Central University of Punjab

Ph.D. in Bioinformatics

Session 2021--

Department of Computational Sciences

School of Basic Sciences

Programme Outcome

The above mentioned programmes will enrich students with the fundamental knowledge of theoretical/computational sciences in the field of basic as well as applied research. On successful completion of the Ph.D. programme the students will able to:

1. Design independent research problems in the field of Theoretical / Computational Sciences

2. Examine real-life problems with the help of computational tools

3. Execute research in this new spectrum of multidisciplinary area of science at the national and international platform.

4. Construct themselves as an Industrious research personnel

SEMESTER I							
S. No.	Paper Code	Course Title	Course Type	Hours			
				L	T	P	Cr
1	CCS.701	Research Methodology	CC	2	0	0	2
2	CCS.703	Review Writing and Presentation	CC	2	0	0	2
3	CCS.751	Research and Publication Ethics		2	0	0	2
4	CCS.752	Teaching Assistantship		0	0	2	1
5	UNI.753	Curriculum, Pedagogy and Evaluation		1	0	0	1
Opt any two of the following courses:							
4	CCS.705	Sequence and Structural Bioinformatics	DE	3	0	0	3
5	CCS.707	Mathematics for Computational Sciences	DE	3	0	0	3

6	CCS.708	Scientific Programming	DE	3	0	0	3
7	CCS.709	Scientific Programming Lab (Practical)	SBE	0	0	6	3
8	CCS.715	Molecular Dynamics	DE	3	0	0	3
9	CCS.716	Molecular Dynamics Lab (Practical)	SBE	0	0	6	3
10	CCS.718	Biomolecular Structure Modelling and Drug Design	DE	3	0	0	3
11	CCS.719	Comparative Database Analysis	DE	3	0	0	3
12	CCS.720	Sequence Analysis	CC	3	0	0	3
13	CCS.721	Computational Genomics and Proteomics	CC	3	0	0	3
	Total				14 Credits		

Mode of Transaction
Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Evaluation Criteria

As per UGC guidelines on adoption of CBCS. CC: Core Course, DE: Discipline Elective, SBE: Skill Based Elective

SEMESTER I

Course Title: Research Methodology
Paper Code: CCS.701
Total Lectures: 30

L	T	P	Cr
2	0	0	2

Learning Outcomes: At the end of the course, the students will be able to:
- prepare a research plan, reading and gain knowledge from scientific papers
- develop skills for scientific writing, research proposal writing, ethics, plagiarism, and lab safety issues

Unit I   **5 Hours**
General principles of research: Meaning and importance of research, critical thinking, formulating hypothesis and development of research plan, review of literature, interpretation of results and discussion.

Unit II   **10 Hours**
Technical writing: Scientific writing that includes the way of writing Synopsis, research paper, poster preparation and presentation, and

dissertation.

Unit III   **5 Hours**
Library: Classification systems, e-Library, web-based literature search engines

Unit IV   **10 Hours**
Entrepreneurship and business development: Importance of entrepreneurship and its relevance in career growth, characteristics of entrepreneurs, developing entrepreneurial competencies, types of enterprises and ownership (large, medium SSI, tiny and cottage industries, limited, public limited, private limited, partnership, sole proprietorship) employment, self-employment and entrepreneurship, financial management-importance and techniques, financial statements- importance and its interpretation, and Intellectual Property Rights (IPRs).

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Suggested Readings

1. Kothari, C. R. (2014). Research methodology (s). New Age International (p) Limited. New Delhi.
2. Sahay, Vinaya and Pradumna Singh (2009). Encyclopedia of Research Methodology in life sciences. Anmol Publications. New delhi
3. Kauda J. (2012). Research Methodology: A Project Guide for University Students. Samfunds literature Publications.
4. Dharmapalan B. (2012). Scientific Research Methodology. Narosa Publishing House ISBN: 978-81-8487-180-7.

Course Code: CCS.751

Course Title: Research and Publication Ethics

L	T	P	Credits
2	0	0	2

Total Hours: 30

Unit I Philosophy and Ethics   **3 hours**

- Introduction to Philosophy : definition, nature and scope, content, branches

- Ethics : definition, moral philosophy, nature of moral judgements and reactions

Unit II Scientific Conduct   5 hours

- Ethics with respect to science and research
- Intellectual honesty and research integrity
- Scientific misconducts : Falsification, Fabrication, and Plagiarism (FFP)
- Redundant publications : duplicate and overlapping publications, salami slicing
- Selective reporting and misrepresentation of data

Unit III: Publication Ethics   7 hours

- Publication ethics : definition, introduction and importance
- Best practices/ standards setting initiatives and guidelines: COPE, WAME, etc.
- Conflicts of interest
- Publication misconduct : definition, concept, problems that lead to unethical behaviour and vice versa, types
- Violation of publication ethics, authorship and contributor ship
- Identification of publication misconduct, complaints and appeals
- Predatory publishers and journals

Unit IV Open Access publishing   4 hours

- Open access publications and initiatives
- SHERPA/RoMEO online resource to check publisher copyright & self-archiving policies
- Software tool to identify predatory publication developed by SPPU
- Journal finder/journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer, Journal Suggester etc.

Unit V Publication Misconduct   4 hours

- Group Discussions: Subject specific ethical issues, FFP, authorship; conflicts of interest; complaints and appeals: examples and fraud from India and abroad
- Software tools: Use of plagiarism software like Turnitin, Urkund and other open source software tools

Unit IV Databases and Research Metrics   7 hours

- Databases: Indexing databases; Citation database: Web of Science, Scopus etc.

- Research Metrics: Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score; Metrics : h-index, g-index, i10 index, almetrics

Course Code: CCS.752

Course Title: TEACHING ASSISTANTSHIP

L	T	P	Credit
0	0	2	1

Total Hours: 30

Learning Outcome:

At the end of this skill development course, the scholars shall be able to

1. familiarize themselves with the pedagogical practices of effective class room delivery and knowledge evaluation system
2. manage large and small classes using appropriate pedagogical techniques for different types of content

Activities and Evaluation:

- The scholars shall attend Master degree classes of his/her supervisor to observe the various transaction modes that the supervisor follows in the class room delivery or transaction process one period per week.
- The scholars shall be assigned one period per week under the direct supervision of his/her supervisor to teach the Master degree students adopting appropriate teaching strategy(s).
- The scholars shall be involved in examination and evaluation system of the Master degree students such as preparation of questions, conduct of examination and preparation of results under the direction of the supervisor.
- At the end of the semester, the supervisor shall conduct an examination of teaching skills learned by the scholar as per the following evaluation criteria:
- The scholars shall be given a topic relevant to the Master degree course of the current semester as his/her specialization to prepare lessons and deliver in the class room before the master degree students for one hour (45 minutes teaching + 15 minutes interaction).
- The scholars shall be evaluated for a total of 50 marks comprising content knowledge (10 marks), explanation and demonstration skills (10 marks), communication skills (10 marks), teaching techniques employed (10 marks), and classroom interactions (10).

Course Code: UNI.753

Course Title: CURRICULUM, PEDAGOGY AND EVALUATION

L	T	P	Credit
1	0	0	1

Learning outcomes: **Total Hours: 15**

After completion of the course, scholars shall be able to:

- analyze the principles and bases of curriculum design and development
- examine the processes involved in curriculum development
- develop the skills of adopting innovative pedagogies and conducting students' assessment
- develop curriculum of a specific course/programme

Course Content

Unit I   Bases and Principles of Curriculum   **4 hours**

1. Curriculum: Concept and Principles of curriculum development, Foundations of Curriculum Development.
2. Types of Curriculum Designs- Subject centered, learner centered, experience centered and core curriculum. Designing local, national, regional and global specific curriculum. Choice Based Credit System and its implementation.

Unit II   Curriculum Development   **4 hours**

1. Process of Curriculum Development: Formulation of graduate attributes, course/learning outcomes, content selection, organization of content and learning experiences, transaction process.
2. Comparison among Interdisciplinary, multidisciplinary and trans-disciplinary approaches to curriculum.

Unit III Curriculum and Pedagogy   **3 hours**

1. Conceptual understanding of Pedagogy.
2. Pedagogies: Peeragogy, Cybergogy and Heutagogy with special emphasis on Blended learning, Flipped learning, Dialogue, cooperative and collaborative learning
3. Three e- techniques: Moodle, Edmodo, Google classroom

Unit IV   Learners' Assessment   **4 hours**

1. Assessment Preparation: Concept, purpose, and principles of preparing objective and subjective questions.
2. Conducting Assessment: Modes of conducting assessment – offline and online; use of ICT in conducting assessments.
3. Evaluation: Formative and Summative assessments, Outcome based assessment, and scoring criteria.

Transaction Mode

Lecture, dialogue, peer group discussion, workshop

Evaluation criteria

There shall be an end term evaluation of the course for 50 marks for duration of 2 hours. The course coordinator shall conduct the evaluation.

Suggested Readings

- Allyn, B., Beane, J. A., Conrad, E. P., & Samuel J. A., (1986). Curriculum Planning and Development. Boston: Allyn & Bacon.
- Brady, L. (1995). Curriculum Development. Prentice Hall: Delhi. National Council of Educational Research and Training.
- Deng, Z. (2007). Knowing the subject matter of science curriculum, Journal of Curriculum Studies, 39(5), 503-535. https://doi.org/10.1080/00220270701305362
- Gronlund, N. E. & Linn, R. L. (2003). Measurement and Assessment in teaching.
- Singapore: Pearson Education
- McNeil, J. D. (1990). Curriculum: A Comprehensive Introduction, London: Scott,
- Foreman/Little
- Nehru, R. S. S. (2015). Principles of Curriculum. New Delhi: APH Publishing Corporation.
- Oliva, P. F. (2001). Developing the curriculum (Fifth Ed.). New York, NY: Longman
- Stein, J. and Graham, C. (2014). Essentials for Blended Learning: A Standards-Based Guide. New York, NY: Routledge.

Web Resources

- https://www.westernsydney.edu.au/__data/assets/pdf_file/0004/467095/Fundamentals_of _Blended_Learning.pdf
- https://www.uhd.edu/academics/university-college/centers-offices/teaching-learningexcellence/Pages/Principles-of-a-Flipped-Classroom.aspx
- http://leerwegdialoog.nl/wp-content/uploads/2018/06/180621-Article-The-BasicPrinciples-of-Dialogue-by-Renate-van-der-Veen-and-Olga-Plokhooij.pdf

Course Title: Review Writing and Presentation
Paper Code: CCS.703
Total Lectures: 60

L	T	P	Cr
0	0	4	2

Course Objectives and Learning Outcomes: The objective of this course

would be to ensure that the student learns the aspects of the Review writing and seminar presentation. Herein the student shall have to write a 5000 words review of existing scientific literature with simultaneous identification of knowledge gaps that can be addressed through future work.

The evaluation criteria for "Review Writing and Presentaion" shall be as follows:

Maximum Marks: 100

S.No.	Criteria	Marks
1.	Review of literature	25
2.	Identification of gaps in knowledge	15
3.	References	10
4.	Content of presentation	15
5.	Presentation Skills	20
6.	Handling of queries	15
	Total	100

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Course Title: Sequence and Structural Bioinformatics
Paper Code: CCS.705
Total Lectures: 45

L	T	P	Cr
3	0	0	3

Course Objectives and Learning Outcomes: The objective of this subject is to ensure that a student learns advanced concepts in Bioinformatics.

Unit I   **10 Hours**
Biological data Types of biological data (various omics)
Biological Databases Nucleic acid and protein sequence and protein structure databases Overview of available Bioinformatics resources on the web

Unit II   **10 Hours**
DNA sequence analysis
Sequence annotation and sequence analysis - Phylogeny of gene (blast, fasta, HMMer) and residue conservation. Primer design and Tm Calculation, DNA Restriction pattern analysis.Condon bias and its effect on the protein expression with reference to various expression system.

Unit III   **10 Hours**
Bioinfo tools
Protein sequence and structure insights (PSSI) X-ray, NMR, Comparative modeling, ab initio, threading methods. Structure refining techniques Energy minimization approaches (Steepest descent, Conjugate gradient etc), Basis of Molecular dynamics simulations and its application.

Unit IV   **15 Hours**
Simulation methods : algorithm for time dependence; leapfrog algorithm, Verlet algorithm, Boltzmann velocity, time steps, duration of the MD run, Starting structure, analysis of MD job, uses in drug designing, ligand protein interactions. Various methods of MD, Monte Carlo, systematic and random search methods. Differences between MD and MC, Energy, Pressure, Temperature, Temperature dynamics, simulation softwares. Various methods of MD, Monte Carlo, systematic and random search methods.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Suggested Readings

1. Andrew R.Leach (2001) Molecular Modelling Principles and applications . II ed . Prentice Hall.
2. A.D. Baxevanis *et. al.*, (2005) Current Protocols in Bioinformatics, Wiley Publishers
3. David W. (2001) Mount Bioinformatics Cold Spring Harbor Laboratory Press, ISBN 0-87969-608-7
4. P. A. Pevzner, (2004) Computational Molecular Biology, Prentice Hall of India Ltd, ISBN81-203-2550-8
5. D.E.Krane and M.L.Raymer (2003) Fundamental concepts of Bioinformatics Pearson Education ISBN 81-297-0044-1
6. N.Gautham (2006) Bioinformatics Narosa publications.   ISBN-13: 9781842653005
7. Fenniri, H. (2000) "Combinatorial Chemistry – A practical approach", Oxford University Press, UK.
8. Lednicer, D. (1998) "Strategies for Organic Drug Discovery Synthesis and Design"; Wiley International Publishers.
9. Gordon, E.M. and Kerwin, J.F (1998) "Combinatorial chemistry and molecular diversity in drug discovery" Wiley-Liss Publishers.

Course Title: Mathematics for Computational Sciences

L	T	P	Cr
3	0	0	3

Paper Code: CCS.707
Total Lectures: 45

Learning Outcomes: At the end of the course, the students will be able to:
   1. identify and describe the basic mathematical techniques that are commonly used by chemist.

2. develop skills in vectors, matrices, differential calculus, integral calculus and probability.
3. apply the principles to a number of simple problems that have analytical solutions.
4. design different methods to problems related to chemistry.

Unit I   **10 Hours**
Matrices & Vector Calculus: matrix algebra, Caley-Hamilton theorem, Eigen values and Eigen vectors, curvilinear coordinates. (Vector calculus: properties of Gradient, divergence and Curl, spherical and cylindrical coordinates)
Differential calculus: Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima, exact and inexact differentials with their applications to thermodynamic properties.

Unit II   **10 Hours**
Integral calculus: basic rules for integration, integration by parts, partial fraction and substitution, reduction formulae, applications of integral calculus, functions of several variables, partial differentiation, co-ordinate transformations
Fourier Transforms: Fourier series, Dirichlet condition, General properties of Fourier series, Fourier transforms, their properties and applications,

Unit III   **10 Hours**
Delta, Gamma, and Beta Functions: Dirac delta function, Properties of delta function, Gamma function, Properties of Gamma and Beta functions.
Special Functions: Legendre, Bessel, Hermite and Laguerre functions, recurrence relations, Orthogonality and special properties. Associated Legendre functions: recurrence relations, Parity and orthogonality, functions, Green's function,

Unit IV   **15 Hours**
Differential Equations Solutions of Hermite, Legendre, Bessel and Laugerre Differential equations, basics properties of their polynomials, and associated Legendre polynomials, Partial differential equations (Laplace, wave and heat equation in two and three dimensions), Boundary value problems and Euler equation.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Suggested Readings

1. E. Kreyszig, (2011) *Advanced Engineering Mathematics,* Wiley India Pvt. Ltd., New Delhi, India.
2. L. A. Pipes, (1985) *Applied Mathematics for Engineers and Physicist,* McGraw-Hill, Noida, India.

3. D. G. Zill, (2012) *Advanced Engineering Mathematics,* Jones & Barlett Learning, Massachusetts, USA.
4. P. K. Chattopadhyay, (2000) *Mathematical Physics,* New Age International (P) Ltd., New Delhi.
5. E.Steiner, (2008) The chemistry Mathematics Book, Oxford University Press .
6. F. Daniels, (1959) Mathematical for Physical Chemistry : Mc. Graw Hill .
7. D.M. Hirst, (1979) Chemical Mathematics Longman .
8. Tebbutt, (1994) Basic Mathematics for Chemists, Wiley .
9. G. Arfken, H. Weber and F. Harris, (2012) *Mathematical Methods for Physicists,* Elsevier Academic Press, Massachusetts, USA.

Course Title: Scientific Programming

L	T	P	Cr
3	0	0	3

Paper Code: CCS.708
Total Hours: 45

Learning Outcomes: At the end of the course, the students will be able to:
- identify and describe the basic art of scientific programming related to Fortran 95/2003.
- demonstrate concepts related to variables, I/O, arrays, procedures, modules, pointers and parallel programming.
- develop skills to write programs related to standard problems and as well as to chemistry.

Unit I   **10 Hours**
Introduction to Computers and Fortran language: History and evolution of Fortran language, Basic elements of Fortran: Character sets, structure of statements, Structure of a Fortran Program, compiling, linking and executing the Fortran program.

Unit II   **10 Hours**
Constants and variables, assignment statements and arithmetic calculations, intrinsic functions, Program design and branching structures, loop and character manipulation.

Unit III
15 Hours
Basic I/O concepts, Formatted READ and WRITE
statements, Introduction to Files and File Processing, Introduction to Arrays and procedures, Additional features of arrays and procedures- 2-D and multidimensional arrays, allocatable attays in procedures, derived data types.
Pointers and dynamic data structures- using pointers in assignment statements, with arrays, as components of derived data types and in procedures, Introduction to object oriented programming in Fortran.

Unit IV   **10 Hours**
What is parallel programming, Why use paralle programming, Parallel Architecture, Open MP & MPI, Models of Parallel Computation, Parallel Program Design, Shared Memory & Message Passing, Algorithms, Merging & Sorting.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Suggested Readings

1. Chapman, (2006) Fortran 95/2003 for Scientists and Wngineers, McGraw-Hill International Edition, New York .
2. V. Rajaraman, (1997) Computer Programming in Fortran 90 and 95, PHI Learning Pvt. Ltd, New Delhi .
3. W. H. Press, S. A. Teukolsky, W. H. Vetterling, B. P. Flannery, (1996) Fortran Numerical Recipes Volume 2 (Fortran 90), Cambridge University Press .
4. M J Quinn (2003) Parallel Programming in C with MPI and OpenMP.
5. IAnanth Grama, George Karypis, Vipin Kumar, and Anshul Gupta (2003) ntroduction to Parallel Computing.

Course Title: Scientific Programming Lab (Practical)
Paper Code: CCS.709
Total Hours: 90

L	T	P	Cr
0	0	6	3

Learning Outcomes: The objective of this course is to introduce students to the art of scientific programming. The practical aspects of scientific programming languages Fortran and C will be taught to students in this course. The students after completion of this course will be able to:
- Identify/characterize/define a computational problem
- Design a fortran program to solve the problem
- Create pseudo executable code
- Read most of the basic fortran code

Unit I   **30 Hours**
Structure of a Fortran Program, compiling, linking and executing the Fortran programs. Constants and variables, assignment statements and arithmetic calculations, intrinsic functions, Program design and branching structures, loop and character manipulation.

Unit II   **20 Hours**
Basic I/O concepts, Formatted READ and WRITE statements, Introduction to Files and File Processing, Introduction to Arrays and procedures, Additional features of arrays and procedures- 2-D and multidimensional arrays, allocatable attays in procedures, derived data types.

Unit III   **20 Hours**

Pointers and dynamic data structures- using pointers in assignment statements, with arrays, as components of derived data types and in procedures, Introduction to object oriented programming in Fortran.
Matrix summation, subtraction and multiplication, Matrix inversion and solution of simultaneous equation, Gaussian elimination.

Unit IV   **20 Hours**
What is parallel programming, Why use paralle programming, Parallel Architecture, Open MP & MPI, Models of Parallel Computation, Parallel Program Design, Shared Memory & Message Passing, Algorithms, Merging & Sorting

Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.

Suggested Readings

1. Chapman, (2006) Fortran 95/2003 for Scientists and Wngineers, McGraw-Hill International Edition, New York .
2. V. Rajaraman, (1997) Computer Programming in Fortran 90 and 95, PHI Learning Pvt. Ltd, New Delhi .
3. W. H. Press, S. A. Teukolsky, W. H. Vetterling, B. P. Flannery, (1996) Fortran Numerical Recipes Volume 2 (Fortran 90), Cambridge University Press .
4. M J Quinn (2003) Parallel Programming in C with MPI and OpenMP.
5. Ananth Grama, George Karypis, Vipin Kumar, and Anshul Gupta (2003) ntroduction to Parallel Computing.

Course Title: Molecular Dynamics
Paper Code: CCS.715
Total Lecture: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes: At the end of the course, the students will be able to:
- learn the modelling of small to large molecular environments
- understand various force field for biomoleculra simulation in details
- learn different methods for simulating large systems
- gain the knowledge about different molecular simulation techniques
- understand the dynamics of the structural transitions

which will help them use the techniques of molecular simulations in their further potential careers in academia and industry.

Unit I   **10 Hours**
Molecular Modeling and Structure - molecular modeling today: overview of problems, tools, and solution analysis, minitutorials with protein and nucleic acid structure as example.

Force Fields and Molecular Representation – (a) Intramolecular Interactions, (b) Non-bonded Interactions – London (van der Waals) Interactions, Electrostatic Interactions, (c) Hydrogen Bonds, (d) Constraints and Restraints, (e) United Atom and Other Coarse-Grained Approaches, (f) Non-pairwise Interactions, (g) How accurate are force fields?
Example: Protein, Nucleic Acid, Small Molecule Force Field, Water Models.

Unit II   10 Hours
Methods for Simulating Large Systems
   a) Non-bonded Cutoffs – Shifted Potential and Shifted Force, Switching Functions, Neighbor Lists
   b) Boundaries – Periodic Boundary Conditions, Stochastic Forces at Spherical Boundary
   c) Long-range Interactions – The Ewald Sum, The Reaction Field Method

Unit III   10 Hours
Energy Minimization and Related Analysis Techniques
(a) Steepest Descent, (b) Conjugate Gradient, (c) Newton-Raphson, (d) Comparison of Methods, (e) Advanced Techniques: Simulated Annealing, Branch-and-bound, Simplex, (f) What's the big deal about the minimum?
Introduction to Equilibrium Statistical Mechanics
(a) Phase space, Ergodicity, and Liouville's theorem, (b) Ensemble theory, Thermodynamic averages - Microcanonical Ensemble, Canonical Ensemble, Other MD Simulation Related Ensembles (c) Statistical Mechanics of Fluids

Unit IV   15 Hours
Simulation Methods:
Monte Carlo: (a) MC integration and Markov chains, (b) The Metropolis method, (c) Biased MC
Molecular Dynamics: (a) Classical Mechanics: Equations of Motion, (b) Finite Difference Methods: Verlet Algorithm, Velocity Verlet, The Time Step: Practical Issues, Multiple time-step algorithms (c) Constraint Dynamics: Fundamental concepts, SHAKE and RATTLE, (d) Temperature: Maxwell-Boltzmann distribution of velocities, (e) Temperature Control: Velocity Scaling, Andersen's Method, Nose-Hoover Dynamics, (f) Pressure Control: Andersen's Method, Nose-Hoover Method, Rahman-Perrinilo Method, (g) Calculating properties from MD trajectories, (h) Hybrid MC,
Free Energy: (a) Perturbation Methods, (b) TI (Thermodynamic Integration) Brownian dynamics and the Langevin Equation.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Suggested Readings

1. M.P. Allen and D.J. Tildesley, (2017) Computer Simulation of Liquids 2nd Edition, Oxford University Press.
2. D. Frenkel and B. Smit, (2001) Understanding Molecular Simulation 2nd Edition, Academic Press.
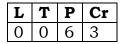
3. A. R. Leach, (2001) Molecular Modelling Principles and Applications 2nd Edition. Pearson.
4. S. Alavi, (2020) Molecular Simulations: Fundamentals and Practice 1st Edition, Wiley-VCH.

Course Title: Molecular Dynamics Lab (Practical)
Paper Code: CCS.716
Total Hours: 90

L	T	P	Cr
0	0	6	3

Learning Outcomes: At the end of the course, the students will be able to:
- learn the basics of Linux environment
- use the remote computing as a tool for high performance computation
- use different energy minimization techniques
- create molecular model from scratch, and high definition images using various graphics tools
- gain the practical in-hand experience of various modeling and classical simulation tools
- learn the use of different insilico techniques for biomolecular simulations

which will enhance their employability in their further potential carrers in academia and industry

1. Linux basics and remote computing
2. Coordinate generations and inter-conversions of small molecules
3. Energy minimizations and optimization, *ab initio methods*
4. Advanced Visualization Software and 3D representations with VMD
5. Introduction to PDB Data
6. Secondary Structure Prediction, Fold Recognition
7. Molecular Dynamics with GROMACS
    a. Water liquid structure and dynamics
    b. Simulation of Ionic Solutions
    c. Simulation of Protein in Water
    d. Simulation of Membrane Proteins
    e. Simulations of DNA
8. Review of Molecular Dynamics Principles

Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.

Suggested Readings

1. M.P. Allen and D.J. Tildesley, (2017) Computer Simulation of Liquids 2nd Edition, Oxford University Press.
2. D. Frenkel and B. Smit, (2001) Understanding Molecular Simulation 2nd Edition, Academic Press.

3. A. R. Leach, (2001) Molecular Modelling Principles and Applications 2nd Edition. Pearson.
4. S. Alavi, (2020) Molecular Simulations: Fundamentals and Practice 1st Edition, Wiley-VCH.

Course Title: Biomolecular Structure Modeling and Drug Design
Paper Code: CCS.718
Total Lectures: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes: On completion of the course the student should be able to:
• describe different types of protein–ligand interactions and characterise binding pockets
• use different search methods to find compounds with specific properties in large compound databases
• set up, perform and evaluate different virtual screening methods using large datasets
• account for and set up molecular dynamics simulations and free energy calculations

Unit I   **10 Hours**
Introduction to Molecular Geometry, Coordinate Space for Optimization of Algorithm of Molecular Geometry, Z-Matrix, Molecular Vibrations, Electrostatic Charges, Electrostatic Charges, Multipole Moments,

Unit II   **10 Hours**
Modelling and structure: From protein sequence to structure, theoretical and practical aspects of protein sequence alignments, secondary, tertiary structure prediction, comparative modeling, Docking, protein-protein and protein-ligand docking.

Unit III   **10 Hours**
Computational drug designing: Structure-based drug design, virtual screening, quantitative structure activity relations, Cheminformatics, Historical Perspective and Viewpoint of Pharmacophore, Functional Groups Considered as Pharmacophores, Ehrlich's "Magic Bullet", Fischer's "Lock and Key", Two-dimensional Pharmacophores, Three-dimensional Approach of Pharmacophores, Criteria for Pharmacophore Model,

Unit IV   **15 Hours**
Pharmacophore Model Generation Software Tools, Molecular Alignments, Handling Flexibility, Alignment Techniques, Scoring and Optimization, Pharmacophores, Validation and Usage, Automated Pharmacophore Generation Methods, GRID-based Pharmacophore Models, Pharmacophores for Hit Identification, Pharmacophores for Human ADME/Tox-related Proteins.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Suggested Readings

1. Grant, Guy H.; Richards, W. Graham (1995) Computational chemistry Oxford: Oxford Univ. Press,
2. Schneider, Gisbert; Baringhaus, Karl-Heinz; Kubinyi, Hugo (2008) Molecular design : concepts and applications Weinheim: Wiley-VCH,
3. Andrew R.Leach (2001) Molecular Modelling Principles and applications . II ed . Prentice Hall.
4. Lednicer, D. (1998) "Strategies for Organic Drug Discovery Synthesis and Design"; Wiley International Publishers.
5. Gordon, E.M. and Kerwin, J.F (1998) "Combinatorial chemistry and molecular diversity in drug discovery" Wiley-Liss Publishers.
6. Molecular and Structural Database, Protein Data Bank, Bioactivity Databases, Gene and Protein Sequence Databases,Cambridge Crystallographic Database, Compound Storage and Management.

Course Title: Comparative Database Analysis

L	T	P	Cr
3	0	0	3

Course Code: CCS.719
Total Lecture: 45

Learning Outcomes: At the end of the course, the students will be able to:

● identify the importance of DNA-Protein Interactions During Transcription
● gain a deep knowledge about the role of bioinformatics-OMIM database, integrated genomic maps, gene expression profiling
● apply probabilistic modeling techniques for the building of transcriptional regulatory networks which will help them to use the techniques of computational proteomics in their further potential careers in academia and industry.

Course Content

Unit I   **12 Hours**

DNA- Protein interaction: Process of DNA-Protein Interactions During Transcription, Network identification and processing. Protein- Protein Interactions: Processing of the Proteome, Prediction of Post-translational modifications, Protein Degradation.

Unit II   **10 Hours**

Role of bioinformatics-OMIM database, integrated genomic maps, gene expression profiling; identification of SNPs, Vector Screening

Unit III   12 Hours

DNA microarray: database and basic tools, Gene Expression Omnibus (GEO), understanding of microarray data, normalizing microarray data, Raw read quality assessment, Mapping data visualization, detecting differential gene expression.

Unit IV   11 Hours
Building predictive models of transcriptional regulatory networks using probabilistic modeling techniques. Viral Informatics: Virome, Comparative metagenomic analysis using VIROME. Metagenomics

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. Sándor Suhai (2002). Genomics and Proteomics. Springer US

2. CAMPBELL (2007). Discovering Genomics, Proteomics and Bioinformatics. Pearson Education

3. Richard P. Grant (2004). Computational Genomics: Theory and Application. Horizon Bioscience

4. Gracia KC, Husi H. (2019) Computational Approaches in Proteomics. Brisbane (AU): Codon Publications, PMID: 31815395.

Web Resources

1. http://virome.dbi.udel.edu

Course Title: Sequence Analysis

L	T	P	Cr
3	0	0	3

Course Code: CCS.720
Total Hours: 45

Learning Outcomes: The outcomes of the subject is to ensure that a student can understand and apply the main algorithms and methods used in

pairwise and multiple alignment

searching of sequence databases

hidden Markov models of biological sequences

finding and discovery of motifs in biological sequences

understand the biological contexts in which to apply biological sequence analysis

Course Content

Unit I   13 Hours

Basic concepts of sequence similarity, identity and homology, homologues, orthologues, paralogues and xenologues Pairwise sequence alignments: basic concepts of sequence alignment, Needleman and Wunsch, Smith and Waterman algorithms for pairwise alignments, gap penalties

Unit II   10 Hours

Scoring matrices: basic concept of a scoring matrix, PAM and BLOSUM series, Comparison of PAM and BLOSUM, Tools such as BLAST (various versions of it) and FASTA.

Unit III   12 Hours

Multiple sequence alignments (MSA): basic concepts of various approaches for MSA (e.g. progressive, hierarchical etc.). Algorithm of CLUSTALW (including interpretation of results), concept of dendrogram and its interpretation.

Unit IV   10 Hours

Sequence patterns and profiles: Basic concept and definition of sequence patterns, motifs and profiles, profile-based database searches using PSI- BLAST, analysis and interpretation of profile-based searches.

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings
- David W.Mount (2001) Bioinformatics. Cold Spring Harbor Laboratory Press, ISBN 0-87969-608-7
- P. A. Pevzner (2004) Computational Molecular Biology. Prentice Hall of India Ltd, ISBN81-203-2550-8

- D.E.Krane and M.L.Raymer (2003) Fundamental concepts of Bioinformatics. Pearson Education ISBN 81-297-0044-1
- N.Gautham (2006) Bioinformatics. Narosa publications ISBN-13: 9781842653005
- Andreas D. Baxevanis, Gary D. Bader, David S. Wishart (2020) Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins 4th Edition.Wiley Publishers, ISBN-10 : 1119335582
- Yoon, Byung-Jun, Qian, Xiaoning (2021) Recent Advances in Biological Network Analysis. Springer International Publishing, ISBN 978-3-030-57172-6.

Web Resources
1. https://iop.vast.ac.vn/theor/conferences/smp/1st/kaminuma/SWI SSPROT/index.html
2. http://ggdc.dsmz.de/

Course Title: Computational Genomics and Proteomics

L	T	P	Cr
3	0	0	3

Course Code: CCS.721
Total Lecture: 45

Learning Outcomes: At the end of the course, the students will be able to:

- learn the importance of DNA-Protein Interactions During Transcription

- gain a deep knowledge about the role of bioinformatics-OMIM database, integrated genomic maps, gene expression profiling

- apply probabilistic modeling techniques for the building of transcriptional regulatory networks which will help them to use the techniques of computational proteomics in their further potential careers in academia and industry.

Course Content
Unit I
12 Hours

DNA- Protein interaction: Process of DNA-Protein Interactions During Transcription, Network identification and processing. Protein- Protein

Interactions: Processing of the Proteome, Prediction of Post-translational modifications, Protein Degradation.

Unit II
10 Hours
Role of bioinformatics-OMIM database, integrated genomic maps, gene expression profiling; identification of SNPs, Vector Screening

Unit III
12 Hours

DNA microarray: database and basic tools, Gene Expression Omnibus (GEO), understanding of microarray data, normalizing microarray data, Raw read quality assessment, Mapping data visualization, detecting differential gene expression.

Unit IV
11 Hours
Building predictive models of transcriptional regulatory networks using probabilistic modeling techniques. Viral Informatics: Virome, Comparative metagenomic analysis using VIROME. Metagenomics

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. Sándor Suhai (2002). Genomics and Proteomics. Springer US

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3. Richard P. Grant (2004). Computational Genomics: Theory and Application. Horizon Bioscience

4. Gracia KC, Husi H. (2019) Computational Approaches in Proteomics. Brisbane (AU): Codon Publications, PMID: 31815395.

Web Resources

1. http://virome.dbi.udel.edu