

# **Central University of Punjab**



**Ph.D. in Bioinformatics**

**Session 2023**

**Department of Computational Sciences**

**School of Basic Sciences**

## **Graduate Attributes**

Students graduating from the Ph.D. in Bioinformatics will contribute to the teaching and research needs in computational biology and life sciences in academia, industry and research institutions at local, regional, national and international levels. They will be part of the scientific workforce that will transform health and agriculture sectors employing higher order thinking skills and capabilities. On successful completion of this programme the students will be able to:

- Design independent research problems and choose suitable methodologies in Bioinformatics
- Examine real-life biological problems with the help of computational tools
- Execute research in this new spectrum of multidisciplinary area of science at the national and international platform
- Construct themselves as an Industrious research personnel
- Continue life-long learning as an autonomous learner and apply and nurture critical and creative thinking.

SEMESTER I							
S. No.	Course Code	Course Title	Course Type	Hours			Cr
				L	T	P	
1	CCS.701	Research Methodology	CC	2	0	0	2
2	CCS.751	Research and Publication Ethics	CC	2	0	0	2
3	CCS.703	Review Writing and Presentation	CC	0	0	4	2
4	UNI.753	Curriculum, Pedagogy and Evaluation	CC	1	0	0	1
5	CCS.752	Teaching Assistantship	CC	0	0	2	1
<b>Opt any two of the following courses:</b>							
6	CCS.722	Molecular Structural Biology	DE	3	0	0	3
7	CCS.723	NGS methods and data analytics	DE	3	0	0	3
8	CCS.724	Protein Engineering and Design	DE	3	0	0	3
9	CCS.726	Omics Technologies	DE	3	0	0	3
10	CCS.727	Biomolecular Simulations and Drug Design	DE	3	0	0	3
11	CCS.708	Scientific Programming	DE	3	0	0	3
12	CCS.709	Scientific Programming Lab (Practical)	DE	0	0	6	3
13	CCC.715	Molecular Dynamics	DE	3	0	0	3
14	CCS.716	Molecular Dynamics Lab (Practical)	DE	0	0	6	3
	Total			<b>14 Credits</b>			

### Course Structure of the Programme

#### 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**

**Course Code: CCS.701**

**Course Type: CC**

**Total Hours: 30**

L	T	P	Cr
2	0	0	2

### **Course Learning Outcomes (CLO):**

On completion of this course, students will be able to:

CLO1: Perform Literature survey, critically analyse the scientific problem and develop a research plan

CLO 2: Write a good to technical report, manuscripts and scientific proposals

CLO 3: Use reference management systems and perform literature reviews using online resources

CLO4: Describe the importance of IPR and develops interest in entrepreneurship

Units/ Hours	Contents	Mapping with CLO
I 5 Hours	<p><b>General principles of research:</b> Meaning and importance of research, critical thinking, formulating hypothesis and development of research plan, review of literature, interpretation of results and discussion.</p> <p><b>Learning Activities:</b> Perform literature survey, Research paper presentation, Peer discussion,</p>	CLO1
II 10 Hours	<p><b>Technical writing:</b> Scientific writing that includes the way of writing Synopsis, research paper, poster preparation and presentation, and dissertation.</p> <p><b>Learning Activities:</b> Writing and Evaluation of research proposals, technical presentation, group discussion</p>	CLO2
III 5 Hours	<p><b>Library:</b> Classification systems, e-Library, web-based literature search engines</p> <p><b>Learning Activities:</b> Perform literature survey, Peer discussion, brain storming</p>	CLO3
IV 10 Hours	<p><b>Entrepreneurship and business development:</b> 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</p> <p><b>Learning Activities:</b> Concept built with real examples, case studies, Student presentation and group discission.</p>	CLO4

**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). Encyclopaedia 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.
5. Gould, J. R. (2020). Directions in Technical Writing and Communication. Routledge.
6. Denisova-Schmidt, E. (2021). Book Review: A Roadmap to the Future of Academic Integrity Research. Academy of Management Learning & Education.

**Course Title: Research and Publication Ethics**

**Course Code: CCS.751**

**Course Type: CC**

**Total Hours: 30**

L	T	P	Cr
2	0	0	2

**Course Learning Outcomes (CLO):**

On completion of this course, students will be able to:

CLO1: Describe with the ethics of research.

CLO2: Outline the good practices to be followed in research and publication.

CLO3: Describe various aspects of Publication ethics

CLO4: Appreciate the importance of Open access publication

CLO5: Identify the misconduct, fraud and plagiarism in research.

CLO6: Utilize various online resources and software to analyse their research output.

Units/ Hours	Contents	Mapping with CLO
I 5 Hours	<b>Philosophy and Ethics</b> 1. Introduction to philosophy: definition, nature and scope, concept, branches 2. Ethics: definition, moral philosophy, nature of moral judgements and reactions  <b>Learning Activities:</b> Case studies, Student presentation and group discussion.	CLO1
II 5 Hours	<b>Scientific Conduct</b> 1. Ethics with respect to science and research 2. Intellectual honesty and research integrity 3. Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP) 4. Redundant publications: duplicate and overlapping publications, salami slicing 5. Selective reporting and misrepresentation of database  <b>Learning Activities:</b> Case studies, Problem based learning, Student presentation and group discussion.	CLO2
III 5 Hours	<b>Publication Ethics</b> 1. Publication ethics: definition, introduction and importance 2. Best practices/standards setting initiatives and guidelines: COPE, WAME, etc. 3. Conflicts of interest 4. Publication misconduct: definition, concept, problems that lead to unethical behavior and vice versa, types	CLO3

	<p>5. Violation of publication ethics, authorship and contributorship  6. Identification of publication misconduct complaints and appeals  7. Predatory publishers and journals</p> <p><b>Learning Activities:</b> Case studies, Problem based learning, Student presentation and group discussion</p>	
IV 5 Hours	<p><b>Open Access Publishing</b></p> <ol style="list-style-type: none"> <li>1. Open access publication and initiatives</li> <li>2. SHERPA/RoMEO online resource to check publisher copyright &amp; self-archiving policies</li> <li>3. Software tool to identify predatory publications developed by SPPU</li> <li>4. Journal finder/journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer Journal Suggester etc.</li> </ol> <p><b>Learning Activities:</b> Case studies, Problem based learning, Student presentation and group discussion.</p>	CLO4
V 5 Hours	<p><b>Publication Misconduct:</b></p> <p><b>A. Group Discussion:</b></p> <ol style="list-style-type: none"> <li>1. Subject specific ethical issues, FFP, authorship</li> <li>2. Conflicts of interest</li> <li>3. Complaints and appeals: examples and fraud from India and abroad</li> </ol> <p><b>B. Software Tools:</b></p> <p>Use of plagiarism software like Turnitin, Urkund and other open-source software tools</p> <p><b>Learning Activities:</b> Case studies, Problem based learning, Student presentation and group discussion.</p>	CLO5
VI 5 Hours	<p><b>Databases and Research Metrics</b></p> <p><b>A. Databases</b></p> <ol style="list-style-type: none"> <li>1. Indexing databases</li> <li>2. Citation databases: Web of Science, Scopus, etc.</li> </ol> <p><b>B. Research Metrics</b></p> <ol style="list-style-type: none"> <li>1. Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score</li> <li>2. Metrics: h-index, g-index, i10 index, altmetrics</li> </ol> <p><b>Learning Activities:</b> Concept mapping, Problem based learning, Student presentation and group discussion.</p>	CLO6

**Transactional Modes:** Class room teaching. guest lecture, group discussion, and practical sessions.

## **Suggested Readings**

1. Lillie, W. (1967). *An Introduction to Ethics*. Allied Publishers Pvt. Ltd.; 1 edition.
2. MacKenzie, J.S. (2005). *A Manual of Ethics*. Cosimo Classics.
3. Committee on Publication Ethics (COPE). *How to handle authorship disputes: a guide for new researchers*. 2003. Available at: [publicationethics.org/files/2003pdf12.pdf](http://publicationethics.org/files/2003pdf12.pdf). Accessed on June 17, 2017.
4. Elsevier. *Publishing Ethics Resource Kit (PERK)*. (2017) Available at: [elsevier.com/editors/perk/plagiarism-complaints](http://elsevier.com/editors/perk/plagiarism-complaints).



**Course Title: Review Writing and Presentation**

**Course Code: CCS.703**

**Course Type: CC**

**Total Hours: 60**

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
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 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 Presentation” shall be as follows:

Maximum Marks: 100

<b>S.No.</b>	<b>Criteria</b>	<b>Marks</b>
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: Curriculum, Pedagogy and Evaluation****Course Code: UNI.753****Course Type: CC****Total Hours: 15**

L	T	P	Cr
1	0	0	1

**Course Learning Outcomes (CLO):**

On completion of this course, students will be able to:

CLO1: Analyze the principles and bases of curriculum design and development

CLO2: Examine the processes involved in curriculum development

CLO3: Develop the skills of adopting innovative pedagogies and conducting students' assessment

CLO4: Develop curriculum of a specific course/programme

<b>Units/ Hours</b>	<b>Contents</b>	<b>Mapping with CLO</b>
I 4 Hours	<b>Bases and Principles of Curriculum</b> Curriculum: Concept and Principles of curriculum development, Foundations of Curriculum Development. 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.	CLO1
II 4 Hours	<b>Curriculum Development</b> Process of Curriculum Development: Formulation of graduate attributes, course/learning outcomes, content selection, organization of content and learning experiences, transaction process. Comparison among Interdisciplinary, multidisciplinary and trans-disciplinary approaches to curriculum.	CLO2
III 3 Hours	<b>Curriculum and Pedagogy</b> Conceptual understanding of Pedagogy. Pedagogies: Peeragogy, Cybergogy and Heutagogy with special emphasis on Blended learning, Flipped learning, Dialogue, cooperative and collaborative learning Three e- techniques: Moodle, Edmodo, Google classroom	CLO3
IV 4 Hours	<b>Learners' Assessment</b> Assessment Preparation: Concept, purpose, and principles of preparing objective and subjective questions. Conducting Assessment: Modes of conducting assessment – offline and online; use of ICT in conducting assessments. Evaluation: Formative and Summative assessments, Outcome based assessment, and scoring criteria	CLO4

## **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**

1. Allyn, B., Beane, J. A., Conrad, E. P., & Samuel J. A., (1986). *Curriculum Planning and Development*. Boston: Allyn & Bacon.
2. Brady, L. (1995). *Curriculum Development*. Prentice Hall: Delhi. National Council of Educational Research and Training.
3. Deng, Z. (2007). Knowing the subject matter of science curriculum, *Journal of Curriculum Studies*, 39(5), 503-535.  
<https://doi.org/10.1080/00220270701305362>
4. Gronlund, N. E. & Linn, R. L. (2003). *Measurement and Assessment in teaching*. Singapore: Pearson Education
5. McNeil, J. D. (1990). *Curriculum: A Comprehensive Introduction*, London: Scott, Foreman/Little
6. Nehru, R. S. S. (2015). *Principles of Curriculum*. New Delhi: APH Publishing Corporation.
7. Oliva, P. F. (2001). *Developing the curriculum* (Fifth Ed.). New York, NY: Longman
8. 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.westernsydney.edu.au/_data/assets/pdf_file/0004/467095/Fundamentals_of_Blended_Learning.pdf)
- <https://www.uhd.edu/academics/university-college/centers-offices/teaching-learning-excellence/Pages/Principles-of-a-Flipped-Classroom.aspx>
- <http://leerwegdialoog.nl/wp-content/uploads/2018/06/180621-Article-The-Basic-Principles-of-Dialogue-by-Renate-van-der-Veen-and-Olga-Plokhooij.pdf>

**Course Title: TEACHING ASSISTANTSHIP**

**Course Code: CCS.752**

**Course Type: CC**

**Total Hours: 30**

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
1	0	0	1

**Course Learning Outcomes:**

On completion of this course, students will be able to:

CLO1: Familiarize themselves with the pedagogical practices of effective class room delivery and knowledge evaluation system

CLO2: 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 Title: Molecular Structural Biology**

**Course Code: CCS.722**

**Course type: DE**

**Total Hours: 45**

L	T	P	Cr
3	0	0	3

**Course Learning Outcomes (CLO):**

On completion of this course, students will be able to:

CLO1: Describe the macromolecular structures and the experimental methods to determine it

CLO2: Apply various structure analysis tools to assign protein fold, biological function and analyse the intramolecular interactions.

CLO3: Predict the protein tertiary structures from its amino acid sequence.

CLO4: Describe DNA synthesis from a structural perspective

CLO5: Describe the importance of structure in various processes ranging from cell signalling, systems biology and macromolecular assemblies

<b>Units/ Hours</b>	<b>Contents</b>	<b>Mapping with CLO</b>
I 12 Hours	<p><b>Introduction to protein structures:</b> Introduction to biological macromolecules, Structural organization of proteins, Factors responsible for Protein folding and stability, Structure determination methods - X-ray crystallography, NMR, Cryo-electron microscopy, SAXS and Neutron scattering. Introduction to PDB Data-file formats, visualizing Structures, reading coordinate files, potential challenges. Structure validation - Ramachandran plot. Software for quality check. Structural Genomics initiatives.</p> <p><b>Learning Activities:</b> Peer discussion, visualization and analysing of protein structures, training on various structural databases and validation, Visit and demonstration of X-ray, NMR and EM facilities.</p>	CLO1
II 10 Hours	<p><b>Structure comparison and structure prediction:</b> Protein structure comparison and alignment, sequence-structure relationship, Structure comparison, multiple structure alignment. Structural domains, Relationship between structure and function, assigning function from structure.</p> <p>Secondary structure prediction methods, Protein-Comparative modeling, Threading, <i>Ab initio</i> modeling, introduction to Deep-learning algorithms in protein structure prediction, Introduction to Membrane Protein Structure Prediction CASP experiments.</p>	CLO2 CLO3

	<p><b>Learning Activities:</b> Hands-on training structure comparison, prediction, Peer group discussion, Student seminars on recent developments</p>	
<p>III 12 Hours</p>	<p><b>Structural perspective of DNA synthesis, transcription and translation:</b></p> <p>Replication, mechanism of DNA synthesis, requirements for DNA synthesis in a bacterium, initiation of bacterial DNA replication, unwinding of the DNA – helicase and helicase loader, priming the DNA synthesis, disentanglement of replication products, a glimpse of eukaryotic replication.</p> <p>Bacterial transcription, eukaryotic transcription, prokaryotic regulation, eukaryotic regulation, post-transcription modifications and mRNA processing</p> <p>RNA – processing, splicing, editing, translation – protein synthesis -the ribosome; initiation of translation – prokaryotic, eukaryotic; translation elongation – Decoding, peptidyl transfer, translocation, translation termination; post-translation modifications.</p> <p><b>Learning Activities:</b> Peer discussion, visualization and analysing of protein structures.</p>	<p>CLO4</p>
<p>IV 11 Hours</p>	<p><b>Structure in cell signaling to systems biology:</b></p> <p>Cell signaling, pathway as signal amplifier, signaling by phosphorylation, cAMP signaling pathway; GPCR and Kinase mediated MAPK pathway; structural basis for immune response; structural systems biology; macromolecular assemblies, ATPases, molecular self-assembly - viral capsids, structural assemblies utilized in the study of macromolecular dynamics.</p> <p><b>Learning Activities:</b> Peer discussion, visualization and analysing of protein structures.</p>	<p>CLO5</p>

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

### Suggested Readings

1. Branden, C. and Tooze, J. (1999). Introduction to Protein Structure, Garland Publishing Inc., 2e
2. Pal, S. (2020). Fundamentals of Molecular Structural Biology. Academic Press. ISBN: 9780128148556.
3. Gu, J. and Bourne, P. E. (2009) Structural Bioinformatics, John Wiley & Sons, 2e,

4. Liljas, A and L. Liljas, J. Piskur, G. Lindblom, P. Nissen and M. Kjeldgaard. (2009) Textbook of Structural Biology. World Scientific Publishing Co.
5. Rupp, B. (2009) Biomolecular Crystallography: Principles, Practice, and Application to Structural Biology. Garland Science.
6. Gromiha, M.M., (2010) Protein Bioinformatics, From Sequence to Function, Academic Press, USA, 1e.
7. Zhou, Y., Kloczkowski, A., Faraggi, E., and Yang, Y. (2017). Prediction of protein secondary structure. Humana Press. ISBN: 9781493964048, 9781493964048.
8. Kihara, D. (2014). Protein structure prediction. New York, NY, USA: Humana Press. ISSN: 1064-3745.
9. Anderson, W. F. (2014). Structural genomics and drug discovery. Methods and Protocols, 1. Humana Press. ISBN: 9781493903535, 9781493903535.
10. Select reviews from the journal *Current Opinion in Structural Biology*

**Web resources:**

NPTL <http://nptel.ac.in/syllabus/syllabus.php?subjectId=104102016>

MIT OpenCourseWare

<http://ocw.mit.edu/courses/biological-engineering/20-442-molecular-structure-of-biological-materials-be-442-fall-2005/>

**Course Title: NGS methods and data analytics****Course Code: CCS.723****Course type: DE****Total Hours: 45**

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
3	0	0	3

**Course Learning Outcomes (CLO):**

On completion of this course, students will be able to,

CLO1: Describe the experimental procedures involved in DNA sequencing

CLO2: Compare various NGS chemistries and NextGen Sequencing platforms

CLO3: Describe the different workflows in the analysis of NGS data

CLO4: Describe NGS data analysis from multiple and single cell sequencing

CLO5: Describe the big data and real-time application in various fields

<b>Units/ Hours</b>	<b>Contents</b>	<b>Mapping with CLO</b>
I 11 Hours	<p><b>NGS and its application to Genome, Transcriptome and Epigenome Sequencing.</b></p> <p>Introduction to NGS platforms (Roche 454, AB SOLiD, Illumina, Ion Torrent, PacBio, Nanopore sequencing).</p> <p>Total RNA and mRNA seq, targeted RNA-seq and small noncoding RNA-seq, single-cell RNA-sequencing (scRNA-seq); Epigenomics: Methylation sequencing (Methylated DNA immunoprecipitation sequencing (MeDIP-Seq), bisulfite sequencing (BS-seq), CHIP-Seq.</p> <p><b>Learning Activities:</b> Peer discussion, Seminars on application of the techniques, Visit and demonstration of NGS platforms</p>	CLO1 & CLO2
II 11 Hours	<p><b>NGS data Analysis workflow file formats and tools</b></p> <p>Primary, secondary and Tertiary analysis; Sequence quality evaluation - Phred Scores; Quality Control and Preprocessing; post alignment quality and bias control; Types of NGS data; File formats - FASTQ, SAM, BAM, VCF; Online NGS databases. Introduction to Galaxy, Bioconductor, velvet.</p> <p><b>Learning Activities:</b> Hands-on training in sequence analysis, Seminars on application of the techniques, Case studies, research paper discussion</p>	CLO3
III 12 Hours	<p><b>NGS Data Analysis</b></p> <p>Sequence alignment algorithms-short reads alignment - Suffix tree, indexing, Burrows-Wheeler transformation; Genome Assembly using deBruijn Graphs; Types of NGS data; File formats - FASTQ, SAM, BAM, VCF; Online NGS databases.</p>	CLO4



	<p>DNA Seq data analysis - Sequence mappability, Refined alignment, Quality recalibration, Variant identification, Variant quality recalibration.</p> <p>RNA-Seq data analysis-Differential Expression Analysis Workflow; Aligning Reads to Reference; Transcriptome Assembly; Alignment programs; Spliced alignment Quantitation and Annotation-Based Quality Control; quantitation of gene expression</p> <p>ChIP-Seq - Principle, Experimental workflow; ChIP-Seq data analysis-ChIP-Seq Peak Calling; Software for ChIP-Seq Peak Calling; Peak Annotation; DNA-protein binding site identification; The ENCODE Project.</p> <p><b>Learning Activities:</b> Discussion and seminars on application of the techniques, Case studies, research paper discussion</p>	
<p>IV 11 Hours</p>	<p><b>NGS Applications</b></p> <p>Large-scale (Genome 10K project; Tree of life sequencing project); cell and cell compartment applications (Single-cell and Mitochondria genome sequencing); Disease-targeted sequencing (Inherited and complex human diseases); Human gut microbiome and Metagenomic impact on human diseases and health; Precision medicine using personal genome sequencing; animal and plant diversity analysis using whole genome sequencing. Epigenomics, epigenetics of the immune system, epigenomics to improve cancer therapies- case studies</p> <p><b>Learning Activities:</b> Peer discussion, hands-on training in sequence analysis, Seminars on application of the techniques, Case studies, research paper discussion</p>	<p>CLO5</p>

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

**Suggested Readings:**

1. Brown, S. M. (2013). Next-Generation DNA Sequencing Informatics. Cold Spring Harbor Laboratory Press, 1/e.
2. Xinkun Wang. (2016). Next-Generation Sequencing Data Analysis. Talyor and Francis Group.

3. Low, L., & Tammi, M. (2017). Introduction to next generation sequencing technologies. *Bioinformatics: A Practical Handbook Of Next Generation Sequencing And Its Applications*.
4. Korpelainen et al (2015). *RNA-seq Data Analysis – A Practical Approach*, CRC Press, Taylor & Francis Group, 1e.
5. Jianping Xu. (2014). *Next-generation sequencing: Current Technologies and Applications*. Caister Academic Press, 1/e.

**Course Title: Protein Engineering and Design****Course Code: CCS.724****Course type: DE****Total Hours: 45**

L	T	P	Cr
3	0	0	3

**Course Learning Outcomes (CLO):**

On completion of this course, students will be able to:

CLO1: Describe the protein folding process, mechanism and its importance.

CLO2: Choose a suitable experimental technique to introduce desired amino acid modifications to wild type proteins

CLO3: Design and modify sequence for a protein with a desired structure and/or property

CLO4: Design the protein molecules with the desired bonded and non-bonded interactions using computational methods

CLO5: Describe the importance of protein designing for various applications.

Units/ Hours	Contents	Mapping with CLO
I 10 Hours	<p><b>Protein Folding and Engineering Methods:</b> Protein structural features, Protein Folding: Theory and Experiment- Protein Renaturation, Determinants of Protein Folding, Folding Pathways, Folding Accessory Proteins. Introduction to Conformational Diseases. Protein stabilising factors, Protein Denaturation, Explaining the Stability of Thermostable Proteins</p> <p><b>Protein Engineering Methods</b> Protein expression systems (<i>E. coli</i> and <i>S. cerevisiae</i>), optimization of protein production and purification.</p> <p>In vitro mutagenesis- chemical mutagenesis – oligonucleotide - based mutagenesis - cassette mutagenesis – PCR based mutagenesis - saturation mutagenesis favouring the mutants. Protein engineering using non-canonical amino acids - methodologies; applications-side chain packing - backbone mutations- dissecting collagen mutations</p> <p><b>Learning Activities:</b> Peer discussion, demonstration using physical and computer models on folding process, Student seminars</p>	CLO1 CLO2
II 13 Hours	<p><b>Strategies for Protein Design:</b> Protein design; strategies for the design of structure - self-assembly - ligand-induced assembly - assembly via covalent cross-linking - assembly of peptides on a synthetic template. Strategies for the design of</p>	CLO3

	<p>function-novel functions by retrofitting natural proteins - incorporation of binding sites into <i>de novo</i> proteins - design of catalytically active proteins - membrane proteins and ion channels - design of new materials.</p> <p><b>Learning Activities:</b> Peer discussion, Case studies, research paper discussion, Problem based learning</p>	
<p>III 10 Hours</p>	<p><b>Computational Protein Design:</b> Methods of Computational Protein Design, core and full repacking, predicting native protein core sequences; altering protein folds. Geometry and stereochemistry-based design, Case studies on Computationally Designed Proteins.</p> <p><b>Learning Activities:</b> Problem based learning, demonstration using and computer models and experimental evidences, Classroom presentation</p>	CLO4
<p>IV 12 Hours</p>	<p>Tools and applications of Protein Engineering, Food and detergent industry applications, Environmental applications, Medical and nanobiotechnology applications. Modulating protein interactions by rational approach. Future challenged of computational protein design.</p> <p>Case studies on recent research articles.</p> <p><b>Learning Activities:</b> Peer discussion, Case studies, research paper discussion, Problem based learning</p>	CLO5

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

### Suggested Readings

1. Zhao,H. (2021) Protein Engineering: Tools and Applications, Wiley-VCH Verlag GmbH & Co
2. Park, S.J., and Cochran, J.R. (2010). Protein Engineering and Design, 1/e, Taylor and Francis Inc., CRC Press, USA.
3. Carey, P.R. (1996) Protein Engineering and Design, 1/e, Academic Press Inc, USA.
4. Samish,I. (2017). Computational Protein Design, 1/e, Humana Press, New York.
5. Branden, C. I., & Tooze, J. (1999)., Introduction to Protein Structure, 2/e, Garland Science, USA.
6. Stefan, L. and Uwe, T.B. (Eds), (2012) Protein Engineering Handbook: Volume 3, 1/e, Wiley-VCH Verlag GmbH & Co.

### Web resources:

NPTEL

1. [https://onlinecourses.nptel.ac.in/noc21\\_cs100/preview](https://onlinecourses.nptel.ac.in/noc21_cs100/preview)

2. [https://onlinecourses.nptel.ac.in/noc21\\_bt14/preview](https://onlinecourses.nptel.ac.in/noc21_bt14/preview)

MIT Open Courseware

1. <https://ocw.mit.edu/courses/biology/7-344-antibiotics-toxins-and-protein-engineering-spring-2007/>
2. <https://ocw.mit.edu/courses/biology/7-91j-foundations-of-computational-and-systems-biology-spring-2014/video-lectures/lecture-12-introduction-to-protein-structure-structure-comparison-and-classification/>

**Course Title: Omics Technologies**  
**Course Code: CCS.726**  
**Course type: DE**  
**Total Hours: 45**

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
3	0	0	3

**Course Learning Outcomes (CLO):**

On completion of this course, students will be able to:

CLO1: Outline the genome sequencing projects and the experimental procedures involved in genome mapping and sequencing

CLO2: Correlate the genomic variations and biological functions

CLO3: Interpret transcriptome profiling data from microarray and RNAseq

CLO4: Explain various proteomics tools for proteome analysis

CLO5: Explain the role of genomic circuits in the functioning of biological systems

<b>Units/ Hours</b>	<b>Contents</b>	<b>Mapping with CLO</b>
I  12 Hours	<p><b>Introduction to Genomics</b></p> <p>Genomics– genotype-phenotype relation – Concept of gene, RNA content of the cell, the link between the transcriptome and the proteome, Varieties of genome organization &amp; genetic features of virus, bacteria and eukaryotes: Sequencing Genomes; Chain-termination sequencing; Next-generation sequencing; Mapping Genomes; Eukaryotic genome sequencing projects, Genome Annotation; imprinting, methylation and cancer.</p> <p><b>Learning Activities:</b> Classroom presentation and discussion, hands-on training on protein-DNA interaction analysis, Problem based learning.</p>	CLO1
II  10 Hours	<p><b>Genomic Variation, Gene Expression and the transcriptome</b></p> <p>Variation in genome, gene mutation, mutation and allele, SNPs - SNPs in malaria resistance; variations in medication responsiveness, mutations causing cancer, SNP Genotyping; Genome-Wide Association Studies, Introduction to Comparative genomics.</p> <p>Genomic microarrays- cancer diagnosis and treatments; improving health care - efficacy of BCG vaccine; predicting effective drugs in different types of cancers; genomic responses to leptin treatments; advantages of RNA sequencing; Gene Expression Databases.</p>	CLO2 CLO3

	<p><b>Learning Activities:</b> Research paper discussion, Hands-on training on biological databases, Problem based learning.</p>	
<p>III 12 Hours</p>	<p><b>Introduction to Proteomics</b> Gene ontology terms; protein identification and quantitation: 2D gels, liquid chromatography and tandem mass spectrometry; De novo Peptide sequencing; Peptide Spectrum Matching via Database Search and Spectral Library Search; Post-translational Modifications: Quantitative proteomics, clinical proteomics and disease biomarkers; protein microarray; the role of single-protein molecules and single-cell proteomes; Structural Proteomics; New directions in proteomics; Protein-DNA and Protein-protein interactions</p> <p><b>Learning Activities:</b> Peer discussion, Hands-on training on Genomic databases and data visualization, Problem based learning.</p>	<p>CLO4</p>
<p>IV 11 Hours</p>	<p><b>Introduction to Metabolomics and Genomic Circuits</b> Integrative Genomics, Metabolomics- Analysis of Cellular Constituents; Metabolic Profiling; Metabolic and Biochemical Databases. Natural gene circuits - gene toggle switches - lambda phage switch. Dissecting a gene's circuitry-gene regulation- gene expression in Endo 16-regulation of transcription; engineered genetic toggle switches.</p> <p><b>Learning Activities:</b> Peer discussion on probabilistic approaches for transcriptional networks, Hands-on training on biological networks, quiz.</p>	<p>CLO5</p>

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

### Suggested Readings

1. Suhai, S (2002). Genomics and Proteomics. Springer US
2. Campbell (2007). Discovering Genomics, Proteomics and Bioinformatics. Pearson Education
3. Informatics, G., and Berger, S. (2021). Viral Meningitis: Global Status: 2021 edition. GIDEON Informatics Inc. ISBN: 1498833098, 9781498833097.
4. Lesk, A. (2019). Introduction to bioinformatics. Oxford university press. ISBN: 9780198794141.
5. Grant, P.R. (2004). Computational Genomics: Theory and Application. Horizon Bioscience
6. Gracia ,K.C, Husi H. (2019) Computational Approaches in Proteomics. Brisbane (AU): Codon Publications, PMID: 31815395.
7. Guzzi, P.H. (2016). Microarray Data Analysis: Methods and Applications. Humana Press. ISBN: 1493931725, 9781493931729.

**Course Title: Biomolecular Simulations and Drug Design****Course Code: CCS.727****Course type: DE****Total Hours: 45**

L	T	P	Cr
3	0	0	3

**Course Learning Outcomes (CLO):**

On completion of this course, students will be able to,

CLO1: Describe the modelling of small to large molecular environments

CLO2: Describe the concept of molecular mechanics force fields and select an appropriate energy function/force field for a given problem

CLO3: Choose an appropriate energy minimization method for the required simulation study.

CLO4: Apply different methods for simulating large molecular systems

CLO5: Describe a pharmacophore model from a set of drug molecule and quantify the structure activity relationship

CLO6: Perform and evaluate different virtual screening methods using large datasets

Units/ Hours	Contents	Mapping with CLO
I 11 Hours	<p><b>Molecular Modeling and Structure</b> Introduction to Molecular modelling, Coordinate systems, potential energy surfaces for simple molecules. mini tutorials with protein and nucleic acid structure as examples.</p> <p>The simple molecular mechanics force field; general features of molecular mechanics force fields. Force Fields and Molecular Representation – Intramolecular Interactions, Non-bonded Interactions – London (van der Waals) Interactions, Electrostatic Interactions, Hydrogen Bonds, Constraints and Restraints, United Atom and Other Coarse-Grained Approaches, Non-pairwise Interactions, accuracy of the force fields.</p> <p><b>Learning Activities:</b> Peer discussion, Demonstration using physical and computer model, Problem based learning, Analysing Experimental data.</p>	CLO1 & CLO2



<p>II 12 Hours</p>	<p><b>Energy Minimization and Related Analysis Techniques</b> Steepest Descent, Conjugate Gradient, Newton-Raphson, Comparison of Methods, Advanced Techniques: Simulated Annealing, Branch-and-bound, Simplex, What's the big deal about the minimum?</p> <p>Phase space, Ergodicity, and Liouville's theorem, Ensemble theory, Thermodynamic averages - Microcanonical Ensemble, Canonical Ensemble, Other MD Simulation Related Ensembles</p> <p><b>Learning Activities:</b> Hands-on training, Peer discussion, Research paper presentation</p>	<p>CLO3</p>
<p>III 11 Hours</p>	<p><b>Methods for Simulating Large Systems</b> Non-bonded Cutoffs – Shifted Potential and Shifted Force, Switching Functions, Neighbor Lists. Boundaries – Periodic Boundary Conditions, Stochastic Forces at Spherical Boundary. Long-range Interactions – The Ewald Sum, The Reaction Field Method</p> <p>Molecular dynamics using simple models, Molecular dynamics with continuous potentials, finite difference and predictor-corrector integration methods, choosing the time step. Calculating properties by integration; implementation of the Metropolis Monte Carlo method; Monte Carlo simulation of rigid and flexible molecules; Lattice and continuous polymer models.</p> <p><b>Learning Activities:</b> Hands-on training on simulation, Peer discussion, Case studies, research paper discussion.</p>	<p>CLO4</p>
<p>IV 11 Hours</p>	<p><b>Drug design</b> Introduction to drug designing, Structure guided drug design, molecular docking and scoring methods, de novo ligand design, fragment-based drug design, role of structure prediction methods. ADMET, drug metabolism, toxicity and pharmacokinetics. Lipinski rule of 5, Identification and validation strategies. Drug Target classification, Concept of Pharmacophore, Functional group considered as pharmacophore, Structure-based drug design, docking, QSAR, Artificial intelligence in drug discovery and development. Anticancer Agents, Antiviral Drugs, Antibiotics and drug resistance.</p> <p><b>Learning Activities:</b> Peer discussion, Case studies, research papers, Hands-on training on drug designing</p>	<p>CLO5 &amp; CLO6</p>

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

## Suggested Readings

1. Leach R. (2001). *Molecular Modelling Principles and Applications* 2nd Edition. Pearson.
2. Frenkel D. and Smit B. (2001). *Understanding Molecular Simulation* 2nd Edition, Academic Press.
3. Buschmann, H., & Holenz, J. (2018). *Biomolecular Simulations in Structure- Based Drug Discovery*. Germany: Wiley. ISBN:9783527342655
4. Alavi S. (2020). *Molecular Simulations: Fundamentals and Practice* 1st Edition, Wiley-VCH.
5. Bhatt, T. K., & Nimesh, S. (Eds.). (2021). *The design and development of novel drugs and vaccines: Principles and protocols*. Academic Press. ISBN: 9780128214718.
6. Renaud, J. P. (Ed.). (2020). *Structural biology in drug discovery: Methods, Techniques, and Practices*. John Wiley & Sons. ISBN: 9781118900406.
7. Allen, M. P., & Tildesley, D. J. (2017). *Computer Simulation of Liquids* 2nd Edition, Oxford University Press.
8. Stromgaard, K., Krosgaard-Larsen, P., & Madsen, U. (2016). *Textbook of Drug Design and Discovery*. CRC Press, 5e, 2016.

**Course Title: Scientific Programming**  
**Course Code: CCS.708**  
**Course Type: DE**  
**Total Hours: 45**

L	T	P	Cr
3	0	0	3

**Course Learning Outcomes (CLO):**

On completion of this course, students will be able to:

CLO1: Write programs to solve scientific problems using Fortran

CLO2: Describe the Use branching structures, loops in programming

CLO3: Demonstrate concepts related to variables, I/O, arrays, procedures, modules, pointers and parallel programming.

CLO4: Develop skills in parallel programming in develop effective skills in scientific programming

Units/ Hours	Contents	Mapping with CLO
I 10 Hours	<b>Introduction to Computers and Fortran language:</b> 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.  <b>Learning Activities:</b> Brain-storming and Problem Solving	CLO1
II 10 Hours	Constants and variables, assignment statements and arithmetic calculations, intrinsic functions, Program design and branching structures, loop and character manipulation.  <b>Learning Activities:</b> Brain-storming and Problem Solving	CLO2
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 arrays 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.  <b>Learning Activities:</b> Brain-storming and Problem Solving	CLO3
IV 10 Hours	What is parallel programming, Why use parallel programming, Parallel Architecture, Open MP & MPI, Models of Parallel Computation, Parallel Program	CLO4

	Design, Shared Memory & Message Passing, Algorithms, Merging & Sorting.  <b>Learning Activities:</b> Brain-storming and Problem Solving	
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**Transactional Modes: Lecture;** Tutorial; Problem solving; Self-learning.

**Suggested Readings**

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

**Course Title: Scientific Programming Lab (Practical)**

**Course Code: CCS.709**

**Course Type: SBE**

**Total Hours: 90**

L	T	P	Cr
0	0	6	3

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.

**Course Learning Outcomes (CLO):**

On completion of this course, students will be able to:

CLO1: Identify/characterize/define a computational problem

CLO2: Design a Fortran program to solve the scientific problem

CLO3: Create pseudo executable code

CLO4: Describe various important aspects of the basic Fortran code

Units/ Hours	Contents	Mapping with CLO
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.  <b>Learning Activities:</b> Peer discussion, real world application, brain storming and Problem Solving.	CLO1
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 arrays in procedures, derived data types.  <b>Learning Activities:</b> Peer discussion, real world application, brain storming and Problem Solving.	CLO2
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.  <b>Learning Activities:</b> Peer discussion, real world application, brain storming and Problem Solving.	CLO3

IV 20 Hours	<p>What is parallel programming, Why use parallel programming, Parallel Architecture, Open MP &amp; MPI, Models of Parallel Computation, Parallel Program Design, Shared Memory &amp; Message Passing, Algorithms, Merging &amp; Sorting.</p> <p><b>Learning Activities:</b> Peer discussion, real world application, brain storming and Problem Solving.</p>	CLO4
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**Transactional Modes:** Laboratory based practical; Problem solving; Self-learning.

### Suggested Readings

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

**Course Title: Molecular Dynamics**  
**Course Code: CCS.715**  
**Course Type: DE**  
**Total Hours: 45**

L	T	P	Cr
3	0	0	3

**Course Learning Outcomes:**

On completion of this course, students will be able to:

- CLO1: Describe the modelling of small to large molecular environments  
 CLO2: Describe the concept of molecular mechanics force fields and select an appropriate energy function/force field for a given problem  
 CLO3: Describe different methods to calculate non-bonded interactions and long range interactions in a molecular system  
 CLO4: Choose an appropriate energy minimization method for the required simulation study.  
 CLO5: Apply different methods for simulating large molecular systems.

Units/ Hours	Contents	Mapping with CLO
I 10 Hours	<p><b>Molecular Modeling and Structure</b> - molecular modeling today: overview of problems, tools, and solution analysis, minitutorials with protein and nucleic acid structure as example.</p> <p><b>Force Fields and Molecular Representation</b> – (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.</p> <p><b>Learning Activities:</b> Peer discussion, real world application, brain storming and Problem Solving.</p>	CLO1 & CLO 2
II 10 Hours	<p><b>Methods for Simulating Large Systems</b></p> <ul style="list-style-type: none"> <li>a) Non-bonded Cutoffs – Shifted Potential and Shifted Force, Switching Functions, Neighbor Lists</li> <li>b) Boundaries – Periodic Boundary Conditions, Stochastic Forces at Spherical Boundary</li> <li>c) Long-range Interactions – The Ewald Sum, The Reaction Field Method</li> </ul> <p><b>Learning Activities:</b> Peer discussion, real world application, brain storming and Problem Solving.</p>	CLO3

<p>III 10 Hours</p>	<p><b>Energy Minimization and Related Analysis Techniques</b>  (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</p> <p><b>Learning Activities:</b> Peer discussion, real world application, brain storming and Problem Solving.</p>	<p>CLO4</p>
<p>IV 15 Hours</p>	<p><b>Simulation Methods:</b>  <b>Monte Carlo:</b> (a) MC integration and Markov chains, (c) The Metropolis method, (c) Biased MC</p> <p><b>Molecular Dynamics:</b> (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,</p> <p><b>Free Energy:</b> (a) Perturbation Methods, (b) TI (Thermodynamic Integration)  Brownian dynamics and the Langevin Equation</p> <p><b>Learning Activities:</b> Peer discussion, real world application, brain storming and Problem Solving.</p>	<p>CLO5</p>

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

### Suggested Readings

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



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

L	T	P	Cr
0	0	6	3

**Course Learning Outcomes:**

On completion of this course, students will be able to:

CLO1: Use the Linux environment for scientific computing

CLO2: Use the remote computing as a tool for high performance computation

CLO3: Use different energy minimization techniques

CLO4: Create macromolecular models from the amino acid sequence, and high-definition images using various graphics tools

CLO5: Use of different *in-silico* techniques for biomolecular simulations which will enhance their employability in their further potential carriers in academia and industry

**List of Exercises**

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