20MSC510T					Theoretical & Computational Chemistry					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
2	1	0	3	3	25	50	25	--	--	100

COURSE OBJECTIVES

- The objective of unit I is to ensure that students learns the basic of UNIX and LINUX programming.
- The objective of unit II is to ensure that students learn about molecular mechanics and how it is implemented into chemistry.
- The objective of unit III is to ensure that students learn how electronic structure calculations can be used as an adjunct to their experimental research.
- The objective of unit IV is to ensure that students understand the role of cheminformatics in drug design process.

Unit I INTRODUCTION **4 hours**

Introduction to the LINUX and UNIX operating system, LINUX/UNIX commands, Difference in UNIX and LINUX operating systems, Comparison of LINUX operating system with windows.

Unit 2 ELECTRONIC STRUCTURE THEORY-I **16 hours**

Molecular mechanics: Introduction, Basic theory, Concept of potential energy surface. Force field and its components (stretch- Morse Potential, bend, out-of-plane bending, torsional, van der Waals and electrostatic energy).

Electronic structure methods: Basics of electronic structure calculations, Semi-empirical methods and Ab-initio methods, Advantages of Semi-empirical methods.

Unit 3 ELECTRONIC STRUCTURE THEORY-II **10 hours**

Density functional methods: Basic theory, building geometry, Basis set, functional's, Notation, Level of theory, Optimization and computable properties like absorption, energy, optimized bond lengths, bond angles, dihedral angles, charge calculations.

Unit 4 CHEMINFORMATICS IN DRUG DESIGN **10 hours**

Computer-aided drug discovery: Classification of CADD, Ligand-based drug design, Structure-based drug design, Virtual screening.

Ligand based drug design: Basic concept, Pharmacophore modelling and QSAR (brief overview), common softwares for implementing ligand-based drug design.

Structure-based drug design: Basic concept, Pharmacophore modelling and Molecular docking (brief overview), common softwares for implementing structure-based drug design.

COURSE OUTCOMES

Upon completion of the course, student will be able to
CO1 – Understand the types of operating systems.
CO2 – Explain the concept of molecular mechanics and its implementation.
CO3 – Describe the role of electronic structure calculations in defining the experimental research.
CO4 – Explain the role of CADD in drug discovery process.
CO5 – Describe the use of different computational softwares.
CO6 – Utilize the softwares to evaluate the structural parameters related to small organic compounds.

REFERENCE BOOKS:

Unit 1

1. Linux Fundamentals by Paul Cobbault, Publication date 2015-05-24 CEST.
2. Online tutorial pdf: https://www.tutorialspoint.com/unix/unix_tutorial.pdf (UNIX computer operating system by tutorial points)

Unit 2 and 3

1. Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems. David C. Young Copyright (2001 John Wiley & Sons, Inc.)
2. Exploring Chemistry with electronic structure methods, 2nd edition, James V. Foresman.

Unit 4

1. Chemoinformatics in Drug Discovery: Methods and Principles in Medicinal Chemistry, Vol. 23, edited by Tudor I. Oprea.
2. Computational Drug Design: A Guide for Computational and Medicinal Chemists, By D. C. Young.
3. The Practice of Medicinal Chemistry, 4th edition, edited by Camille Georges Wermuth, David Aldous Pierre Raboisson Didier Rognan.

SEMESTER EXAMINATION PATTERN

Max. Marks: 100	**Exam Duration: 3 Hrs**
Part A/Question: 10 questions of 2 marks each with internal choice	20 Marks
Part B/Question: 8 questions of 10 marks each with internal choice	80 Marks