BANASTHALI VIDYAPITH

Certificate/Diploma Course

Curriculum Structure

1. Certificate Course in Molecular Modelling and Drug Design – 2020
2. Diploma in Computational Biology – 2020

BANASTHALI VIDYAPITH
P.O. BANASTHALI VIDYAPITH
(Rajasthan)-304022

July, 2019

159

No. F. 9-6/81-U.3

Government of India
Ministry of Education and Culture
(Department of Education)

New Delhi, the 25th October, 1983

NOTIFICATION

In exercise of the powers conferred by section 3 of the University Grants Commission Act, 1956 (3 of 1956) the Central Government, on the advice of the Commission, hereby declare that Banasthali Vidyapith, P. O. Banasthali Vidyapith, (Rajasthan) shall be deemed to be a University for the purpose of the aforesaid Act.

Sd/
(M. R. Kolhatkar)
Joint Secretary to the Government of India

NOTICE

Changes in Bye-laws/Syllabi and Books may from time to time be made by amendment or remaking, and a Candidate shall, except in so far as the Vidyapith determines otherwise, comply with any change that applies to years she has not completed at the time of change.

Departmenrt of Bioscience and Biotechnology
Part-Time Courses

S.N.	Course Title	Duration	Total Hours	Minimum Eligibility
	One Semester Course -			
1.	Certificate Course in Molecular Modelling and Drug Design	I Semester (T–4, P–4)	Theory – 60 Practical – 30	M.Sc./ (Bioscience/ Biotechnology/ AMBT/Computer Science), M. Pharm. and M. Tech. (Biotechnology)
	Two Semester Course –			
1.	Diploma in Computational Biology	I Semester (T–4, P–4)	Theory – 60 Practical – 30	M.Sc. (Bioscience/ Biotechnology/ AMBT/Computer Science). M. Pharm. M. Tech. (Biotechnology)
		II Semester (T–3, P–4, Proj–2)	Theory – 45 Practical – 30 Project – 15	

1. Passing grade is 40% separately in written examination & practical examination and 50% in aggregate.

2. It will be necessary for a candidate to pass in theory part as well as in the practical part separately.

3. Successful candidates should be classified as follows:-

(i) 75% marks or above Distinction

(ii) 60% marks or above First Division

(iii) 50% marks or above Second Division

Scheme of Examination for Certificate/Diploma Courses
Scheme of Examination

	Exam Dura-tion	Contact Hour/ Week			Cont. Ass. Marks			Ann. Ass. Marks			Total Marks			Min. Pass. Marks		
One Semester Course		**T**	**P**	**Proj.**	**T**	**P**	**Proj.**	**T**	**P**	**Proj.**	**T**	**P**	**Proj.**	**T**	**P**	**Proj.**
Certificate Course in Molecular Modelling and Drug Design	3 Hours	4	4	0	20	10	0	40	20	0	60	30	0	24	12	0

Two Semester Course		Exam Dura-tion	Contact Hour/ Week			Cont. Ass. Marks			Ann. Ass. Marks			Total Marks			Min. Pass. Marks		
Diploma in Computational Biology	I Sem.	3 Hours	4	4	0	20	10	0	40	20	0	60	30	0	24	12	0
	II Sem.	3 Hours	3	4	2	15	10	5	30	20	10	45	30	15	18	12	6

Certificate Course in Molecular Modelling and Drug Design

Preamble: The Certificate Course in Molecular Modelling and Drug Designing has been structured to provide theoretical and practical knowledge of computational methods used in biomolecular studies and the drug discovery programs to the students with background in biology, chemistry and pharmaceutical sciences. Further, this course also include basic flavor of computer programming in order to enable the students to solve complex biological problems computationally. Theoretical introduction to drugable targets and biomolecular structures helps in understanding the complexities in drug discovery process. The hands on experiences with software and programming further augment the skills to take on the challenges of drug discovery. The trained students will be benefitted in placement interviews of pharmaceutical industries as well as in research program of nationwide institution.

Theory

Learning Outcome:

Upon successful completion of the course, students should be able to:

- 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 chemoinformatics data.

Syllabus

Section – A

- Protein: Structure of protein; Hierarchical organization of protein structure – primary, secondary, tertiary and quaternary structure.
- Ramachandran map. Introduction to enzymes as drug targets; enzymatic activity and its inhibition (Case study of COX-1, HIV-protease and AChE).
- Transcription factors as drug target, membrane proteins as drug targets.
- DNA: Structure of DNA, types of base pairing – Watson-Crick and Hoogstein; Structural properties of A-, B- and Z- DNA.

- DNA as drug target (Case study of Cis-platin).
- Targeting Biomolecular Interactions: protein – protein interactions and DNA – protein interactions.
- Introduction to receptors; Drug – receptor interaction; Forces involved in drug receptor interaction.

Section – B

- Drug discovery and design: Structure based drug discovery process. Methods and Tools in Computer-aided drug design.
- Modeling drug - target interaction; molecular docking, and virtual screening.
- Principles of Pharmacokinetics and Pharmacodynamics: ADME, Bioavailability of drugs - Lipinski's rule; Concept of Pharmacophore and QSAR.
- Lead Optimization**;** functional group replacements: isosteres and bioisosteres.
- Molecular modelling for drug discovery: Molecular mechanics: energy of a molecule under stretch, bend, torsional strain, van der Waals and dipole-dipole interactions.
- 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.

Section – C

- Perl Programming: Data types: Scalar, Array and Hash Variables: their representation, applications and manipulations.
- Perl Regular Expression: concepts and applications in biological data handling, Pattern-matching, Substitutions, Transliteration, split and join functions.
- Concept on File handling, Opening, Closing and editing a File, Opening, Reading and Closing a Directory
- Perl Subroutines: Advantage of Subroutines, Scoping and Subroutines, Arguments, Passing Data to Subroutines, Modules and Libraries of Subroutines. Introduction to Bioperl.

Suggested Books:

- Berg J.M., Tymoczoko J.L. & Stryer, L. (2006) *Biochemistry* (6th Ed.); W.H. Freeman and Co New York.
- Leach A.R. (2001) *Molecular Modeling: Principles and Applications* (2nd Ed.). Prentice Hall, USA.
- Gervasio F. L. & Spiwok V. (Ed.) (2019) *Biomolecular Simulations in Structure-Based Drug Discovery*. Wiley-VCH Verlag GmbH & Co.
- Riccardo, B. (Ed) (2012) *Computational Drug Discovery and Design* Humana Press.
- Wall L., Christiansen T. & Orwant J. (2007) *Programming Perl* (3rd Ed). O'Reilly.

Laboratory

Learning Outcome:

Upon successful completion of the course, students should be able to:

- Write Perl programs to analyze and interpret biological data.
- Model and analyze 3D structure of drug targets.
- Handle software for drug designing and virtual screening.

Syllabus

Drug Designing Exercises

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 Autodock and MGLTools and Pharmacophore analysis.

Perl Exercises

1. Use of various arithmetic and logical operators.
2. Programming based on string manipulation (concatenation, splitting etc.).
3. Regular expression and its applications, use of s/// and tr/// operators.
4. Pattern matching to locate and count motifs in a string.
5. Calculating nucleotide frequency and GC content. Hydropathy index calculation of proteins.
6. Constructing arrays, addition and removal of elements from array, exploring array.
7. Use hashes in conversion of three letter code to one letter code and protein translation.
8. Perl subroutines, generating random DNA and its comparison with real DNA.
9. File handling, reading data from a file writing data to a file and editing a file.
10. Directory handling, make a directory, change current working directory, reading files from a directory.

Diploma in Computational Biology

Aim and Scope: This course is designed to train the students, without any formal training of bioinformatics, in the field of computational biology. The course aims to introduce the major's disciplines of computational biology. The trained students will be benefitted in placement interviews of pharmaceutical industries as well as in research program of nationwide institution. This course will enable the student to appear in Bioinformatics National Certificate Exams conducted by DBT every year.

I Semester

Theory: Molecular Modelling and Drug Designing

Learning Outcome

Upon successful completion of the course, students should be able to:

- 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 chemoinformatics data.

Syllabus

Section – A

- Protein: Structure of protein; Hierarchical organization of protein structure – primary, secondary, tertiary and quaternary structure.
- Ramachandran map. Introduction to enzymes as drug targets; enzymatic activity and its inhibition (Case study of COX-1, HIV-protease and AChE).
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- DNA: Structure of DNA, types of base pairing – Watson-Crick and Hoogstein; Structural properties of A-, B- and Z- DNA.
- DNA as drug target (Case study of Cis-platin).
- Targeting Biomolecular Interactions: protein – protein interactions and DNA – protein interactions.
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- Drug discovery and design: Structure based drug discovery process. Methods and Tools in Computer-aided drug design.
- Modeling drug - target interaction; molecular docking, and virtual screening.
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- Lead Optimization**;** functional group replacements: isosteres and bioisosteres.
- Molecular modelling for drug discovery: Molecular mechanics: energy of a molecule under stretch, bend, torsional strain, van der Waals and dipole-dipole interactions.
- 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.

Section – C

- Perl Programming: Data types: Scalar, Array and Hash Variables: their representation, applications and manipulations.
- Perl Regular Expression: concepts and applications in biological data handling, Pattern-matching, Substitutions, Transliteration, split and join functions.
- Concept on File handling, Opening, Closing and editing a File, Opening, Reading and Closing a Directory
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Laboratory - I

Learning Outcome:

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- Handle software for drug designing and virtual screening.

Syllabus

Drug Designing Exercises

1. Molecular visualization tool (applications such as molecular interaction, Molecular surface visualization, electrostatics, H-bond calculation etc. with PyMol) and Visualization of structural motifs.
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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.
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Perl Exercises

1. Use of various arithmetic and logical operators.
2. Programming based on string manipulation (concatenation, splitting etc.).

3. Regular expression and its applications, use of s/// and tr/// operators.
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5. Calculating nucleotide frequency and GC content. Hydropathy index calculation of proteins.
6. Constructing arrays, addition and removal of elements from array, exploring array.
7. Use hashes in conversion of three letter code to one letter code and protein translation.
8. Perl subroutines, generating random DNA and its comparison with real DNA.
9. File handling, reading data from a file writing data to a file and editing a file.
10. Directory handling, make a directory, change current working directory, reading files from a directory.

II – Semester

Theory: Computational Biology

Learning Outcomes: After successful completion of the course students should be able to:

- Solve problems of sequencing projects by applying the computational tools and understand the molecular evolution process.
- Analyze the biological networks to identify potential node for various application in molecular biology

Syllabus

Section – A

- Sequence Analysis – Concepts of sequence comparison, identity and homology, definitions of homologues, orthologues, paralogues and xenologues. Scoring matrices: concept and applications of PAM.
- Algorithms: Needleman and Wunsch, Smith and Waterman algorithms for pairwise alignments and application.
- Concept and application of multiple sequence alignments.
- Database searchin: introduction to BLAST.

Section – B

- Molecular Evolution – Gene Phylogeny versus Species Phylogeny, Forms of Tree Representation.
- Phylogenetic Tree Construction Methods and Programs: Distance-Based Methods, Character-Based Methods.
- MatLab: Introduction to MatLab environment, vector and matrices, expression, subscripts and manipulating matrices.
- Programming with MatLab: Flow control, script and function files.
- Graphics: Plotting (2D and 3D) graphs.
- Introduction to Bioinformatics toolbox.

Section – C

- Biological Networks - Basic properties of Network: Degree, average degree and degree distribution.
- Network Models- Erdos-Renyi model, Small-world effect, clustering coefficient. Scale-free networks, Power laws, The Barabasi-Albert Model.

- Biological networks, Intra-cellular networks: Gene-regulatory network, Protein-interaction network, Metabolic networks and Signaling network

Suggested Books:

- Bromham L. (2016) *An Introduction to Molecular Evolution and Phylogenetics.* Oxford University Press.
- Newman M.E.J. (2010) *Networks: An Introduction*, Oxford University Press.
- Selzer P. M., Marhöfer R. J. & Koch O. (2018) *Applied Bioinformatics: An Introduction* (2nd Ed.). Springer International Publishing AG.
- Gilat A. (2016) MATLAB: *An introduction with application* (6th Ed.). John-Wiley Publication.

Laboratory - II

Learning Outcome:

Upon successful completion of the course, students should be able to:

- Perform sequence and phylogenetic analysis.
- Analyse data using MATLAB.

Syllabus

Computational Biology Exercises

1. Pair wise sequence alignment (both global and local sequence alignments).
2. Blast tools.
3. Multiple sequence alignment.
4. Molecular Phylogeny (Phylogenetic tree reconstruction).
5. Prediction of coding region in given nucleotide sequence (GenemarkS).
6. Demonstration and analysis of Biological networks (Protein – Protein Interaction and Metabolic).

MatLab Exercises

1. Introduction to MatLab working environment.
2. Working with matrices
3. Writing biology oriented simple programs.
4. Matlab Graphics (Plotting 2D and 3D Graphs).
5. Introduction to Bioinformatics Toolbox.
6. Data analysis and Statistics with Matla