COURSE TITLE	**CHEM-INFORMATICS**
COURSE CODE	**01CB0606**
COURSE CREDITS	**3**

Objective:

1 To provide a comprehensive understanding of chemical structure databases, facilitate hands-on experience with Cheminformatics tools, and explore the practical applications of Cheminformatics in drug design

Course Outcomes: After completion of this course, student will be able to:

1 Apply chemical structure representation methods and use chemical databases for data retrieval.

2 Apply chemical structure searching, visualization, and optimization tools for molecular analysis.

3 Analyze molecular structures using QSAR, pharmacophore modeling, and docking techniques in drug design.

4 Evaluate chemoinformatics-based approaches in the drug discovery pipeline.

5 Design computational strategies and molecular models for lead identification and optimization in drug discovery.

Pre-requisite of course: Basic knowledge of Bioinformatics

Teaching and Examination Scheme

Theory Hours	Tutorial Hours	Practical Hours	ESE	IA	CSE	Viva	Term Work
2	0	2	50	30	20	25	25

Contents : Unit	Topics	Contact Hours
1	**Introduction** Introduction to Chemoinformatics, History and Evolution of Chemoinformatics, Use of Chemoinformatics, Prospects of Chemoinformatics. Databases: Chemical Structure Databases (PubChem, Drug bank). Modelling of small molecules and Structure Elucidation	5
2	**Representation of Molecules** Representation of Molecules and Chemical Reactions. Different Types of Notations, SMILES Coding, Structure of Mol files and Sdf files (Molecular converter, SMILES Translator), RDFile, and many more	5

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Contents : Unit	Topics	Contact Hours
3	**Chemoinformatics databases** Literature Databases; Chemical Databases; Structure Databases, Medline; GenBank. PIR; CAS Registry; National Cancer Institute (NCI) Database. Databases of Small Molecules (ZINC), pubchem, chemspider.	5
4	**Searching Chemical Structure** Searching Chemical Structure: Full Structure Search; SubStructure Search; Similarity Search. Three dimensional Search Methods. Structure Visualisation. Drawing the Chemical Structure: 2D and 3D Drawing Tools (ACD Chemsketch) Structure Optimization	6
5	**Chemoinformatics in drug design** Definition of drugs, Structure-Based Drug Design, QSAR. Pharmacophore Design, Ligand-Based Design, De Novo Drug Design Virtual Screening / Docking of Ligands. Protein structure-Fragment-Based Drug Design, ADMET Prediction.	7
Total Hours		**28**

Suggested List of Experiments:

Contents : Unit	Topics	Contact Hours
1	**Module1:** To compare 2D and 3D formats of the chemicals / molecules	2
2	**Module1:** To compare information on specific molecules from chemical structure databases	2
3	**Module2:** To create Molecular Model and Structure Elucidation of small molecules	2
4	**Module2:** To compare SMILES, Mol files, and SDF files using molecular converter tools	2
5	**Module3:** To Perform similarity searches on PubChem using known molecules	2
6	**Module3:** To generate chemical structure using Marvin sketch	2
7	**Module3:** To generate chemical structures using Chemsketch	2
8	**Module3:** To generate chemical structures using ChemDraw	2
9	**Module4:** To identify and convert one format into another format	2
10	**Module4:** To compare molecules by ADMET analysis	2

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Suggested List of Experiments:

Contents : Unit	Topics	Contact Hours
11	**Module4:** To compare screened chemicals based on rule of five	2
12	**Module5:** To perform binding energy analysis of the screened chemicals	2
13	**Module5:** To compare the binding energies of the compounds	2
14	**Module5:** To visualize the binding complexes and justify the screening criteria	2
Total Hours		**28**

Textbook :

1 Chemoinformatics -A Textbook, Johann Gasteiger and Thomas Engel, Germany: Wiley-VCH, 2003

2 Handbook of Chemoinformatics-From Data to Knowledge, Johann Gasteiger, Germany: Wiley-VCH, 2003

References:

1 An Introduction to Chemoinformatics, An Introduction to Chemoinformatics, Andrew R. Leach, Valerie J. Gillet, UK: Springer, 2007

2 Chemoinformatics: Theory, Practice, and Products, Chemoinformatics: Theory, Practice, and Products, Bunin, Barry A. Dordrecht, UK: Springer, 2010

3 Chemoinformatics: Concepts, Methods, and Tools for Drug Discovery, Chemoinformatics: Concepts, Methods, and Tools for Drug Discovery, Bajorath, Juergen,Totowa, N.J., USA: Humana Press, 2004

4 Computer Applications in Pharmaceutical Research and Development, Computer Applications in Pharmaceutical Research and Development, Ekins, Sean, Hoboken, N.J., Germany: Wiley, 2006

Suggested Theory Distribution:

The suggested theory distribution as per Bloom's taxonomy is as follows. This distribution serves as guidelines for teachers and students to achieve effective teaching-learning process

Distribution of Theory for course delivery

Remember / Knowledge	Understand	Apply	Analyze	Evaluate	Higher order Thinking / Creative
20.00	30.00	20.00	10.00	10.00	10.00

Instructional Method:

1 The course delivery method will depend upon the requirement of content and need of students. The teacher in addition to conventional teaching method by black board, may also use any of tools such as demonstration, role play, Quiz, brainstorming, MOOCs etc.

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Instructional Method:

2 The internal evaluation will be done on the basis of continuous evaluation of students in the laboratory and class-room.

3 Practical examination will be conducted at the end of semester for evaluation of performance of students in laboratory.

Supplementary Resources:

1 https://chem.libretexts.org/Courses/Intercollegiate_Courses/Cheminformatics/01%3A_Introduction/1.09%3A_Cheminformatics_Resources

2 https://www.udemy.com/course/cheminformatics-and-medicinal-chemistry/

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