SCHEME AND SYLLABUS OF

CERTIFICATE COURSE

IN

MOLECULAR MODELING AND DRUG DESIGNING
(w.e.f. academic session 2022-23)

Department of Microbiology and Bioinformatics

Atal Bihari Vajpayee Vishwavidyalaya

Bilaspur (C.G.)

(A State University, Established by the Government of Chhattisgarh)

1. **About the Department**

Department of Microbiology and Bioinformatics was established in Atal Bihari Vajpayee Vishwavidyalaya (formerly Bilaspur University), in the year 2013, with the objective of imparting quality education in the field of Microbiology and Bioinformatics. The Department has always produced quality professionals, holding important positions in Microbiology and Bioinformatics industry in Chhattisgarh, India and abroad. The Department has excellent infrastructure with well-equipped laboratories for conducting teaching, learning and research in the areas of Microbiology, Bioinformatics, Biotechnology, Botany and relevant disciplines. The Department has well qualified and experienced faculty members, who were always engaged with teaching and research. The staff holds funding from various government organizations and has published good number of books and research publications in reputed journals.

2. **About the Course**

The certificate programme in Molecular Modeling and Drug Designing is recognized qualification provides better understanding on biological concept, applications and analysis of big data from available biological databases. Those completing the course are awarded a CERTIFICATE and will be able to apply this knowledge for solving problems and making decisions associated with the technical and practical applications in *in silico* methods.

3. Scope

Molecular Modeling and Drug Designing has a wide scope and opportunities all around the world. Most of the biological data is available in several databases and better understanding of the unknown and complex bigdata is quite complicated by manual methods. The certificate course provides job-oriented knowledge and applications in scientific methods which caters the need of society. Bioinformatics has wide scope in education, software industries, pharmaceuticals, medical, marketing and several platforms in research.

4. Outcome of the Course

- To impart comprehensive overview of the scientific and technical aspects of Molecular modeling and Drug Designing.
- To workout in databases, sequence analysis and drug designing
- To demonstrate several packages and software's available in Molecular Modeling and Drug Designing.
- Understand the structural organization and of drugable targets.
- Learn the drug discovery process and role of computational techniques.
- Develop programming skills for analyzing the bioinformatics and chemo-informatics data.

5. Eligibility Criteria

All those who have completed their Senior School Certificate Examination (Class XII) with Mathematics/Biology.

6. **Fees Structure**

One time registration/tuition fees of Rs. 3000/-

7. Intake Capacity – 15 seats

8. Course Duration – 6 months/ 24 weeks.

9. Attendance
Minimum attendance of 75 % is required in the classes for appearing in the examination.

10. Examination Scheme

S. No.	Papers	Maximum Marks	Minimum Marks	Credits
1.	Paper I- Theory (Molecular Modeling and Drug Designing)	100	40	4
2.	Paper II- Practical (Molecular Modeling and Drug Designing Lab)	100	40	2
Total		200	80	6

11. Syllabus

Theory

Title: Molecular modeling and drug designing

Module 1: Protein: Structure of protein; Hierarchical organization of protein structure – primary, secondary, tertiary and quaternary structure.

Module 2: Ramachandran map. Introduction to enzymes as drug targets; enzymatic activity and its inhibition (Case study of COX-1, HIV-protease and AChE).

Module 3: Transcription factors as drug target, membrane proteins as drug targets.

Module 4: DNA: Structure of DNA, types of base pairing – Watson-Crick and Hoogstein; Structural properties of A-, B- and Z- DNA.

Module 5: DNA as drug target (Case study of Cis-platin).

Module 6: Targeting Bimolecular Interactions: protein – protein interactions and DNA – protein interactions.

Module 7: Introduction to receptors; Drug – receptor interaction; Forces involved in drug receptor interaction.

Module 8: Drug discovery and design: Structure based drug discovery process. Methods and Tools in Computer-aided drug design.

Module 9: Modeling drug - target interaction; molecular docking, and virtual screening.

Module 10: Principles of Pharmacokinetics and Pharmacodynamics: ADME, Bioavailability of drugs - Lipinski's rule; Concept of Pharmacophore and QSAR.

Module 11: Lead Optimization; functional group replacements: isosteres and bioisosteres.

Module 12: Molecular modelling for drug discovery: Molecular mechanics: energy of a molecule under stretch, bend, torsional strain, van der Waals and dipole-dipole interactions.

Module 13: Molecular dynamics simulations: introduction to Newtonian dynamics, Leapfrog Integrations. Implicit and explicit Solvation models, Periodic boundary conditions, Temperature and pressure control in molecular dynamics simulations.

Laboratory

Title: Molecular modeling and drug designing lab

1. Molecular visualization tool (applications such as molecular interaction, Molecular surface visualization, electrostatics, H-bond calculation etc. with PyMol) and Visualization of structural motifs.
2. Analysis of PDB (NMR and X – ray) structures (Quality of structure, analyzing molecular interactions, protein – ligand/ protein – protein if any, from PDB).
3. Homology based protein structure prediction.
4. Quality estimation of modeled protein structure (ProCheck, PROSA, Verify3D, Errat and MolProbity).
5. Contact map based protein structure comparison.
6. Energy minimization based mutational analysis of proteins.
7. Protein – Ligand docking using iGEMDOCK and MGLTools and Pharmacophore analysis.
8. Design of ligands and find QSAR properties

Suggested Books

1. Berg J.M., Tymoczoko J.L. & Stryer, L. (2006) Biochemistry (6th Ed.); W.H. Freeman and Co New York.
2. Leach A.R. (2001) Molecular Modeling: Principles and Applications (2nd Ed.). Prentice Hall, USA.
3. Gervasio F. L. & Spiwok V. (Ed.) (2019) Biomolecular Simulations in Structure-Based Drug Discovery. Wiley-VCH Verlag GmbH & Co.
4. Riccardo, B. (Ed) (2012) Computational Drug Discovery and Design Humana Press.

Online resources

https://www.britannica.com
https://encyclopedia2.thefreedictionary.com
http://www.free-ebooks.net/
https://www.scribd.com
https://www.wikipedia.org/

BUDGET PLAN FOR THE CERTIFICATE COURSE

S.No.	Income /course	Amount (in Rupees)
a)	Intake- 15 candidates with course fee 3000 rupees	45,000/-
S.No.	Expenditure Detail	Amount (in Rupees)
1.	Instruments and tools (one time)	0 (Established)
2.	Contingencies	8,000/-
3.	Stationary and printing	10,000/-
4.	TA and Conveyance	--
5.	Teaching (300 per class - 40 classes)	12,000
6.	Total	30,000

Year wise plan

S.No.	Expenditure Detail	Amount (in Rupees)
1.	For first year	30,000/-
2.	From second year (Contingencies and Teaching)	20,000/-