School of Interdisciplinary Engineering and Sciences (SINES)
National University of Sciences & Technology (NUST)

NUST
Defining futures

Title: Computational Enzymology

Objectives: The objectives of enzymology revolve around gaining a comprehensive understanding of enzymes, their properties, mechanisms, regulation, and applications. This knowledge contributes to various fields, including biochemistry, molecular biology, biotechnology, medicine, and drug discovery.

Outcomes: On completion, students will be able to apply theoretical knowledge to:

1. explain biochemical reaction in sense of thermodynamics, kinetics and molecular interactions
2. use catalytic strategies in interpreting mechanisms of enzymatic action
3. apply appropriate methods for determination of catalytic parameters and activity of enzymes and resolve problems considering kinetics and thermodynamics of enzymatic reactions

Course Code: CSE-914

Credit Hours: 3-0

Course Contents:

1. Enzymology-Historical Aspect
2. Computational Methods in Enzymology
3. Structural Components of Enzymes and their Functions
4. Enzyme kinetics
5. Enzymes in Humans
6. Chemical Reaction Investigations in Enzyme Catalysis
7. Challenges in Enzyme Modeling

Course Contents with proposed contact Hours (Weekly plan):

Lecture wise Breakdown

W#1	Topics	Lect #
1	Enzymology-Historical Aspect	1-2
2	Computational Methods in Enzymology (a) Hybrid Potentials for Large Bio-molecular Systems (b) Conformational Search on High-Dimensional Energy Surface (c) Conjugate Peak Refinement Method	3-4
3	(d) Boundary Interactions at the QM/MM Interface (e) Combined Quantum Mechanical/Classical Molecular Dynamics Simulations	5-6
4	Structural Components of Enzymes and their Functions (a) Overview of Protein Chemistry (b) Enzyme Commission Nomenclature	7-8
5	(c) Enzymatic and Non-Enzymatic Catalysis	9-10

	(d) Catalytic Approaches Adopted by Enzymes	
6	Enzyme kinetics (a) Steady state kinetics (b) Isotope effects	11-12
7	(c) Transient Phase kinetics (d) pH-Rate profiles (e) Allosteric Regulations	13-14
8	Revision	15-16
9	**Mid Semester Exam**	17-18
10-12	Enzymes in Humans Different kinds of enzymes in humans and their function (examples and explanation of six main categories of enzymes; oxidoreductases, transferases, hydrolases, lyases, isomerases, and ligases	19-24
13	Chemical Reaction Investigations in Enzyme Catalysis Reaction Mechanisms revealed by QM/MM investigations (a) Biomolecular Motors (b) RAS-GAP Signaling protein	25-26
14	(c) EcoRV enzyme (d) Lactate and Maltate Dehydrogenases (e) Acetylcholinestrase	27-28
15	(e) Carbonic Anhydrase (f) Ni-Fe Hydrogeanse (g) HIV Protease	29-30
16	Challenges in Enzyme Modeling	31-32
17	Presentations + Revision + Problem Solving Assignment-1: Paper Submission	33-34
18	**End Term** ☺	35-36

Details of lab work/workshop practice, if applicable:

Lab sessions will mainly focus on the hands-on training in connection with the lectures taught in class. Details are mention in the week wise breakdown.

Recommended reading, including textbooks, reference books with dates

6. Robert A. Copeland, “Enzymes: A Practical Introduction to Structure, Mechanism, and Data Analysis”, Wiley; 3rd edition, **2023**

7. N.S. Punekar, “ENZYMES: Catalysis, Kinetics and Mechanisms”, Springer; 1st ed. **2018**

8. Lodola, A., Mulholland, A.J., “Computational Enzymology. In: Monticelli, L., Salonen, E. (eds) Biomolecular Simulations. Methods in Molecular Biology”, vol 924. Humana Press, Totowa. **2013**

9. T. Devasena, “Enzymology”, Oxford University Press; 1st edition, **2012**

10. Frey PA, Hegeman AD: Enzyme Reaction Mechanisms, Oxford University Press, **2007**.

11. Buchholz K, Bornscheuer UT: *Biocatalysts and Enzyme Technology*,Wiley-Blackwell, **2012.**

12. "Encyclopedia of Computational Chemistry", 5th volume, John Wiley and Sons, Inc. 1998.

13. Relevant publications

Nature of Assessments

Homework/ Assignments:	5%
Quizzes:	5%
MSE:	30%
Final Exam:	40%
Project:	20%