SRI RAMAKRISHNA MISSION VIDYALAYA COLLEGE OF ARTS AND SCIENCE (AUTONOMOUS), COIMBATORE - 641 020

Name of the Programme: M.Sc Chemistry **Month &Year of Revision:** February 2019

S.No.	Course Title	Course Code	% of Revision
1	CORE: Computational Chemistry and Molecular Modelling	19PCH3C09	100%

Note:

No.of Courses offered by the Department (A)	22
No.of Courses revised in BoS (>20% Revision) (B)	1
Formula for Syllabus revision: (B/A)*100	**4.54%**

Programme: M.Sc. Chemistry Course Code: 19PCH3C09

CORE–10: CORE: Computational Chemistry and Molecular Modelling

Year: II Semester: III Credits: 5 Total Hours: 5 x 15 = 75

Unit I : Molecular Mechanics

Force fields and molecular representations of matter - potential energy functions, inter- and intra-molecular interactions, empirical parameters, constraints and restraints, united atom and coarse-grained approaches, non-pairwise interactions. Energy minimization techniques- steepest descent, conjugate gradient, Newton-Raphson, simulated annealing, branch-and-bound and simplex.

Unit II : Molecular Dynamics

Elementary concepts of Ensembles and fluctuations, non-bonded cutoffs, long-range interactions, periodic boundaries, partition function, ensemble averaging and ergodicity. Trajectory analysis - conformational analysis and normal mode analysis. Brownian dynamics, free energy perturbation methods and Monte Carlo simulation.

Unit III : Quantum Mechanics

Basis set: Slater and Gaussian functions, contractions, polarization and diffuse functions, split-valence sets, correlation-consistent sets, core-valence sets, general contractions.

Semi-empirical method: π-methods, valence electron methods - extended Hückel, neglect of differential overlap methods - Austin Model 1, Parameter Model 3.

Ab initio theory: restricted and unrestricted Hartree-Fock, electron correlation, many body perturbation theory, coupled cluster theory and multi configuration self-consistent field theory.

Density functional theory: homogeneous electron gas, Coulomb hole, exchange hole, use of density functional theory in quantum chemistry, Kohn-Sham equations, exchange, correlation and hybrid functional.

QM/MM Method: Mixed methods like the combination of quantum chemical methods and molecular mechanics (QM/MM) for the description of biochemical problems with specific reference to the interaction between drug and receptor.

Unit IV : MM Modelling

MM Modelling I: Biomolecular structure modelling, visualization and database

MM Modelling II: Parameterization of force field

MM Modelling III: Ligand docking and binding pocket analysis

MM Modelling IV: Tool handling

MM Modelling V: Solvation modelling explicit *vs* implicit

MM Modelling VI: Energy minimization techniques and conformation analysis

MM Modelling VII: Molecular dynamics simulation and analysis

MM Modelling VIII: Monte Carlo simulation in chemical and biochemical applications

Unit V : QM Modelling

QM Modelling I: Electronic structure building

QM Modelling II: Basis Sets and Basis Set Superposition Error

QM Modelling III: Single point and geometry optimization calculation

QM Modelling IV: Atomic charges, dipole moment, polarizability and hyper polarizability

Electronic spin - $\hat{S}^2$ operator and degeneracy

Group theory - molecular point groups and term symbols

QM Modelling V: Vibrational frequency analysis, symmetry analysis, harmonic vs fundamental frequencies, zero-point vibrational energies, Hessian index and distinguishing minima from transition states

QM Modelling VI: Reaction profiles in gas phase reaction, solvent effects, thermodynamic properties and intrinsic reaction coordinates analysis

QM Modelling VII: Prediction of theoretical UV-vis, IR and NMR Spectroscopy

QM/MM Modelling VIII: Protein-Ligand interaction, modelling enzymatic reaction profile

References

1. F. Jensen, *Introduction to Computational Chemistry*, Wiley, New York, 1999.
2. Christopher J. Cramer, *Essentials of Computational Chemistry: Theories and Models*, 2nd Ed. Wiley & Sons, New York, 2004.
3. Andrew R. Leach, *Molecular Modelling: Principles and Applications*, 2nd Ed., Prentice Hall, 2001.
4. David Young, *Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems*, John Wiley & Sons, 2004.
5. A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory*, 1st Ed, Dover, 1989.

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