to find complex patterns in the DNA and protein sequences.
- Parsing FASTA files
- Parsing Genbank files.

# **Unit 5: References, Subroutines and introduction to BioPERL(8hours)**

- Referencing and dereferencing of scalars and arrays
- Reading and writing a 2-dimensionl matrix in PERL
- Writing subroutines (pass by value and pass by reference) for the programs of units 1 and 2.
- Writing PERL modules
- Learning the usage of CPAN
- Creating simple BioPERL objects.

#### **Text Books:**

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Schwartz et al. (2011), Learning PERL. O'Reilly
James Tisdall (2001), Beginning PERL for Bioinformatics. O'Reilly
James Tisdall (2007), Mastering PERL for Bioinformatics. O'Reilly
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# **Additional Readings:**

20. Christiansen et al. (2012), Programming PERL. O'Reilly



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#### **SEMESTER I**

Course Code: CBB 402

**Course Name:** Modern Biology **Instructor Name:** Dr P. Aparoy

**Credits Equivalent:** 2 Credits (One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

**Course Objectives**: The course is designed to:

- Introduce students the principles of modern biology
- Describe mechanisms that regulate biological systems, including: replication, transcription and translation.
- Acquaint the role of bioinformatics in evolution

#### **Attendance Requirement:**

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

#### **Evaluation Criteria**:

Mid Term Examination: 25%
 End Term Examination: 50%

**3.** Continuous Internal Assessment : 25%

- a) Class Test 10%
- b) Class Room Participation 10%
- c) Attendance 5%

#### **Course Contents:**

#### **UNIT -I:** Genes and Chromosomes

(3 Hours)

- Chromosomal Elements
- DNA Super coiling
- Structure of Chromosomes

# **<u>UNIT-II</u>**: Bioinformatics in Exploring Evolution

(3 Hours)

- Role of Sequence Alignments in Exploring Evolution
- Role of Three-Dimensional Structure in Exploring Evolution
- Introduction to Evolutionary Trees

# **UNIT -III:** DNA metabolism

(5 Hours)

- DNA replication
- DNA repair
- DNA recombination

#### **UNIT-IV:** RNA metabolism

(5 Hours)

- DNA dependent synthesis
- RNA dependent synthesis
- RNA processing

#### **UNIT -V:** Protein metabolism

(4 Hours)

- Genetic code
- Protein synthesis
- Post translational modification

#### **Prescribed Text Books:**

- **1.** Nelson & Cox, Lehninger. (2017). Principles of Biochemistry 7<sup>th</sup> edition, W. H. Freeman Publications
- **2.** Jeremy M. Berg, Lubert Stryer, John L. Tymoczko, Gregory J. Gatto. (2015). Biochemistry 8<sup>th</sup> edition, W. H. Freeman Publications
- **3.** U. Satyanarayana, U. Chakrapani. (2017) Biochemistry : 5<sup>th</sup> edition. Elsevier Health Sciences



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# **SEMESTER I**

Course Code: CBB 403

Course Name: Introduction to Statistics and Probability

Instructor Name: Dr P. Aparoy

#### **Credits Equivalent: 2**

2 Credits (One credit is equivalent to 10 hours of lectures / organized classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

#### **Course Objectives:**

CBB-403 will introduce the students to the concepts and methods of statistics, covering topics such as data organization, data presentation, data analysis, probability, estimation and hypothesis testing.

#### **Attendance Requirement:**

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

#### **Evaluation Criteria:**

1. Mid Term Examination: 25% 2. End Term Examination: 50%

3. Continuous Internal Assessment: 25%

a) Class test: 10%

b) Class room participation: 10%

c) Attendance: 5%

#### **Course Contents:**

#### **Unit-I: Frequency Distributions and Graphs**

(2 Hrs)

Introduction to Statistics; Frequency Distributions; Dot Plots; Bar Charts or Bar Graphs; Histograms; Frequency Polygons; Stem-and-Leaf Displays or Plots; Time Series Graphs; Pie Graphs or Pie Charts; Pareto Charts

**Unit-II: Numerical Measures** (4Hrs)

- Measures of Central tendency:
   Mean, Median, Mode Notation and Formulae, Mean, Median and Mode for grouped data, relative merits of Mean, Median and Mode
- Measures of Dispersion:
   Range, Semi-interquartile range, Standard Deviation and Variance; Empirical
   Rule: The normal curve, Percentile and Quartile, Detecting Outliers

#### **Unit-III: Correlation and Regression**

(4 Hrs)

- Introduction to correlation; A numerical Index to Correlation; Pearson Product-Moment Correlation Coefficient; Interpretation of Correlation Coefficient: Explained and Unexplained Variation; Spearman Rank Correlation
- Introduction to Regression; Criterion for the Line of Best Fit; Another Measure of Ability to Predict: The Standard Error of Estimate

#### **Unit-IV: Probability**

(5 Hrs)

• Introduction and Basic Concepts of Probability; Probability of Simple and Combined Events; Various Laws of Probability; Bayes' Theorem; Random Variables and their Distribution; Binomial Distribution; Normal Distribution; Interpreting Scores in Terms of *z* Score; Sampling Distribution; Central Limit Theorem

#### **Unit-V: Introduction to Statistical Inference**

(5 Hrs)

• Principles of Hypothesis Testing; One and Two tailed tests; *z*-test; *t*-test; Chi-Square test; ANOVA

#### **Reference Books**

- Murray Spiegel, John Schiller, R. Alu Srinivasan, Debasree Goswami. (2017). Probability and Statistics, McGraw Hill Education; 3 edition
- Roger E. Kirk (2007) Statistics: An Introduction, Cengage Learning; 5th edition
- Neil A. Weiss (2012) Introductory Statistics, 9th edition



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#### **SEMESTER I**

CourseCode:CBB431

CourseName: Bioanalytical Techniques

Course Instructor: Mr. Satpal

CreditsEquivalent: 2Credits

2 Credits (One credit is equivalent to 10 hours of lectures / organized classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

#### **Course Objectives**: The course is designed to:

- Introduce students about the techniques used to study biochemical analysis of cellular structures and macromolecules
- Acquaintstudentstothebasicprinciplesofvariousimmunochemic altechniques
- Toun derstandthetech niquestomonitorhowthestructureanddynamicsofbiom oleculesenablesspecificbiologicalfunctions

#### **Attendance Requirement:**

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75 % attendance is a must failing which a student may not be permitted to appear in examination.

#### **Evalua tion Criteria:**

1. MidTermExamination:25%

2. EndTermExamination:50%

3. Continuous Internal Assessment: 25%

a. Assignment:10%

b. ClassTest:5%

C. Presentation:10%

#### **Course Contents:**

#### **UNIT-1**: Introduction to Centrifugation and Microscopy

- Basic principles of centrifugation and types of centrifuges
- Preparative and Analytical Centrifugation
- Light Microscope
- Stereomicroscope

# **UNIT-II**: Mass Spectrometric Techniques

- Introduction, Ionisation
- Mass analyzers, Detectors
- Structural Information by tandem mass spectrometry
- Analysing protein complexes

# **<u>UNIT-III</u>**: ElectrophoreticTechniques

- Introduction ,Electrophoresis of proteins
- Electrophoresis of proteins
- Electrophoresis of nucleic acids
- Electrophoresis of nucleicacids and capillaryelectrophoresis

#### **UNIT-IV: Chromatographic Techniques**

- Principle of chromatography
- Liquidchromatography and highperformance liquidchromatography
- Adsorption, Partition and Ion Exchangechrolnatography.
- Molecular exclusion, gasliquid and thinlayerchromatography

#### **UNIT-V**: Spectroscopic Techniques

- Introduction to Spectroscopic Techniques
- X-Ray Spectroscopy; applications
- Nuclear magnetic resonance spectroscopy; applications
- Circular Dichromism and Electron spin spectroscopy; application

#### **Prescribed Text and Reference Books:**

- 1) BiochemistryandMolecularBiology,7thedition,KeithWilsonandjohnWalker
- 2) Fundamentals of Bioanalytical Techniques And Instrumentation, Ghosal & Srivastava, 2009, Published by Ashoke K. Ghosh.
- 3) Introduction to Biophysical Methods for Protein and Nucleic Acid Research , Jay A. Glasel, Murray P.Deutscher and Murray P. Deutscher, ISBN: 978-0-12-286230-4
- $4). Biophysical Techniques, Iain Campbell, 368 pages, 16 February\ 2012.$

Sr.No.	Journal articles (specific articles, Complete reference)
1	Spectroscopic Methods in Biochemistry -Principles and Applications,© Jorg H. Kleinschmidt WS 2000/ 2001
2	A review of chromatographic methods for the assessment of phospholipids in biological samples,2005; Brianna L Peterson and Brian S. Cummings, BIOMEDICAL CHROMATOGRAPHY, Biomed. Chromatogr. 20: 227-243 (2006)
3	An Introduction to Mass Spectrometry, 1998,Scott E. Van Bramer

#### **Relevant Websites**

Sr.No.	Web address	Salient Features
1	(http://www.sciencedirect.com/science/journal	Methodological aspects of biochemistry, biophysics,



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# <u>SEMESTER I</u>

Course Code: CBB-418
Course Name: Biomolecules
Course Instructor: Mr. Satpal

**Credits Equivalent:** 2 Credits (One credit is equivalent to 10 hours of lectures / organized classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

#### **Course Objectives**: The course is designed to:

- Introduce students about the structure and function of Biomolecules.
- Study various forces responsible for their molecular structures.
- Study their role in body metabolism.

#### **Attendance Requirement:**

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination

#### **Evaluation Criteria:**

- 1. Mid Term Examination: 25%
- 2. End Term Examination: 50%
- 3. Continuous Internal Assessment: 25%
  - a) Presentation 10%
  - b) Class Participation 10%
  - c) Attendance 5%

#### **Course Contents:**

# **Unit-1: Water and its Property**

(4 Hours)

- Physiochemical properties of water
- Dissociation and Association constant, pI, pKa
- Ionization of water-Weak acids and Weak bases, Buffering in biological system
- Hesselberg-Henderson equation

#### .Unit-2: Carbohydrates

(4 Hours)

- Structure and function of -Monosaccharides- disaccharides- oligosaccharides
- Structure and Biological functions of Homo and Heteropolysaccharides
- Biosynthesis and Degradation of Glucose and Glycogen
- Glycolipids and Peptidoglycans

#### **Units-3: Lipids**

(4 Hours)

- Lipids Classification- structure and properties
- Fatty acids- saturated and unsaturated fatty acids
- Phospholipids, Glycoplipids, Sphingolipids and Cholesterol
- Structure and biological role of prostaglandins, thromboxanes and leukotrienes

#### **Units-4: Nucleic Acids**

(4 Hours)

- Structure and Function: Physical and Chemical properties of Nucleic acids
- Double helical model of DNA and Forces responsible for A, B and Z- DNA
- DNA denaturation and renaturation- hypochromicity- Tm
- Application of DNA microarray

#### **Units-5: Proteins**

(4 Hours)

- Amino acid Structure and function
- Structural organization of proteins- Primary, Secondary, Tertiary and Quaternary,
- Ramachandran plot and super secondary structure
- Forces stabilizing protein structure and shape, Protein denaturation and folding

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#### **Text Book:**

- 1. Nelson.D.L, Cox. M. M. Lehninger's Principle of Biochemistry. 4th ed. Freeman, 2004
- 2. Murray. R.K, Granner.D.K, Mayes. P. A, Rodwell. V. W. Harper's Biochemistry. 27th ed. McGraw Hill, 2006.

# **Suggested Reading:**

- 1. Dixon & Webb. Enzymes. 3rd ed. Longmans, 1979.
- 2. Berg.J.M, Tymoczko.J.L, Stryer, L. Biochemistry. 6 th ed. Freeman, 2006.
- 3. Adams. R.L, Knowler.J.Leader. D.P. Biochemistry of Nucleic Acids. Cambridge Univ. Press, 1998.



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#### **SEMESTER I**

**Course Code: CBB 405** 

**Course Name: Basics of Bioinformatics Course Instructor:** Mrs. Neha Chaudhary

**Credits:** 

Credits Equivalent: 2 Credits (One credit is equivalent to 10 hours of lectures / organized classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/projects/dissertation/thesis; seminars, etc.)

#### **Attendance Requirement:**

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination

#### **Evaluation Criteria:**

Mid Term Examination: 25% 2. End Term Examination: 50%

Continuous Internal Assessment: 25% 3.

Presentation 10%

Class Participation 10% b)

c) Attendance 5%

#### **Course Contents:**

#### UNIT - I: **Introduction and Historical Background**

- What is Bioinformatics, introduction.
- Historical developments and evolution of Bioinformatics.
- Importance of Bioinformatics in Life Sciences

#### **UNIT - II:** Biological Databases

- Introduction
- Primary and Secondary Databases
- **Nucleotide Sequence Databases**
- Protein Sequence Databases (Swissprot, Uniprot)
- SCOP, CATH and FSSP

Information retrieval from databases

# **UNIT - III:** Assessing Pairwise Sequence Similarity

- Types of alignment: Local and Global
- Scoring matrices
- BLAST Types and how it works
- Comparing FASTA and BLAST

# **UNIT - IV:** Sequence alignment: Local and global

- Needleman Wunsch and Smith Waterman algorithms
- Exercises on pairwise alignment

# **UNIT - V:** Phylogenetic Analysis

- Concepts in Molecular Evolution
- Phylogenetic Trees and Dendrograms
- How to Construct a tree
- Methods in Phylogenetic reconstructions

# **Suggested Reading:**

- 1. Bioinformatics: Sequence and Genome Analysis by David W. Mount.
- 2. Introduction to Bioinformatics by Arthur M Lesk.
- 3. Introduction to Bioinformatics by T K Attwood, D J Perry-Smith and Samiron Phukan.



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#### **SEMESTER I**

Course Code: CBB 405

**Course Name:** Practical course on Bioinformatics Tools

**Course Instructor:** Mrs. Neha Chaudhary

#### **Course Content:**

**Lab I:** Information retrieval from databases

**Lab II:** Chemical structure softwares

**Lab III:** Sequence alignment tools

Lab IV: BLAST: A sequence similarity search tool

Lab V: Modeller: Structure prediction by Homology modeling

**Lab VI:** Phylogenetic tree construction



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# **SEMESTER III**

Course Code: CBB 518

Course Name: Elements of Systems Biology

**Instructor Name:** Dr Vikram Singh

**Credits Equivalent:** 4 Credits

(One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

**Course Objectives**: This course will be centered on (i) the theoretical and practical aspects of modellingin systems biology – both deterministic and stochastic and (ii) the study of biological networks. Students will become acquainted with the key concepts and computational approaches of both these fields.

"Systems Biology" finds its major application in the research field known as "Synthetic Biology" (aiming to design and realize modified or new biological parts). Students will also become familiar with necessary mathematical and computational concepts of Synthetic Biology.

Students having prior knowledge of any programming language will be encouraged to write their own codes for simulating and analysing model biological systems.

#### **Attendance Requirement:**

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination

#### **Evaluation Criteria**:

Mid Term Examination: 25%
 End Term Examination: 50%

3. Continuous Internal Assessment: 25%

a. Attendance: 5%

b. Class-room participation: 5%

c. Class test: 5%

d. Presentation and assignment: 10%

#### **Course Contents**

#### **Unit 1: Introductory interdisciplinary concepts** (8 hours)

- Definition and scope of systems and synthetic biology. Introduction to biological complexity -- Self organization, Emergence, Chaos, Robustness.
- First-order systems: Fixed points and stability, Population growth.
- Bifurcations (with examples) in first order systems: Saddle node, Pitch fork, Transcritical.
- Basic notion of bifurcations in second order systems: Period doubling, Hopf.

#### **Unit 2: Deterministic modelling in systems biology**

(8 hours)

- Chemical kinetics, Michaelis-Menten kinetics, Hill equations
- Feedback in gene regulation: positive, negative, mutual inhibition
- Deterministic methods of systems modelling (Euler and RK4), with numerical applications on
  - a) Simple examples of autocatalysis, linear degradation etc.
  - b) Examples from natural systems: Predator-Prey, p53-mdm2.
  - c) Examples from synthetic systems: Brusselator, Repressilator.

#### **Unit 3: Stochastic modelling in systems biology**

(8 hours)

- Introduction to noise in biological systems. Intrinsic vs. extrinsic noise. System behaviour and role of noise.
- Stochastic Methods for modelling biological systems (Master equation, Gillespie's stochastic simulation algorithm)
- Application of Gillepsie's SSA on Brusselator, Predator-Prey and other simple examples.

#### Unit 4: Design principles of biological networks

(8 hours)

- Introduction to networks: Hamiltonian path vs. Eulerian path; Basic terminology; Topology of genetic, metabolic and ecological networks.
- Network models: Erdös-Renyi, Small-world, Scale-free.
- Global Properties: Average path length, network diameter, centrality measures, clustering coefficients etc. Modular and hierarchical networks.
- Local Properties: Regulatory motifs and graphlets in networks. Motifs in TRNs: discussion on FFL, SIM and other motifs.

- Elementary graph algorithms: Breadth-first search, Depth-first search, Topological sort, Strongly connected components. Growing a minimum spanning tree.
- Finding shortest path: Single source shortest path, All pairs shortest paths
- Network clustering: Clique based clustering, Center based clustering
- Basics of flux balance analysis.

#### **Text Books:**

- 21. **Steven H. Strogatz** (1994), Nonlinear Dynamics and Chaos: With Applications to Physics, Biology, Chemistry, and Engineering. Perseus Books, Massachusetts.
- 22. Szallasi et al. (2010), System Modelling in Cellular Biology. MIT Press.
- 23. **Junker and Schreiber (2008),** Analysis of Biological Networks. Wiley-Interscience, New Jersy.

# **Additional Readings:**

- 2 Uri Alon (2006), An Introduction to the Systems Biology. Chapman and Hall.
- 3 Mark Newman (2010), Networks: An Introduction. Oxford University Press.
- 4 Klipp et al. (2009), Systems Biology in Practice. Wiley-VCH.
- 5 **BO Palsson (2006),** Systems Biology. Cambridge University Press.
- 6 Press et al. (2007), Numerical Recipies in C. Cambridge University Press.
- 7 **Singh and Dhar (2015),** Systems and Synthetic Biology, Springer



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#### **SEMESTER III**

**Course Code: CBB 515** 

**Course Name:** Computer Aided Drug Discovery

**Course Instructor:** Dr P. Aparoy

**Credits Equivalent:4** Credits (One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

#### **Course Objectives:**

This course will be centred on

- When to use CADD methods in your research (and when not to).
- Which methods are best to use to solve your particular research problems.
- Structure Based and Ligand based drug design approaches and examples.
- Role of Scaffold Hopping in modern drug discovery

#### **Attendance Requirement:**

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

#### **Evaluation Criteria**:

1. Mid Term Examination: 25%

2. End Term Examination: 50%

3. Continuous Internal Assessment: 25%

- a) Class room participation 5 %
- b) Assignments 5 %
- c) Class test 10 %
- d) Presentations 5 %

#### **Course contents:**

#### **Unit –I: Introduction to Drug Discovery and Proteins**

(5 classes)

- Introduction: Drug Discovery process
- Differences between traditional and computational drug discovery
- Proteins: Amino acids; Levels of Protein Structure
- Anfinsen's experiment and dogma

#### **Unit –II: Introduction to Molecular Modelling** (10 classes)

- Force Field
- Intermolecular interactions
- Energy minimization; Local and global minima
- Types of energy minimisation methods

#### Unit –III: Structure Based Drug Design

(10 classes)

- Protein Structure Prediction; Homology modelling
- Docking and its applications : Various search algorithms and scoring functions
- *De novo* drug design methods
- Virtual screening and its applications
- Molecular Dynamics

#### **Unit –IV: Ligand Based Drug Design**

(10 classes)

- QSAR
- Pharmacophore Modelling
- Pseudoreceptor Modelling
- Scaffold Hopping

# **Unit –V : Clinical Trials and Drug Discovery**

(5 classes)

- Success stories of CADD
- Clinical trials

# **Reference books:**

- Andrew Leach (2009) Molecular Modelling: Principles and Applications, Pearson Education (ISBN-13: 9788131728604).
- Kenneth M. Merz, Dagmar Ringe, Charles H. Reynolds (2010) Drug Design: Structure- and Ligand-Based Approaches, Cambridge University Press ( ISBN-13: 9780521887236)
- Lipkowitz, KB, Boyd, DB, Eds (1997) Reviews in Computational Chemistry; John Wiley & Sons, Inc.: Hoboken, NJ, USA (ISBN: 9780471192480)

#### **Additional Readings**

1. David L. Nelson, Michael M. Cox (2017) Lehninger Principles of Biochemistry 7<sup>th</sup> Edition, WH Freeman publisher

- 2. Laurie AT, Jackson RM. Methods for the prediction of protein-ligand binding sites for structure-based drug design and virtual ligand screening. Curr Protein Pept Sci. 2006 Oct;7(5):395-406. Review. PubMed PMID: 17073692.
- 3. Krieger E, Nabuurs SB, Vriend G. Homology modeling. Methods Biochem Anal. 2003;44:509-23. Review. PubMed PMID: 12647402.
- 4. Dias R, de Azevedo WF Jr. Molecular docking algorithms. Curr Drug Targets. 2008 Dec;9(12):1040-7. Review. PubMed PMID: 19128213.
- 5. Oda A, Tsuchida K, Takakura T, Yamaotsu N, Hirono S. Comparison of consensus scoring strategies for evaluating computational models of protein-ligand complexes. J Chem Inf Model. 2006 Jan-Feb;46(1):380-91. PubMed PMID: 16426072.
- Warren GL, Andrews CW, Capelli AM, Clarke B, LaLonde J, Lambert MH, Lindvall M, Nevins N, Semus SF, Senger S, Tedesco G, Wall ID, Woolven JM, Peishoff CE, Head MS. A critical assessment of docking programs and scoring functions. J Med Chem. 2006 Oct 5;49(20):5912-31. PubMed PMID: 17004707.
- 7. Bissantz C, Kuhn B, Stahl M. A medicinal chemist's guide to molecular interactions. J Med Chem 53 (2010) 5061-5084.
- 8. Sun H. Pharmacophore-based virtual screening. Curr Med Chem. 2008;15(10):1018-24. Review. PubMed PMID: 18393859.
- 9. Hans-Joachim Böhm, Alexander Flohr, Martin Stahl, Scaffold hopping, Drug Discovery Today: Technologies, Dec 2004; 1 (3):217–24.

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# **SEMESTER III**

Course Code: CBB 516

**Course Name:** Molecular Evolution and Biodiversity

Course Instructor: Dr. Satpal

**Credits Equivalent:** 4 Credits (One credit is equivalent to 10 hours of lectures / organized classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

#### Course Objectives: The course is designed to:

- Make students familiar with laws of genetics.
- Understand mechanism behind the process of molecular evolution.
- Study various techniques which are used to study genetic patterns and evolutionary history.
- Study genetic processes that result in biodiversity.

#### **Attendance Requirement:**

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination

#### **Evaluation Criteria:**

Mid Term Examination: 25%
 End Term Examination: 50%

3. Continuous Internal Assessment: 25%

a) Presentation 10%

b) Class Participation 10%

c) Attendance 5%

#### **Course Content:**

# UNIT I: INTRODUCTION TO MOLECULAR EVOLUTION (8 hours)

Introduction to Molecular evolution: Meaning and importance of Molecular evolution, heredity and variation, Variations- nature and types, Genetic basis of evolution, Mendelian laws of inheritance, Exceptions in Mendel 's laws and organization and structure of gene, evolution of Genetic code, Molecular clock, phylogeny

#### UNIT II: EVOLUTION AT MOLECULAR LEVEL

(8 Hours)

Mutation and its types: Point mutation, Gene duplication, Chromsomal rearrangement, polyploidy and aneuploidy

DNA Damage and Repair: Types of DNA Repair: Base Excision Repair Nucleotide Excision Repair, Mismatch Repair, Double Strand Break Repair

Protein and DNA alignment, distances among sequences, parsimony, Models of

molecular evolution: Neutral and nearly neutral theory, tree as evolutionary hypothesis

#### **UNIT III: MOLECULAR TECHNIQUES**

(8 Hours)

Molecular techniques: RFLP, RAPD, SSR, AFLP, VNTR, Plasmid Fingerprinting Hybridization techniques: FISH, Nucleic acid probes or hybridisation probe Polymerization chain reaction and its various types: Allele specific PCR, Helicase Dependent PCR, Real Time PCR, Assembly PCR, Inverse PCR, Anchor Dependent PCR or solid phase PCR, *In situ* PCR, RT PCR, Nested PCR DNA sequencing methods: Sanger dideoxy method, Maxam Gilbert method

# UNIT IV: MOLECULAR EVOLUTION IN BACTERIAL PATHOGENS (8 Hours)

Molecular epidemiology of pathogenic bacteria, Applications in Epidemiology Diagnostics and Interventions, Strategies of genome evolution, gene acquisition Horizontal gene transfer (HGT)

Evolution in *Mycobacterium tuberculosis* and *M. leprae* Reductive evolution: Case of *Mycobacterium leprae* and *Yersinia pestis* 

#### UNIT V: BIODIVERSITY (8 hours)

Biodiversity: Genetic, species and ecosystem diversity. Biodiversity at global and national levels.

Genetic variations, genetic drift, factors that affect genetic variations Approaches to biodiversity conservation: species and landscape approach, Ecosystem approach

#### PRESCRIBED TEXT AND REFERENCE BOOKS:

- 1. John H.Gillespie. (2004), Population genetics: A concise guide, (2<sup>nd</sup>edn), John Hopkins
- 2. P.Higgs and T.Atwood. (2005), Bioinformatics and Molecular Evolution, John Wiley and Sons
- 3. Molecular Biology of the gene (2004), Watson, Baker, Bell, Gann, Levine and Losick, (5<sup>th</sup> edn)

#### **Additional Readings:**

- 1. Purves, Sadava, Orians and Heller, Life-The Science of Biology (7<sup>th</sup> edn)
- 2. Bebjamin and Pierce (2005), Genetics, A Conceptual Approach (2<sup>nd</sup> edn)
- 3. D.C.Reanney Hicks and Smith. (1973), Molecular Evolution, Frontiers of Biology
- 4. Richard B. Primack. (2002). Essentials of Conservation Biology (3rd edition)
- 5. Eldon John Gardner, Michael J. Simmons, D. Peter Snustad. Principles of Genetics (8th edition)
- 6. T. A. Brown. (2010). Gene Cloning and DNA Analysis: An Introduction (6<sup>th</sup> edition)
- 7. T.A. Brown (2002). Genomes 2, BIOS scientific Publishers

#### **Journal Articles**

- 1. Evolution of Mycobacterium tuberculosis (2013). Adv Exp Med Biol.; 783:81-91.
- 2. Genomic fluidity and pathogenic bacteria: applications in diagnostics, epidemiology and intervention (2008). *Nat Rev Microbiol*. 6(5): 387-94.
- 3. *Mycobacterium leprae*: genes, pseudogenes and genetic diversity (2011). *Future Microbiol*6(1): 57–71. Doi: 10.2217/fmb.10.153
- 4. Studying Genomes Through the Aeons: Protein Families, Pseudogenes and Proteome Evolution (2002). *Journal of Molecular Biology*.
- 5. Horizontal Gene Transfers in prokaryotes show differential preferences for metabolic and translational genes (2009). *BMC Evolutionary Biology*.

#### **LECTURE PLAN**

Lectures	Topics	Prescribed	Chapter
		Text Book	No.
Lecture – 1	Introduction to Molecular evolution:	Book-4	26
	Meaning and importance of Molecular		
	evolution		
Lecture – 2	Heredity and variation	Book-4	9,24
Lecture – 3	Variations- nature and types	Book-4	9,24
Lecture – 4	Genetic basis of evolution	Book-4	26
Lecture – 5	Mendelian laws of inheritance &	Book-5	2
	Exceptions in Mendel 's laws		
Lecture – 6	Organization and structure of gene	Book-4	9
Lecture – 7	Evolution of Genetic code	Book-3	15
Lecture – 8	Molecular clock & phylogeny	Book-4	26
Lecture – 9	Mutation and its types: Point mutation	Book-10	14
Lecture – 10	Gene duplication, Chromsomal	Book-10	14
	rearrangement		
Lecture – 11	Polyploidy and aneuploidy	Book-5	9
Lecture – 12	DNA Damage and Repair: Types of DNA	Book-10	14
	Repair: Base Excision Repair		
Lecture – 13	Nucleotide Excision Repair & Mismatch	Book-10	14
	Repair,		
Lecture – 14	Double Strand Break Repair & Protein and	Book-10	14

	DNA alignment		
Lecture – 15	Distances among sequences, parsimony	Book-2	8
Lecture – 16	Models of molecular evolution: Neutral	Book-2	8
	and nearly neutral theory, tree as	20011 2	
	evolutionary hypothesis		
Lecture – 17	Molecular techniques: RFLP, RAPD,	Book-9	10
Lecture – 18	SSR, AFLP	Book-9	10
Lecture – 19	VNTR, Plasmid Fingerprinting	Book-9	10
Lecture – 20	Hybridization techniques: FISH, Nucleic	Book-9	10
Lecture – 20	acid probes or hybridisation probe	DOOK-)	10
Lecture –21	Polymerization chain reaction and its	Book-9	9
	various types:Allele specific PCR,		
	Helicase Dependent PCR,		
Lecture –22	Real Time PCR, Assembly PCR & Inverse	Book-9	9
	PCR		
Lecture –23	Anchor Dependent PCR or solid phase	Book-9	9
	PCR, In situ PCR, RT PCR, Nested PCR		
Lecture –24	DNA sequencing methods: Sanger	Handouts &	
	dideoxy method, Maxam Gilbert method	Web	
	,	Resources	
Lecture –25	Molecular epidemiology of pathogenic	11,12	
	bacteria	,	
Lecture –26	Applications in Epidemiology	11,12	
Lecture –27	Diagnostics and Interventions	11,12	
Lecture –28	Strategies of genome evolution	Book-4	26
Lecture –29	Gene acquisition	Book-4	26
Lecture –30	Horizontal gene transfer (HGT)	15	20
Lecture –31	Evolution in <i>Mycobacterium tuberculosis</i>	11	
Lecture 31	and M. leprae		
Lecture –32	Reductive evolution: Case of	13,14	
	Mycobacterium leprae and Yersinia pestis	,	
Lecture –33	Biodiversity: Genetic	Handouts &	
		Web	
		Resources	
Lecture –34	Species and ecosystem diversity	Handouts &	
	The state of the s	Web	
		Resources	
Lecture –35	Biodiversity at global and national levels	Handouts &	
	20 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1	Web	
		Resources	
Lecture –36	Genetic variations	Book-1	1
Lecture –37	Genetic drift	Book-1	19
Lecture –38	Factors that affect genetic variations	Book-1	19
Lecture –39	Approaches to biodiversity conservation:	Handouts &	
Lecture 37	species and landscape approach	Web	
	species and landscape approach	Resources	
Lecture –40	Ecosystem approach	Handouts &	
Lecture 40	2005) Stelli approuen	Web	
		Resources	
	1	17C3OUTCES	



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# **SEMESTER III**

Course Code: CBB 514

Course Name: Molecular Simulation and Application

Course Instructor: Mrs. Neha Chaudhary

Credits: 4

**Credits Equivalent:** 4 Credits (One credit is equivalent to 10 hours of lectures / organized classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

#### **Attendance Requirement:**

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination

#### **Evaluation Criteria:**

Mid Term Examination: 25%
 End Term Examination: 50%

3. Continuous Internal Assessment: 25%

a) Presentation 10%

b) Class Participation 10%

c) Attendance 5%

#### **Course Content:**

#### **UNIT - I: Molecular Mechanics and molecular simulation**

- Fundamentals of Molecular Mechanics
- Introduction to Force field and Lennard-Jones pair potential
- Potential energy Functions
- Bonded and Non-bonded Interactions

#### **UNIT - II: Molecular dynamics simulation ensembles**

- Energy Minimization: Methods for energy minimization
- Simulations in pressure ensembles
- Simulations in temperature ensembles
- Advantages, limitations and challenges associated

#### UNIT - III: Molecular dynamics simulation: in a nutshell

- Introduction to Molecular dynamics simulation
- Integrating equation of motion
- Periodic Boundary Conditions: Basics of treatment of Boundaries
- Integration algorithm: Verlet and velocity-verlet

#### **UNIT - IV: Applications of molecular simulation**

- Analysis of MD simulation results: structural and energetic
- Understanding protein-ligand interactions
- Refining structure predictions
- Understanding functional mechanisms of proteins

#### **UNIT - V: Approaches to free energy calculation**

- Brief introduction to Free Energy Perturbation
- Thermodynamic integration and Linear Interaction Energy
- MM-PBSA/MM-GBSA based approaches
- Applications of Free Energy Calculations

#### **Suggested Reading:**

- 1. Atkins' Physical Chemistry, Tenth Edition by Peter Atkins and Julio De Paula.
- 2. Understanding Molecular simulation, From Algorithms to Applications by Daan Frenkel and Berend Smit.
- 3. A practical introduction to the simulation of molecular systems by Martin J Field.