Course Code	Course Name	Credits
26CH111	MOLECULAR DESCRIPTORS AND FINGERPRINTS	04

Course Objectives

- To understand the fundamental concepts of molecular descriptors and their types, including constitutional, topological, geometrical, and electronic descriptors.
- To explain the concept and representation of molecular fingerprints in chemical informatics.
- To develop an understanding of chemical similarity, database searching, and their applications in drug design, QSAR, and cheminformatics.

Learning Outcomes

Upon successful completion of this course it is intended that a student will be able to:

- Understand basic molecular descriptors and fingerprints
- Identify their types and simple uses
- Apply basic concepts in chemical data analysis

Unit 1 - Introduction (12 Hrs.)

Definition of molecular descriptors, Importance in chemistry and drug design, Basic idea of cheminformatics.

Unit 2- Molecular Descriptors (12 Hrs.)

Types of descriptors:

i. Constitutional (molecular weight, atom count)
ii. Topological (connectivity, Wiener index)
iii. Geometrical (molecular size, shape)
iv. Electronic (charge, dipole moment)

Unit 3 - Molecular Fingerprints (12 Hrs.)

Definition and concept

Types:

i. Structural (substructure-based)
ii. Path-based
iii. Circular fingerprints (e.g., ECFP – basic idea only)
iv. Binary representation (0s and 1s)

Unit 4 – Similarity and Searching (12 Hrs.)

Concept of chemical similarity, Tanimoto coefficient (basic idea), Application in database searching.

Unit 5 - Applications (12 Hrs.)

Drug discovery, QSAR studies, Virtual screening, Environmental and material chemistry.

Reference Books:

1. Roberto Todeschini, Handbook of Molecular Descriptors, Publisher Wiley-VCH, 2008.
2. Mati Karelson, Molecular Descriptors in QSAR/QSPR, Publisher Wiley-Interscience 2000
3. Hugo Kubinyi ,3D QSAR in drug design: theory, methods and applications , 1993

Websites and eLearning Sources:

1. https://www.youtube.com/watch?v=ajM-nZuoi7k&list=PL3Hxlme4R-Pa77h81Pw3jSq6-5Hj1lJ_-
2. https://www.youtube.com/watch?v=9i9SY6Nd1Zw
3. https://www.youtube.com/watch?v=-oHqQBUyrQ0

COs and Bloom's Taxonomy Mapping – 26CH111		
Course Outcomes	**On completing U.G. program the students will be able to**	**BTL**
CO1	Explain the fundamental concepts of molecular descriptors, fingerprints, and their role in chemistry and drug design.	K1
CO2	Classify and describe different types of molecular descriptors such as constitutional, topological, geometrical, and electronic.	K2
CO3	Interpret molecular fingerprints and understand their binary representation and types (structural, path-based, circular).	K3, K4
CO4	Apply basic concepts of chemical similarity and use measures like the Tanimoto coefficient for database searching.	K5
CO5	Evaluate the applications of molecular descriptors and fingerprints in QSAR, drug discovery, and cheminformatics.	K6

BTL K1 and K2 – remembering and understanding, K3- Applying, K4 – Analyse, K5- Evaluate and K6- Create

Relationship Matrix– 26CH111													
Course Outcomes	**Programme Outcomes (POs)**						**Programme Specific Outcomes (PSOs)**						**Mean Score of Cos**
	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PSO1**	**PSO2**	**PSO3**	**PSO4**	**PSO5**	**PSO6**	
CO1	3	2	1	1	1	1	3	2	2	2	1	1	1.7
CO2	3	3	2	1	1	1	3	2	2	2	2	1	1.9
CO3	3	3	3	2	1	1	3	3	2	2	2	2	2.3
CO4	3	3	3	2	2	1	3	3	3	2	2	2	2.4
CO5	3	3	3	3	2	2	3	3	3	3	2	2	2.7
												Total	2.2

Mean Score: 3- High, 2- Medium/Moderate, 1-Low