Central University of Himachal Pradesh

(Established under Central Universities Act 2009
PO BOX: 21, DHARAMSHALA, DISTRICT KANGRA – 176215, HIMACHAL PRADESH
www.cuhimachal.ac.in

SEMESTER- IV

Course Code: CBB-513
Course Name: Chemoinformatics
Credits Equivalent: 4

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:

This introductory course will provide a broad overview of Chemoinformatics. The course will cover an introduction to basic theory of chemoinformatics and new advances in this area. This course is also designed to give the student insights into the fundamentals of chemoinformatics with emphasis on its relation to drug development and discovery. It emphasizes the description of computational models and algorithms used in chemoinformatics.

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 Attendance: 5%
    b. Assignment: 10%
    c. Class room participation: 10%

Course Contents:

Unit I - Representation and manipulation of 2D and 3D molecular structures (8 Hours)

- Introduction
- Computer representation of Chemical Structures
- Structure and Substructure searching
- Structure-Generation Programs and Conformational Search and analysis.
- Systematic Conformational Search and Random Conformational search
- Application of 3D Pharmacophore mapping

Unit II – Molecular descriptor and computational models. (8 Hours)

Descriptor calculated from 2D structure.

- Descriptor based on 3D structure.
- Deriving QSAR equation: simple and multiple linear regression.
- Designing a QSAR experiment
- Interpretation and application of QSAR equation

Unit III – Similarity methods and selection of diverse set of compounds (8 Hours)

- Similarity based on 2D fingerprints.
- 3D similarity.
- Cluster analysis.
- Dissimilarity based selection and Cell based methods.
- Optimization methods
- Comparison and evaluation of selection methods.

Unit IV – Virtual screening and analysis of high-throughput screening data (10 Hours)

- Introduction
- Drug-likeness and compound filters
- Concept of Structure based virtual screening
- ADMET properties and their prediction

Unit V – Combinatorial chemistry and libraries design (6 Hours)

- Introduction to combinatorial chemistry
- Diverse and focussed libraries.
- Library enumeration.
- Combinatorial library design strategies.

Prescribed Text Books:

1. **An introduction to chemoinformatics**: Andrew R. Leach, Valerie J. Gillet ISBN: 978-1-4020-6290-2.
2. **Chemoinformatics: concepts, methods, and tools for drug discovery.** Bajorath, Jürgen, ed. Vol. 275. Humana Press, 2004.

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SEMESTER- IV

Course Code: CBB 525

Course Name: Enzyme Kinetics

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 about the structure & function of enzymes
- Acquaint students to the basic principles of enzyme kinetics
- To understand the molecular mechanisms of enzyme catalysis
- To understand the enzyme inhibition and its types

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%
- Continuous Internal Assessment : 25%
  a) Presentation 10%
  b) Class Participation 10%
  c) Attendance 5%

Course Contents:

UNIT -I: Introduction to Enzymes (4 Hours)

- Enzymes, Enzyme commission's system of classification and significance of EC number
- Mechanism of action of enzyme catalysis and factors affecting catalytic power and specificity
- Structure of Proteins
- Monomeric and Oligomeric Enzymes

UNIT -II: Introduction to bioenergetics, catalysis and kinetics (4 Hours)

- Concepts of bioenergetics
- Factors affecting rates of chemical reactions
- Kinetics of uncatalysed chemical reactions
- Kinetics of enzyme catalysed reactions

UNIT -III: Kinetics of Single substrate Enzyme Catalysed Reactions (4 Hours)

- Henri and Michaelis-Menten Equation; significance and its modification
- Lineweaver- Burk Plot, Eadie- Hofstee and Hanes Plot
- Eisenthal and Cornish- Bowden plot, Haldane relationship for reversible reactions
- Rapid Reaction Kinetics

UNIT -IV: Enzyme Inhibition (4 Hours)

- Reversible Inhibition: Competitive and Uncompetitive Inhibition
- Non-competitive Inhibition and Mixed Inhibition
- Partial Inhibition and Substrate Inhibition
- Allosteric Inhibition and Irreversible Inhibition

UNIT –V: Kinetics of Multi-Substrate Enzyme- Catalyzed Reactions (4 Hours)

- Ping-pong bi-bi, Random-order and Compulsory-order Mechanisms
- Steady State Kinetics
- Investigation of Reaction Mechanisms using Steady- State Methods
- Investigation of Reaction Mechanisms using Non Steady- State Methods

Prescribed Text Reference Books:

1).Understanding Enzymes,Trevor Palmer,Prentice Hall,4th Ed,1995

2. Biochemistry By Lubert Stryrer,3rd Ed.,1995,W.F. Freeman and Co., New York.

3. Enzyme Structure and Mechanisms, Alan Ferst,W.M. Freeman, New York,1985.

Other Readings

Sr. No.	Jouranls atricles (specific articles, *Complete reference*)
1	Muller J, Morrison DK (2002). Assay of Raf-1 activity. Methods in Enzymology 345: 490-498
2	Reszka, R and Jacobs, A and Voges, J (2005) Liposome-mediated suicide gene therapy in humans. Methods in Enzymology, 391 . 200-208. ISSN 0076-687
3	Methods in enzymology. Vol. 89, carbohydrate metabolism, part D : Edited by , Academic Press, New York, 1982. 656

Relevant Websites

Sr. No.	Web address	Salient Features
1	Methods in enzymology. Vol. 89, carbohydrate metabolism, part D : Edited by , Academic Press, New York, 1982. 656	Lesson of properties of enzymes
2	www.proteinscience.org	All types of enzyme mechanisms are mentioned in this website

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SEMESTER- IV

Course Code: CBB 522
Course Name: Elements of Synthetic Biology
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: The course is designed to introduce students the concepts of synthetic biology – a field of study at the interface of (i) complexity of biological systems and (ii) techniques of traditional engineering. This course is designed to acquaint students about the following basic questions:

- Can we study and understand biology as an engineering discipline?
- Why is it necessary to consider stochasticity while modeling biological processes?
- What are the basic parts and devices that have been successfully bioengineered?
- What are the implications of Synthetic Biology on the society?

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

Evaluation Criteria:
1. Mid Term Examination: 25%
2. End Term Examination: 50%
3. Continuous Internal Assessment: 25%
   - 5% class participation,
   - 20% assignment and presentation

Course Contents

UNIT I: Introductory Interdisciplinary Concepts (3 Hours)

1. Definition and scope of systems biology and synthetic biology.
2. Engineering concepts: parts, devices, circuits -- digital vs. analog, logic gates.
3. Biological complexity: Self organization, Emergence, Robustness.

UNIT II: Modeling methods for Biological Systems (5 Hours)

1. Review of kinetic chemistry, Aspects of noise in designing biological systems.
2. Brief overview of deterministic modeling, master equation and Gillespie's Stochastic Simulation Algorithm.
3. Lambda switch and Chemotactic module in *E coli*.
4. Open source programs: CellDesigner, etc

UNIT III: Standards and parts in Synthetic Biology (4 Hours)

1. Standards: SBML, SBGN, BioPAX
2. MIT Registry of standard biological parts
3. Bio-brick and non-biobrick initiatives, iGEM events
4. Lac operon, Promoter designing, Quorum sensing
5. ZFNs, TALENs, CRISPR/Cas

UNIT IV: Bio-engineered Synthetic Circuits (4 Hours)

1. Gates: AND gate, Counters: Pulse generators, Switches: Toggle switch
2. Oscillators: Repressilator, mammalian oscillator
3. Brief overview of cascades, time delayed circuits, spatial patterning, biosensors, and other logical formula driven circuits.
4. Riboswitches and riboregulators
5. Four and Six-letter genetic code

UNIT V: From Modules to Systems (4 Hours)

1. Integrating gene circuits
2. DNA Origami,
3. Genome Synthesis, Minimal synthetic cell, Multicellular synthetic systems
4. Protocell construction
5. Bio-energetics and Bio-fuels
6. **Safety and Legal issues:** Bio-security, Bio-safety

Text Books:

1. **Chris Myers (2009).** Engineering Genetic Circuits. Chapman & Hall.
2. **Edda Klipp *et al.* (2009).** Systems Biology: A Textbook. Wiley-VCH.
3. **Huimin Zhao (2013).** Synthetic Biology: Tools and Applications. Academic Press.

Additional Readings:

1. **Freemont and Kitney (2012).** Synthetic Biology: A Primer. World Scientific
2. **Fu and Panke (2009).** Systems Biology and Synthetic Biology. Wiley, New Jersy.
3. Presidential Commission for the Study of Bioethical Issues (2010). NEW DIRECTIONS: Ethics of Synthetic Biology and Emerging Technologies. (http://bioethics.gov)
4. Singh V. (2014). Applied Synthetic Biology. ISBN: 1-62699- 019-0. Studium Press LLC, USA.
5. Singh V., and Dhar, P. K. (2015). Systems and Synthetic Biology, Springer Science, 385. ISBN: 978-94- 017-9513- 5.

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SEMESTER- IV

Course Code: CBB 523
Course Name: Practical Course on Systems Biology
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: The course is designed to give students an opportunity for learning the computational techniques to understand biological complexity at systems level. They will be introduced to the softwares implementing deterministic and stochastic modeling algorithms. At the same time they will also be acquainted with the network visualization and analysis softwares. Students having working knowledge of any programming language will be encouraged to write their own codes for simulating and analysing model biological systems. Students will be required to learn the following modeling and analysis suites.

1. CellDesigner, MCell
2. Cytoscape
3. XPPAut

Pre-requisite: CBB 518 – Elements of Systems Biology
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%
    - 5% attendance,
    - 5% class participation,
    - 15% assignment and presentation

Contents:

1. Standards in Systems Biology -- SBML, SBGN, BioPAX
2. Deterministic simulation of a natural biological system.
3. Deterministic simulation of a synthetic biological system.
4. Implementation of Gillespie's stochastic simulation algorithm to model the given chemical reaction system.
5. Introduction to biological network databases – KEGG, STRING, STITCH, DIP, BIND, HPRD, EMP, EcoCyc, MetaCyc, AraCyc etc.
6. To construct and visualize simple biological network.
7. To analyze a given biological network by calculating the following characteristics
    a. Diameter, density
    b. Average path length
    c. Clustering coefficient
    d. Centrality measures (Degree, Closeness, Eccentricity, Betweenness)
    e. Degree distribution
    f. Community detection Etc.
8. To identify motifs and graphlets in a given network.
9. Stability analysis of a given 1-dimensional dynamical system.
10. Stability analysis of a given 2-dimensional biological system.
11. A minor project