Course Code	BIO523
Course Name	Chemoinformatics
Credits	4
Course Offered to	UG/PG
Course Description	The objective of this course is to provide introduction to chemoinformatics, an interdisciplinary area on the interface of chemistry, informatics and biology. The student will be provided with understanding of fundamentals of chemoinformatics and its applications. Through lectures, hands-on exercises and assignments, the student is expected to achieve a good grasp of the concepts and applications of chemoinformatics.

Pre-requisites		
Pre-requisite (Mandatory)	Pre-requisite (Desirable)	Pre-requisite (Other)
None	Knowledge of chemistry, algorithms, programming and machine learning (Desirable)	

Post Conditions			
CO1	CO2	CO3	CO4
Students are able to explain basic concepts of chemoinformatics.	Students are able to explain and implement computation of molecular descriptors and chemical similarity.	Students are able to classify small molecules and interpret results from chemoinformatics analysis.	

Weekly Lecture Plan			
Week Number	Lecture Topic	COs Met	Assignment/Labs/Tutorial
1	Motivation for data and informatics driven view of chemistry, Applications for drug discovery, Scope, opportunities and challenges	CO1	3 hours
2	Introduction to Organic structures and their properties	CO1, CO2	3+2 hours (Exercises)
3	Representation and manipulation of 2D & 3D molecular structures	CO1, CO2	3+2 hours (Exercises + Assignment-1)
4	Open source tools for Chemoinformatics	CO1, CO2, CO3	3+2 hours (Exercises)
5	Molecular descriptors-I	CO1, CO2	3+2 hours (Exercises)
6	Molecular descriptors-II	CO1, CO2	3+2 hours (Exercises + Assignment-2)
7	Computational models and analyss: QSAR	CO1, CO2	3+2 hours (Exercises)
8	Chemical similarity methods-I	CO1, CO2, CO3	3+2 hours (Exercises + Mini Project)
9	Chemical similarity methods-II	CO1, CO2, CO3	3+2 hours (Exercises)
10	Case Studies: Classification of molecules	CO1	3+2 hours (Exercises)
11	Analysis of high-throughput screening data and Virtual screening	CO1	3+2 hours (Exercises)
12	Combinatorial chemistry and library design	CO1	3+2 hours (Exercises)
13	Open challenges in Chemoinformatics	CO1	3+2 hours (Mini-Project Presentations)

Assessment Plan	
Type of Evaluation	% Contribution in Grade
Mid-Sem	20
Assignments	30
Mini-Project	20
End-Sem	30

Resource Material	
Type	Title
Textbook	An Introduction to Chemoinformatics, Leach and Gillet (Springer)
Textbook	Practical Chemoinformatics, Karthikeyan and Vyas (Springer)
Refence Book	Organic Chemistry by Morrison and Boyd (Pearson India)