

20MSC510P					Theoretical & Computational Chemistry- Practical					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
0	0	2	1	2	--	--	--	50	50	100

COURSE OBJECTIVES

- The objective of the practical session is to ensure that students learn the practical aspects of electronic structure calculations of chemical compounds and modelling of bio-molecular structures.

ELECTRONIC STRUCTURE THEORY PRACTICALS (Any 4 practical's)

1. Geometry construction: Linear and ring systems, setting up and running calculations.
2. Energy calculation, Molecular orbital visualization and atomic charges, dipole and higher dipole moments, calculating conformer energy.
3. Frequency calculation, IR, RAMAN & NMR spectra, thermal energy correction and calculation.
4. Isomerization energy calculation, stability calculation, enthalpy of isomerization.
5. Basis set dependence and its limit, potential energy surface and locating stationary points.
6. Use of some softwares to study electronic structure properties like optimized bond lengths, bond angles, dihedral angles and energy.
7. Exercise on modelling of small molecules using Argus lab: water, methane, benzene, cyclohexane: chair and boat form.

CADD THEORY PRACTICAL (Any 4 practical's)

8. Advanced visualizing softwares and 3D representation with CHIMERA or any visualization software.
9. Coordinate generation and interconversion.
10. Superimposition of proteins using CHIMERA or Discovery studio.
11. Virtual Screening using drug-likeness properties.
12. Molecular docking.

COURSE OUTCOMES

Upon completion of the course, student will be able to

- CO1 – Construct the linear and ring systems using softwares.
 CO2 – Can explain the structural properties parameters retrieved during electronic structure calculations.
 CO3 – Describe the role of electronic structure calculations in defining the experimental research.
 CO4 – Utilize the visualization softwares to evaluate the structure of proteins.
 CO5 – Describe the conversion of chemical structure in different formats.
 CO6 – Can superimpose the proteins with the software or manually.

REFERENCE BOOKS:

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.
3. Chemoinformatics in Drug Discovery: Methods and Principles in Medicinal Chemistry, Vol. 23, edited by Tudor I. Oprea.
4. Computational Drug Design: A Guide for Computational and Medicinal Chemists, By D. C. Young.
5. 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

LW (Daily lab performance plus journal
maintain each 25 marks)

50 Marks

LE (Viva-voce plus Lab examination each 25
marks)

50 Marks