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# Sant Gadge Baba Amravati

## University Amravati

# M.Sc.

# **Bioinformatics**

## Programme

# **Objective:**

- 1. The program aims to utilize and understand biological databases to gather, store, retrieve, manage, analyze and integrate biological data for generating new knowledge.
- 2. The program aims to impart extensive understanding and learning of theoretical concepts in Life Sciences.
- 3. Each semester includes at least one core course in life sciences along with computational biology in each semester.
- 4. Basic practical methodology is incorporated as practical sessions in Laboratory courses in each semester.
- 5. Developing and implementing computational logic, learning programming languages, algorithms and software for progressive life science solutions.
- 6. Better understanding of dynamic biological processes and their understanding at molecular level enabled through and correlated using internet and Bioinformatics.
- 7. To develop skilled bioinformatics professionals who have life science background and who are simultaneously proficient in pharmacogenomics, Drug delivery System and Parasitology.
- 8. To introduce new age concepts of big data in the 'omics' era and their analysis.

# Programme Specific Outcomes (PSO):

- 1. Students undertaking the course shall have fundamental knowledge in theoretical Biochemistry, Cell Biology, Molecular Biology, genomic, computational biology and Genetics.
- 2. They will possess basic biochemistry and computational biology practical skills and its application in research and industry.
- 3. Students undertaking the course shall have fundamental knowledge in theoretical Cell Biology, Biochemistry, Mathematics, Statistics, Parasitology and database management, possess basic practical skills in these fields and its application in research and industry.
- 4. Students will learn on various aspects in Biotechnology and have hands on skills in Molecular Techniques.
- 5. Students will learn basic mathematical and statistical concepts and learn to apply them in aiding life science research and analysis.
- 6. As beginners the students will learn to use a computer, internet, scope and applications of bioinformatics.
- 7. Students will later learn to use the vast array of biological databases and their resources. Knowledge in life sciences would be the key and tools, methodologies and softwares used in bioinformatics will give them a comprehensive edge in data analysis.

- 8. Differential skills on basis of bioinformatics and computational biology proficiency would be later validated through academic supervision and systematically guided according to their skill.
- 9. Students as a part of curriculum will learn many programming languages from basic C, HTML etc. to PERL, PYTHON, R Programming, etc.
- 10. Students will be able to use free software, operating systems, work in command line environments and extensively work in databases, their creation and management. This will be ideal for job opportunities for them in IT enabled services as well.
- 11. Drug discovery strategies from life science point of view and the concerted computational approach are learned, evaluated and practiced through experimental sessions and thoroughly learned.
- 12. Students learn Genomics and Proteomics as primary subjects in their quest for biological repositories of information where in they will find their data which they will later analyze using next generation techniques for prediction of function and annotation.
- 13. Students also learn basics of data mining, machine learning, and artificial neural networks as a part of curriculum in bioinformatics which can be considered as a stepping stone in comprehending industry demands and hype surrounding big data analysis.

# **Employability Skills:**

After completion of Programme in Bioinformatics the student/s would be placed in

- 1. Post-Doctoral fellow.
- 2. Data Scientist
- 3. Drug delivery system analyst
- 4. Pharmacogenomics industry
- 5. As a Computational Biologist.
- 6. Biotechnology industry as a biomolecular engineer
- 7. Senior Software Engineer
- 8. Bioinformatics Engineer
- 9. Bioinformatics Analyst
- 10. Parasitic informatician
- 11. As an academician
- 12. As a computer programmer.
- 13. As expert in genomics and proteomics industries.
- 14. As a primer designer.

## Scheme of Teaching, Learning & Examination leading to the Degree in Master of Science in the Programme Bioinformatics (Two year- Four Semester Degree Programme- C.B.C.S.) (M.Sc. Part II) Semester III

S.	Subject	Subject	Teaching & Learning Scheme			Duration	Examination & Evaluation Scheme										
No.		Code	Те	<b>Teaching Periods Per</b>		Credits		of Exam	The	ory	Pra	ctical	Total	Mini	mum		
					Week					Hours					Marks	Pas	sing
			L	Т	Р	Total	L/T	Practical	Total		Theory+	Theory	Internal	External		Marks	Grade
											MCQ	Internal					
											External						
1	DSC-VII Proteomics		3	-	-	3	3	-	3	3	80	20	-	-	100	40	Р
2	AEC- III Wet lab techniques		-	1	-	1	1	-	1	1	-	-	25	-	25	40	Р
3	DSC-VIII System Biology		4	-	-	4	4	-	4	3	80	20	-	-	100	40	Р
4	DSC –IX Bio-programming I		4	-	-	4	4	-	4	3	80	20	-	-	100	40	Р
5	DSC- X Parasite Bioinformatics		4	-	-	4	4	-	4	3	80	20	-	-	100	40	Р
6	Lab- 5Practical Based on DSC VII&VIII		-	-	6	6	-	3	3	*	-	-	-	100	100	50	P
7	Lab- 6 Practical Based on DSC IX& DSC-		-	-	6	6	-	3	3	*	-	-	-	100	100	50	Р
	X																
8	# Internship/ Field Work/ Work Experience																
	@																1
9	Open elective/ GIC/ Open skill/ MOOC*																
	Total					28			22						625		

# L: Lecture, T: Tutorial, P: Practical

# Student may complete their Internship/ Field Work/ Work experience in First or Second or Third semester of Master of Science in the Programme, according to their convenience; @ denotes Non-Examination credits.

Note: Internship/ Apprenticeship/ Field Work Experience (during vacations of semester I to III. This will carry 2 credits for learning of 60 hours or 3 Credits for learning of 90 hours. Its credits and grades will be reflected in final semester IV credit grade report.

-OEC (Optional) can be studied during semester I to IV

Part B								
Syllabus Prescrib	ed for 2022 Year	PG. Programme						
Programme		<b>M.Sc. Bioinformatics</b>						
Semester III								
Code of the Cour	se Subject Title of the Course/ Subject	No. of periods/						
week								
DSC VII	Proteomics	03						
Cos: This course which play deals with biological area, the e application first hand s	<b>Cos :</b> This course will introduce the concepts of Proteomics – its principles and techniques which play a significant role in modern systems biology and related areas. Proteomics deals with the qualitative and quantitative analysis of the proteins that express in a biological system. This course introduces the basics of evolution of proteomics as an area, the experimental aspects of tools and techniques in addressing systems level applications. As a result of this course, the students will have strong foundations and							
Unit-I : (Introduction to Proteomics)	Introduction to Proteomics: Scope and Ap problem: Post translational modification, I studying proteins, protein-protein inte application of proteomics and current r databases.	pplication, Complexity of the Phosphorylation, Methods of eractions (Y2H), Practical research technology, Protein						
Unit-II : (The Proteome and Proteome technology)	Introduction of proteome technologies; Ex profile); Protein separation technology - 21 chromotagraphy, use of affinity chromato NMR, mass spectroscopy and its uses in pr and Reverse Proteomics. Protein microarra	pression proteomics (express D-Gel Electrophoresis, liquid graphy in; X-ray diffraction, rotein identification; Forward y and it types.						
Unit-III : (Computational Protein Structure Prediction)	Secondary structure: Basic principles on v of first, second and third generation are Fasman, GOR methods; concepts in r predictions (Q3, Segment overlap, Mathew Tertiary Structure: Theoretical basis of prediction, choice of appropriate prediction and protocol of Homology Modeling; I principles for fold recognition, threading an ab-initio structure prediction and the b Validation methods	which the prediction methods based; algorithms of Chou measuring the accuracy of 's correlation coefficient etc.) ' the methods for structure on approach; basic principles Databases of models; Basic pproaches, basic principles of proad approaches, Structure						
Unit-IV : (Comparative Proteomics)	Protein structure comparison and classi concepts in 3D structure comparison, purp algorithms such as FSSP database, VAST structures using Rasmol or SPDBViewer of molecular modeling, different types of molecules, Concepts of force fields: represe interactions, Protein Sequence alignment Proteomics	fication: classes, folds; the pose of structure comparison, and DALI. Visualization of or CHIME, Basic concepts in computer representations of entations of atoms and atomic and it tools, Genomics and						

Unit-V :	Molecular force field model, molecular dynamics, MD simulation,								
(Advance	gromacs software, hydrogen bonds, Protein structure minimization,								
Proteomics)	Protein structure comparison and its algorithms.								
Suggested Reading:									
2. Azuaje F., Dopazo J., (2005) "Data analysis and visualization in genomics and									
proteomic	proteomics" John Wiley and Sons								
3. Dubitzky W. Granzow M. Berrar D (2007) "Fundamentals of data mining in genomics and proteomics"									
4. Gu Jenny,	Bourne P. (2009) "Structural bioinformatics" Wiley- Blackwell								
5. Kraj A, Si John Wile	lberring J, (2008) "Proteomics: introduction to methods and applications" v & Sons								
6. Liebler D.	C. (2002), "Introduction to proteomics: tools for the new biology"								
Humana P	ress								
7. Mishra N. John Wile	C., (2010), "Introduction to Proteomics: Principles and Applications" y and Sons								
8. Penningtor function"	n S.R., Dunn M. J. (2001), "Proteomics: from protein sequence to BIOS								
9. Reinders J, Sickmann A., (2009) "Proteomics: methods and protocols" Hum Press									
10. Suhai S. (2	2000) "Genomics and proteomics: functional and computational aspects"								
Springer									
11. Veetstra T and Sons	.D., Yates J.R. (2006) "Proteomics for biological discovery" John Wiley								
12. Polanski A	A., Kimmel M. (2007) "Bioinformatics" Springer Verlag Berlin Heibel								
berg									
Learning	Outcome								
After successfully completing this course, you will have the following competences:									
1. Practical and theoretical knowledge in proteomics.									
2. Knowledg	e about common workflows for the large-scale analysis of proteins.								
3. Fundamen	tal knowledge about quantification of proteomes.								
4. Understan	ding how to identify proteins from mass spectrometry data.								
5. Able to ev	aluate MS/MS data including de novo sequencing.								
6. Insight interaction	o the analysis of post-translational modifications and protein-protein as.								
<ol> <li>On-hands experience with in-gel digestions, LC-ESI and MALDI mass spectrometry and protein identification.</li> </ol>									

Part B							
Syllabus Prescril	oed for 2022 Y	PG. Programme					
Programme			M.Sc. Bioinformatics				
Semester III							
Code of the Cou	se Subject	Title of the Course/ Subject	No. of periods/				
week							
AEC III		Wet lab techniques	03				
Cos: 10. To familiarize the student with emerging field of biotechnology i.e. Recombinant DNA Technology as well as to create understanding and expertise in wet lab techniques in genetic Engineering							
Unit I PCR or Polymerase Chain Reaction, Components, primer, types of PCR, PCR reactions. Purification and analysis of proteins, protein chemistry, chromatography, immunology and spectroscopic methods.							
Suggested Reading:							
11. Wilson K, Goulding KH. (2018) Principles and Techniques of Biochemistry and							
Molecular	Biology, Eig	ht Edition , Edited by Hofman	nn A, Clokie S. Cambridge				
University Press							

12. Plummer DT. (2017) An Introduction to Practical Biochemistry. 3rd Edition
McGraw Hill Education
13. Philips, R. Kondev J, Theriot J, Garcia H. (2012). Physical Biology of the Cell. 2nd
Edition Garland Science.
Learning Outcome:
After completion of this course the student will able to understand the techniques,
protocol and analytical tools required for the walk of Bioinformatics.

Part B		
Syllabus Prescribed for 2022	Year	PG. Programme
Programme		M.Sc. Bioinformatics
Semester III		
Code of the Course Subject	Title of the Course/ Subject	No. of periods/
week		
DSC VIII	System Biology	04
This course would be a focused on mammalia moving from molecula expression deepens and in cellular processes, w other to form modules t core subcellular proces electrical excitability. behaviors such as secre <b>Unit-I : (Introduction to</b>	ble to introduce the student to com an cells, their constituents and ar to modular. As our knowled, we develop lists of molecules (p we need to understand how these that act as discrete functional syst sses such as signal transduction In turn these processes come etion, proliferation and action pot System Biology – Introduc	ntemporary Systems Biology their functions. Biology is ge of our genome and gene roteins, lipids, ions) involved molecules interact with each tems. These systems underlie a, transcription, motility and together to exhibit cellular tentials.
System Biology)	analysis of biological networks Biology, System Biology app Organization of living cells, Systems Biology Markup Lang	; Need for system analysis in roaches, Dynamic Analysis, Components vs. Systems,. uage (SBML)
Unit-II : (System Kinetics)	Biochemical Reaction Kinetics elementary reactions, complex equation for EK, Stochastic M and Km values of enzyme, Enz	s – Rate equation approach, reaction, Michaelis-Menten odelling and Simulation, Ki yme assay and its types.
Unit-III : (Reconstruction of Biochemical Networks)	Metabolic network model simulation, Flux balance analy networks, Signaling Network reconstruction, KEGG, Reactor designer software.	ing, Metabolic network sis, Regulation of metabolic orks, Applications of a ome, Brenda databases; Cell

Unit IV : (Introduction to	Synthetic Biology - Introduction, Emergence of Synthetic						
Synthetic Biology)	biology, Tools in Synthetic biology. Genetic engineering,						
	Biosensors and its applications, Synthetic Life: Synthia; E-						
	cell and V-cell Simulations and Applications. ethical						
	concerns in the field of synthetic biology;						
Unit V : (Introduction to R	R programming – Introduction and preliminaries, Simple						
programming)	manipulation, Objects and Modules, Orders, Arrays, Lists,						
	Reading data from files, Loops and conditions, Functions						
	creation, Packages.						
	Suggested Reading:						
11. B. O. Palsson	"System Biology - Properties of Reconstructed Networks"						
Cambridge Un	iversity Press						
12. Olaf Wolkenha	uuer. (2010) "System Biology – Dynamic Pathway Modeling"						
13. Andres Kriete	, Roland Eils (2006) "Computational systems biology"						
Academic Pres	S						
14. Andrzej K. Ko	onopka (2007) "Systems biology: principles, methods, and						
concepts" CRC	2 Press/Taylor & Francis						
15. Lilia Alberghin	na (2008) "Systems biology: definitions and perspectives" 2						
Edition, Spring	er						
16. Uri Alon (200	7) "An introduction to systems biology: design principles of						
biological circu	uits" Chapman & Hall/CRC						
17. W. N. Venable	es, D. M. Smith; "An Introduction to R (Version 2.8.1.)", R						
developer Con	re team.Bergman N. H. (2007),"Comparative genomics"						
Volume 2, Hur	nana Press						
18. Cantor C.R., S	18. Cantor C.R., Smith C.L., (1993) "Genomics: the science and technology						
behind the Human Genome Project" John Wiley and Sons							
19. Choudhuri S	Carlson D. B. (2008), "Genomics: fundamentals and						
applications" I	nforma Healthcare						
20. Clark M (2000	), "Comparative genomics" Springer						
Learning Out	come:						
1. Describe the principles	s of systems biology						
2. Describe key cellular	processes like transcription, translation, signaling and protein						
secretion in a quantitat	ive fashion						
3. Use matrix notation to	describe the stoichiometry of metabolic networks						
4. Describe metabolic netabolic	etwork reconstruction based on biochemical and genomic						
information	_						
5. Describe how genome	-scale metabolic models (GEMs) can be used for analysis of						
cellular physiology							
6. Describe how constraints and objective functions are underlying principles of flur							
balance analysis							
7. Describe the use of genome-scale metabolic models in research on human disease							
8. Describe how meta-on	nics data can be analyzed						
9. Describe the principles	s of RNAseq						
10. Describe the principles							
	s of proteomics						

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Part B							
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Syllabus Prescribed for 2022 Y	ear P	PG. Programme					
Programme	Γ	M.Sc. Bioinformatics					
Semester III							
Code of the Course Subject	Title of the Course/ Subject	No. of periods/					
week							
DSC IX	Bio-Programming – I	04					
Cos :							
<ol> <li>Student would know about the properties of DNA, RNA, and proteins, the relationships amongthese molecules, and some biological questions that have puzzled researchers.</li> <li>Student would know how to convert a biological question into a computational problem that can besolved using computers.</li> <li>Student would know how to read and understand solutions to computational problems, which willbe formalized as a series of tasks (an algorithm).</li> <li>Student would learn about general approachesfor solving computational problems, and will be able to apply these approaches to newproblems encounter.</li> </ol>							
Unit-I : (Introduction to PERL)Introduction to PERL, History and uses, PERL Basics, types, Basic Operators, Control Statements: if, if else, if else, Loops: do, while, until, for, foreach, labels, l Arrays and associative arrays							
Unit-II : (Introduction to PERL)	Pattern matching: Regular ex functions: structure and invoc file handles, opening, closing, r manipulating files, Perl Module and installing, Object oriented	cpressions, Subroutines and ations, scope Files and I\O: reading and writing, formats, es: CPAN, Bioperl, obtaining PERL					
Unit-III : (Introduction to ODBC)DBM Databases and DBM Hashes, Design of DBI, D Methods, DBI Environment Variables, DBD Interf Modules, Fixed Length Random-Access Database Variable-Length Databases, Win32 Database Interface, F Graphics, Using the GD.pm graphics lib							
Unit-IV : (Introduction to HTML and CGI)Basics structure of HTML, Basics HTML TAGS, UF Encoding, CGI Environment Variables, Handling form Accessing form Input, Extra Path Information, CGI.p Module, Passing Parameters via CGI, Less Typing, Sev Side Includes, Debugging CGI programs, Stepping throu programs, Breakpoints, Line Action							
Unit-V: (HTML References Tags)HTML Tag List, HTML Attributes, Global Attribute Browser Support, Events, Colors, Canvas, Audio/Vide Doctypes, Character Sets, URL Encode, Lang Code Messages, Methods.							
	Suggested Reading:						
8. Arun Jagota (20	8. Arun Jagota (2004) "Perl for Bioinformatics" Arun Jagota						

	9. D. Curtis Jamison (2003) "Perl programming for biologists" Wiley- IEEE
	10. D. Curtis Jamison (2008) "Perl Programming For Bioinformatics &
	Biologists" Wiley-India
	11. James D. Tisdall (2003) "Mastering Perl for bioinformatics" O'Reilly
	Media, Inc
	12. Jules J Berman (2008) "Perl: The Programming Language" Jones & Bartlett
	Learning
	13. Randal L. Schwartz, Tom Phoenix, Brian D. Foy (2008) "Learning Perl"
	O'Reilly Media, Inc
	14. Vittal R. Srinivas (2005) "Bioinformatics: A Modern Approach" PHI
	Learning Pvt. Ltd
	Learning Outcome:
1.	Basic Applications of Computer; Components of ComputerSystem.
2.	Concept of Internet; WWW and Web Browsers; SearchEngines
3.	Data analysis by different computational techniques
4.	Concepts of computer programming languages like C, JAVAhelps in solving
	different complex problem in biology or dataanalysis
5.	Writing scripting for different data analysis

- 6. Command line scripting in DOS and LINUX
- 7. Writing script in R programming to solve biological problem.

Part B								
Syllabus Pres	Syllabus Prescribed for 2022 Year PG. Programme							
Programme	Ν	<b>M.Sc. Bioinformatics</b>						
Semester III								
Code of the C	ourse Subject Title of the Course/ Subject	No. of periods/						
week								
DSCX	Parasite Bioinformatics	04						
Cos:								
1. Genera	1. General concept of parasitology.							
2. Knowl andmar	2. Knowledge of some parasitic diseases that could be transmitted between animals andman (Zoonotic diseases).							
3. Knowl theirtre	3. Knowledge how to protect man and domestic animals from parasites and theirtreatment.							
4. Basic knowledge of parasitism, the different biological inter-relationships and the								
<ul> <li>hostparasite relationships.</li> <li>5. Knowledge of different parasitic examples from all phyla (Protozoa &amp; Metazoa) theirmorphology, biology, life cycles, diagnosis, treatment &amp; control.</li> </ul>								
6. Dissem	6. Dissemination of health awareness of these parasitic diseases.							

to Parasitic Diseases)distribution of strains (Malaria, Leishmaniasis, Trypanosoma, Filariasis), Role of bioinformatics in Diseases monitoring.Unit-II : (Introduction to Parasitic Diseases)Parasite Genome and Proteome Databases (AnoBase, ENSEMBL, PlasmoDB), Vectors of parasites – Biology of vectors; Giardiasis , Sleeping sickness, Chagas disease, Parasite-specific genes/ gene products (e.g. house-keeping genes, genes essential for survival), Resistant Genes.Unit-III : (Techniques to study Parasitic Diseases)Full Genome Comparison, Gene Prediction, Signal sequence prediction, Protein sequence comparison and analysis, Protein structure comparison and analysis, Micro Array and Proteomics Data Analysis, Structural genomics of parasites.Unit-IV : (Introduction to Host-parasite interaction)Host-parasite interaction: Recognition and entry processes of different pathogens like bacteria and viruses into animal and plant host cells; alteration of host cell behavior by pathogens, virus-induced cell transformation, pathogen- induced diseases in animals and plants; cell-cell fusion in both normal and abnormal cells.Unit-V : (Introduction to Host-parasite interaction)Host-Parasite and Host-Vector-Parasite Interactions, Pathway databases (KEGG, BioCyc, Pathguide, REACTOME), Multi-Drug Resistance - Mechanism of MDR: genomic, molecular, cellular, Identification of genes responsible for MDR, Approaches to novel drug discovery for parasite, Challenges and opportunities in vaccine development, Plant Parasites and diseases - Disease resistance genes of plants, Plant-pathogen interactions.						
Initial District DistrictsTrypanosoma, Filariasis), Role of bioinformatics in Diseases monitoring.Unit-II : (Introduction to Parasitic Diseases)Parasite Genome and Proteome Databases (AnoBase, ENSEMBL, PlasmoDB), Vectors of parasites – Biology of vectors; Giardiasis , Sleeping sickness, Chagas disease, Parasite-specific genes/ gene products (e.g. house-keeping genes, genes essential for survival), Resistant Genes.Unit-III : (Techniques to study Parasitic Diseases)Full Genome Comparison, Gene Prediction, Signal sequence prediction, Protein sequence comparison and analysis, Protein structure comparison and analysis, Micro Array and Proteomics Data Analysis, Structural genomics of parasites.Unit-IV : (Introduction to Host-parasite interaction)Host-parasite interaction: Recognition and entry processes of different pathogens, like bacteria and viruses into animal and plant host cells; alteration of host cell behavior by pathogens, virus-induced cell transformation, pathogen- induced diseases in animals and plants; cell-cell fusion in both normal and abnormal cells.Unit-V : (Introduction to Host-parasite interaction)Host-Parasite and Host-Vector-Parasite Interactions, Pathway databases (KEGG, BioCyc, Pathguide, REACTOME), Multi-Drug Resistance - Mechanism of MDR: genomic, molecular, cellular, Identification of genes responsible for MDR, Approaches to novel drug discovery for parasite, Challenges and opportunities in vaccine development, Plant Parasites and diseases - Disease resistance genes of plants, Plant-pathogen interactions.						
InspirationUnit-II : (Introduction to Parasitic Diseases)Parasite Genome and Proteome Databases (AnoBase, ENSEMBL, PlasmoDB), Vectors of parasites – Biology of vectors; Giardiasis , Sleeping sickness, Chagas disease, Parasite-specific genes/ gene products (e.g. house-keeping genes, genes essential for survival), Resistant Genes.Unit-III : (Techniques to study Parasitic Diseases)Unit-IV : (Introduction to Host-parasite interaction)Host-parasite interaction)Unit-V : (Introduction to Host-parasite interaction)Host-parasite interaction)Sugested Reading Host-parasite interactionKurgested Reading Reactrome, Reading Host-parasite interaction)Kurgested ReadingKurgested Reading: Reading: Reading:Kurgested Reading: Reading:Kurgested Reading: Kurgested Reading:Kurgested Reading:Kurgested Reading:						
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Parasitic Diseases)Finalistic Oction and and Notectors of parasites – Biology of vectors; Giardiasis , Sleeping sickness, Chagas disease, Parasite-specific genes/ gene products (e.g. house-keeping genes, genes essential for survival), Resistant Genes.Unit-III : (Techniques to study Parasitic Diseases)Full Genome Comparison, Gene Prediction, Signal sequence prediction, Protein sequence comparison and analysis, Protein structure comparison and analysis, Micro Array and Proteomics Data Analysis, Structural genomics of parasites.Unit-IV : (Introduction to Host-parasite interaction)Host-parasite interaction: Recognition and entry processes of different pathogens like bacteria and viruses into animal and plant host cells; alteration of host cell behavior by pathogens, virus-induced cell transformation, pathogen-induced diseases in animals and plants; cell-cell fusion in both normal and abnormal cells.Unit-V : (Introduction to Host-parasite interaction)Host-Parasite and Host-Vector-Parasite Interactions, Pathway databases (KEGG, BioCyc, Pathguide, REACTOME), Multi-Drug Resistance - Mechanism of MDR: genomic, molecular, cellular, Identification of genes responsible for MDR, Approaches to novel drug discovery for parasite, Challenges and opportunities in vaccine development, Plant Parasites and diseases - Disease resistance genes of plants, Plant-pathogen interactions.						
Tarastic Diseases)Enviring (in the production of parasites = Diology of vectors) (in parasite) (in the parasite intersection in the parasite interaction is equence comparison, Gene Prediction, Signal sequence prediction, Protein sequence comparison and analysis, Micro Array and Proteomics Data Analysis, Structural genomics of parasites.Unit-IV : (Introduction to Host-parasite interaction)Host-parasite interaction of host cell behavior by pathogens, virus-induced cell transformation, pathogen-induced diseases in animals and plants; cell-cell fusion in both normal and abnormal cells.Unit-V : (Introduction to Host-parasite interaction)Host-Parasite and Host-Vector-Parasite Interactions, Pathway databases (KEGG, BioCyc, Pathguide, REACTOME), Multi-Drug Resistance - Mechanism of MDR: genomic, molecular, cellular, Identification of genes responsible for MDR, Approaches to novel drug discovery for parasite, Challenges and opportunities in vaccine development, Plant Parasites and diseases - Disease resistance genes of plants, Plant-pathogen interactions.Suggested Reading:						
Vectors, Ghathasis , Steeping stokless, Chagas disease, Parasite-specific genes / gene products (e.g. house-keeping genes, genes essential for survival), Resistant Genes.Unit-III : (Techniques to study Parasitic Diseases)Full Genome Comparison, Gene Prediction, Signal sequence prediction, Protein sequence comparison and analysis, Protein structure comparison and analysis, Micro Array and Proteomics Data Analysis, Structural genomics of parasites.Unit-IV : (Introduction to Host-parasite interaction)Host-parasite interaction: Recognition and entry processes of different pathogens like bacteria and viruses into animal and plant host cells; alteration of host cell behavior by pathogens, virus-induced cell transformation, pathogen- induced diseases in animals and plants; cell-cell fusion in both normal and abnormal cells.Unit-V : (Introduction to Host-parasite interaction)Host-Parasite and Host-Vector-Parasite Interactions, Pathway databases (KEGG, BioCyc, Pathguide, REACTOME), Multi-Drug Resistance - Mechanism of MDR: genomic, molecular, cellular, Identification of genes responsible for MDR, Approaches to novel drug discovery for parasite, Challenges and opportunities in vaccine development, Plant Parasites and diseases - Disease resistance genes of plants, Plant-pathogen interactions.						
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development, Plant Parasites and diseases - Disease resistance genes of plants, Plant-pathogen interactions. Suggested Reading:						
resistance genes of plants, Plant-pathogen interactions.						
Suggested Reading:						
1. Bush, A. O., Fernandez, J. C., Esch, G.W. & Seed, R. J., "Parasitism", Cambridge						
University Press, 2001.						
2. Melville, S.E., "Parasite genomics protocols", New Jersey. Humana Press, 2004.						
3. Latey, A.N, Pune, "A modern textbook of Parasitology", Narendra prakashan,						
1991.						
4. Wyler, D.J. "Modern parasite biology: cellular immunological and molecular						
aspects", Ed., 1990.						
Learning Outcome:						
1. Identify parasitism, parasites and their examples.						
2. Describe parasitic diseases and modes of diagnosis.						
3. Trace control of parasitic infections.						

4. Understand host-parasite relationship.

## Sant Gadge Baba Amravati University, Amravati

Syllabus	Pres	cri	bed	for	2022	Year
Program	me:	М.	Sc.	Bio	inforı	natics

PG Programme

Semester 1 Code of the Course/Subject

**Title of the Course/Subject** (Laboratory/Practical/practicu m/hands-on/Activity) (No. of Periods/Week)

Practical V

#### Practical Based on DSC VII&VIII

06

## CO:

- 1. Fundamentals of Computer, Basic Applications of Computer; Components of Computer System.
- 2. Concept of Computing, Data and Information
- 3. Basics of Operating System; Popular Operating Systems(Windows, Linux, DOS);
- 4. Data structure and its relevance to biological science
- 5. Communication using the Internet: Basic of Computer networks; LAN, MAN, WAN;
- 6. Concept of Internet; WWW and Web Browsers; Search Engines; Understanding URL
- 7. Design & Structure of biological databases
- 8. Introduction to PERL as scripting language; variables; Array; Initialization and manipulation
- 9. Arithmetic and logical operators; Conditional statement and Loops; Regular Expressions; Function and subroutines
- 10. Application of PERL in Bioinformatics; concatenating DNA fragments; DNA to RNA; Reading protein Files; Finding motifs; ORFs; DNA to protein

## \* List of Practical/Laboratory Experiments/Activities etc.

1	Microbial Database
2	MLVA
3	HBMMD
4	DSMZ
5	RIDOM
6	GPMS

## **Proteomics**

1	Protein Sequence Databases
2	Protein Structure Databases
3	Protein Sequence Analysis by BioEdit
2	Advanced Visualization Software and 3D representations
6	Coordinate generations and inter-conversions
e	Secondary Structure Prediction
7	GORIV
8	Online Secondary structure prediction tools
9	Fold Recognition, ab initio (Rosetta Server)
10	Homology based comparative protein modeling
11	Energy minimizations
12	Validation of models
a.	WHATIF
b.	PROSA
с.	PROCHECK
d.	VERIFY 3D
e.	RAMPAGE
f.	Protein Structure Alignment
g.	Protein Structure Comparison
h.	Modeller9v7

i.	Geno-3D							
j.	Discovery Studio Server							
	Learning Outcome:							
	1. Bioinformatics – an Overview, Definition and							
	History.Information Networks –Internet inBioinformatics,							
	Evolution of Bioinformatics – Scope –Potentials of							
	Bioinformatics, Human Genome Project							
	2. Introduction to Biological Databases: NCBI, EMBL,							
	PIR,SWISS-Prot, PubChem							
	3. Compound, KEGG-Pathway, ChEMBL,							
	BindingDB.Analysis of Three Dimensional Structures of							
	Proteins, RCSB-PDB. Primary and Secondary database							
	4. Various file formats for bio-molecular sequences:							
	genbank,fasta, gcg, msf, nbrf-pir etc.							
	5. Basic concepts of sequence similarity, identity							
	andhomology, definitions of homologues,							
	orthologues, paralogues.							
	6. Scoring matrices: basic concept of a scoring matrix,							
	PAMand BLOSUM series							

### Sant Gadge Baba Amravati University, Amravati

Syllabus Prescribed for 2022 Programme: M. Sc. Bioinfor	Year PG P matics	PG Programme				
Semester 1 Code of the Course/Subject	<b>Title of the Course/Subject</b> (Laboratory/Practical/practicu m/hands-on/Activity)	(No. of Periods/Week)				
Practical VI	Practical based on DSC IX& DSC- X	06				

CO:

- 1. Identify parasitism, parasites and their examples
- 2. Describe parasitic diseases and modes of diagnosis. Trace control of parasitic infections.
- 3. Understand host-parasite relationship.

\* List of Practical/Laboratory Experiments/Activities etc.

1.	Exercise in Structured Programming: Basic Operators and Control Flow, Basic Perl Data Types,
	References, Matrices, Complex/Nested Data Structures, Scope (my, local, our),
	Function/Subroutines, System and User Function, The local Operator, Variable-length Parameter
	Lists, Notes on Lexical Variable, File handle and File Tests, stat and stat Functions, Formats,
	Directory Access & Manipulation, Process Management, Formatting Data, System Information
2.	Exercise in Regular Expressions: Uses of Regular Expressions, Patterns, Single-Character Patterns,
	Grouping Patterns (Sequence, Multipliers, Parentheses as memory, Alternation) Anchoring Patterns,
	Precedence, Matching Operators, Ignoring Case, Different Delimiter, Variable Interpolation, Special
	Read-Only Variables, Substitutions, Split and Join Functions, Dynamic Programming, Approximate
	String Matching
3.	Exercise in CGI: URL Encoding, CGI Environment Variables, Handling forms, Accessing form
	Input, Extra Path Information, CGI.pm Module, Passing Parameters via CGI, Less Typing, Sever
	Side Includes, Debugging CGI programs, Stepping through programs, Breakpoints, Line Action
4.	Exercise in CPAN Database Modules: DBM Databases and DBM Hashes, Design of DBI, DBI
	Methods, DBI Environment Variables, DBD Interface Modules, Fixed Length Random-Access
	Databases, Variable-Length Databases, Win32 Database Interface, Perl Graphics, Using the GD.pm
	graphics library

5.	Exercise in Bioperl: Installing Bioperl, General Bioperl Classes, Sequences (Bio::SeqClass,								
	Sequence Manipulation), features and Location Classes (Extracting CDS), Alignments (AlignIO),								
	Analysis (Blast, Genscan), Databases (Database Classes, Accessing a local database), Implementing								
	REBASE								
6.	Exercise in HTML: Basics structure of HTML, Formatting text with HTML, Adding local and								
	remote links, Adding graphics, creating lists in HTML, Creating tables in HTML, Frames, and								
	Forms.								
7.	Parasite Bioinformatics								
а	ICTV database								
b	Parasite Genome and Proteome Databases.								
8.	Genome Comparison								
9.	Gene Prediction (Parasite)								
10.	Signal sequence prediction (Parasite)								
11.	Protein sequence comparison and analysis								
12.	Protein structure comparison and analysis (from parasite genome)								
	Learning Outcome:								
	1. Right use of microscopes.								
	2. Identification and description of parasites.								
	3. Using computers and internet.								
	4. Characterize methods of resistance and appropriate treatment								
	5. or each disease.								
	6. Conducting documentary about some parasites throughout the Kingdom.								

Scheme of Teaching, Learning & Examination leading to the Degree in Master of Science in the Programme Bioinformatics

(Two year- Four Semester Degree Programme- C.B.C.S.) (M.Sc. Part II) Semester IV

S.	Subject	Subject	Teaching & Learning Scheme			Duration	Examination & Evaluation Scheme										
No.		Code	Teaching Periods Per		Credits		of Exam	Theory Practical		ctical	Total	tal Minimum					
				Week					Hours						Pas	sing	
			L	Т	Р	Total	L/T	Practical	Total		Theory+	Theory	Internal	External		Marks	Grade
											MCQ	Internal					
											External						
1	DSC-XI Bio-programming II		3	-	-	3	3	-	3	3	80	20	-	-	100	40	Р
2	AEC- IVR-programming		-	1	-	1	1	-	1	1	-	-	25	-	25	40	Р
3	DSC-XII Chemo-informatics		4	-	-	4	4	-	4	3	80	20	-	-	100	40	Р
4	DSC -XIII Molecular Modeling and Drug Designing		4	-	-	4	4	-	4	3	80	20	-	-	100	40	Р
5	DSC- XIV Research Methodology, IPR and Bioethics.		4	-	-	4	4	-	4	3	80	20	-	-	100	40	Р
6	SEC-II- Python		2	-	-	2	2	-	2	2					50	20	Р
7	Lab- 7Practical Based on DSC XI, XII,		-	-	6	6	-	3	3	*	-	-	-	100	100	50	Р
8	Lab & Practical Based on Project				6	6	_	3	3	*			_	100	100	50	р
0	# Internation/Field Work/Work Experience		-	-	0	U	-	5	5		_	-	-	100	100	50	1
7																	
10	Open elective/ GIC/ Open skill/ MOOC*	OEC-II	4	-	-	4	4	-	4	3	80	20	-	-	100	40	Р
	Pharmacogenomics																
	Total					30			24						675		

# L: Lecture, T: Tutorial, P: Practical

# Student may complete their Internship/ Field Work/ Work experience in First or Second or Third semester of Master of Science in the Programme, according to their convenience; @ denotes Non-Examination credits.

Note: Internship/ Apprenticeship/ Field Work Experience (during vacations of semester I to III. This will carry 2 credits for learning of 60 hours or 3 Credits for learning of 90 hours. Its credits and grades will be reflected in final semester IV credit grade report.

-OEC (Optional) can be studied during semester I to IV

Part B							
Syllabus Prescribed for 2022 YearPG. Programme							
Programme M.Sc. Bioinformatics							
Semester IV							
Code of the Cour	Code of the Course Subject Title of the Course/ Subject No. of periods/						
week		-					
DSC XI	Bio-programming II	03					
Cos	F88						
11. To facilitat 12. To enable 13. To interpol	e the students in gaining programming skills. the students to design and execute Java, $C++a$ ate biological demands through programming	and Perl scripts					
Unit I :	Basics of JAVA, History, an overview	of JAVA, Object Oriented					
(Introduction to Java)	Programming, Data types- Variables and Ar point types, Operators, Control statements, objects, Assigning object reference var Constructors, Garbage collection, using obj passing, Retaining objects, Recursion, Understanding static; Nested and inner class Using command line arguments.	rays, the simple types, floating Class fundamentals, Declaring iables, Introducing methods, jects as parameters, Argument Introducing Access control, sses, exploring the string class,					
Unit II :	Inheritance: Basics, Member access and in	heritance. Using super: to call					
(Introduction to	super class constructors, Creating a multile	vel hierarchy. The object class					
Java)	Packages and Interfaces: Packages, Defining path, Access protection: Importing pack Implementing interfaces, Applying interfa Exception Handling: Fundamentals, Exception Using try and catch, Displaying a description clauses, Nested statements, throw, throws Creating own exception subclasses, Using ex	a package, Understanding class ages, Defining an interface, aces, Variables in interfaces, on types, Uncaught exceptions, of an exception. Multiple catch s; Java's built in exceptions, aceptions					
Unit III : (Introduction to Unix & Linux)	Introduction to Unix & Linux, History of Un Operating Systems, Kernel, shell and file sy of Linux, Basic Commands of Linux, I Installation of Linux, Interactive Install Network based Installation, Startup an Sequence, Kernel Initialization	hix & Linux, Basic Concepts of stem structure, Basic Concepts Advanced Linux Commands, lation, Kickstart Installation, nd Shutdown scripts, Boot					
Unit IV :	The UNIX Filesystem and Shell Intro: The S	Shell - Executing commands					
(Introduction to	and command options, Interactive features: j	ob control, history; The UNIX					
Unix & Linux)	The system, File Utilities (cp, mv, rm, etc.), c	comm, cmp, diff, Editors: Vi,					
	Filters: cat head tail sort unio: Regular Ev.	es (ps, KIII, wait, sieep);					
	expressions, grep, fgrep, egrep, Sed	pressions and sea. Regular					
Unit V :	Installing Bio-Java, Symbols, Basic Sequence	e Manipulation (DNA to RNA,					
(Introduction to	Reverse Complement, motif as regular exp	ression), Translation (DNA to					
Bio-Java)	Protein, Codon to amino acid, Six frame tran	Islation), Proteomics (Calculate					
	the mass and pl of a peptide), Sequence I/	U (File Formats conversions),					
	modifications) BLAST and FASTA (Bla	n, Range Location, Feature					
	information from parsed results), User Interf	aces.					
Suggested Reading:							
14. Benjamin,	Cummings and Booch, G. (1994) "O	bject Oriented Design and					
Applications"; Second edition, Addison Wesley Publishers.							
15. Horstmann, C.S. (2000) "Computing Concepts with Java 2 Essentials"; Second Edition,							
John wiley	P and Schildt H (1999) "Java-2. The comple	ete Reference" <sup>.</sup> Third Edition					
McGraw H	(ill Publishers.	an Reference, finite Eutitoli,					
17. Bal H, Huj	ol J, (2007) "Java for bioinformatics and bion	nedical application" Springer					
<ol> <li>Lindsey C. S., Tolliver J.S., Lindblad T, (2005) "JavaTech: an introduction to scientific and technical computing with JAVA" Cambridge University Press</li> </ol>							

1. Learn the basics of programing         1. Learn the basics of programming in biology         2. Relate the necessity for programming in biology         3. Handling biological concepts with C++ and Perl scripts         4. Apply programing to analyze genomic sequences         5. Understand Bio-Perl and their application in bioinformatics to handle the complex data         Part B         Syllabus Prescribed for 2022 Year         Programme         Programme         Programme         Programme         Programme         Officity Programming of Course Subject         No. of periods/         week         AEC IV         Programming Col         Cos:         Understand the basics of Fundamentals of R.         Understand the loading, criterional to R.         Understand the loading, criterional to R.         Understand the loading, criterional of R.         Understand the loading, criterional of R.         Understand the loading, criterional of R.         Understand the loading, criterional to R.         Programming         Introduction to R	10. Spining V. D. (2005) "Disinformation A modern Annuagel" DIII logning Dat 144						
<ul> <li>Learn the basics of programming in biology         <ol> <li>Relate the necessity for programming in biology</li> <li>Handling biological concepts with C++ and Perl scripts</li> <li>Apply programing to analyze genomic sequences</li> <li>Understand Bio-Perl and their application in bioinformatics to handle the complex data</li> </ol> </li> <li>Part B         Syllabus Prescribed for 2022 Year PG. Programme Programme M.Sc. Bioinformatics         Semester IV         Code of the Course Subject Title of the Course/ Subject No. of periods/ week         AEC IV R-programming 01         Code of the Course Subject Title of the Course/ Subject No. of periods/ week         AEC IV R-programming 01         Code of the biology, retrieval techniques of data.         Understand the basics of Fundamentals of R.         Understand the basics of Fundamentals of R.         Understand the basics of Fundamentals of R.         Understand how data is analysed and visualized using statistic functions.         6.         Onements – Handling Packages in R: Installing a R Package, Few commands to get started: installed, package(), package, Description(), help(), find, package(), library() - Input and Output – Entering Data from kyboard – Printing fewer digits or more digits – Special Values functions : NA, Inf and – inf. R Data Types: Vectors, List, Matrices, Arrays, Factors, Data Frame – R - Variables (0) Operators, Legical Operators, Asignment Operators, Legical Operators, Asignment Operators, Miscellaneous Operators - R Decision Making: if statement, withe operators, Miscellaneous Operators - R Decision Making: if statement, if – else statement, if – else if textement, with statement – R Loops: repeal loop, while loop, for loop – Loop control statement: break statement, next statement, if – else Virss, Joire Meys, R for Dummics A Wiley Brand, 2nd Edition, John Wiley and Sons, I</li></ul>	19. Sillivas v.	19. Srinivas V.R. (2005) "Bioinformatics: A modern Approach" PHI learning Pvt. Ltd					
<ul> <li>Relate the necessity for programming in biology</li> <li>Handling biological concepts with C++ and Perl scripts</li> <li>Apply programming to analyze genomic sequences</li> <li>Understand Bio-Perl and their application in bioinformatics to handle the complex data</li> </ul> Part B Syllabus Prescribed for 2022 Year PG. Programme Programme M.Sc. Bioinformatics Semester IV Code of the Course Subject Title of the Course/ Subject No. of periods/ week AEC IV R-programming 01 Cos: Understand the basics of Fundamentals of R. Understand the data is analysed and visualized using statistic functions. 6. Unit I Rel Introduction to R: What is R? – Why R? – Advantages of R over Other Programming Languages - R Studio: R command Prompt, R script file, comments I Handling Packages in R: Installing a R Package, Few commands to get started: installed, package(), package Description(), help(), find, package(), library() - Input and Output – Entering Data from keyboard Printing fewer digits or more digits – Social Values functions: NA, Inf and –inf. R Data Types: Vectors, Lists, Matrices, Arrays, Factors, Data Frame – R - Variables: Variable assignment, Data types of Variable, Finding Variable 10, Oreitors - R Deogrators, Assignment Operators, Miscellaneous Operators - R Decision Making: if statement, if – else statement, if – else if statement, switch statement - R Loops: Arithmetic Operators, Relational Operators, McGraw Hill Education (India), 2017, ISBN: 978-93-5260-525-5. 9. Scena Acharya, Data Analytics using R, McGraw Hill Education (India), 2018, ISBN: 978-93-5260-524-8. 10. Tutorials Point (1) simply easy learning. Online Tutorial Library (2018), R Programming Retrieved from https://www.tutorialspoint.com/	1 Lea	ic. arn the basics	of programing				
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<ul> <li>Miscellaneous Operators - R Decision Making: if statement, if – else statement, if – else if statement, switch statement – R Loops: repeat loop, while loop, for loop – Loop control statement: break statement, next statement.</li> <li>Suggested Reading:</li> <li>8. Sandip Rakshit, R Programming for Beginners, McGraw Hill Education (India), 2017, ISBN : 978-93-5260-455-5.</li> <li>9. Seema Acharya, Data Analytics using R, McGrawHill Education (India), 2018, ISBN: 978-93-5260-524-8.</li> <li>10. Tutorials Point (I) simply easy learning, Online Tutorial Library (2018), R Programming, Retrieved from https://www.tutorialspoint.com/r/r_tutorial.pdf.</li> <li>11. Andrie de Vries, Joris Meys, R for Dummies A Wiley Brand, 2nd Edition, John Wiley and Sons, Inc, 2015, ISBN: 978-1-119-05580-8.</li> <li>Learning Outcome:</li> <li>12. Install, Code and Use R Programming Language in R Studio IDE to perform basic tasks on Vectors, Matrices and Data frames.</li> <li>13. Describe key terminologies, concepts and techniques employed in StatisticalAnalysis.</li> <li>14. Define, Calculate, Implement Probability and Probability Distributions to solve awide variety of problems.</li> <li>15. Conduct and Interpret a variety of Hypothesis Tests to aid Decision Making.</li> <li>16. Understand, Analyse, Interpret Correlation and Regression to analyse the underlying relationships between different variables.</li> </ul>		Operators, 1	Relational Operators, Logica	l Operator, Assignment Operators,			
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	underlying relation	nships betwee	en different variables.				

Part B							
Syllabus Prescrib	Syllabus Prescribed for 2022 Year PG. Programme						
Programme		M.Sc. Bioinformatics					
Somostor IV							
Semester IV							
Code of the Cour	se Subject Title of the Course/ Subjec	ct No. of periods/					
week							
DSC XII	<b>Chemo-informatics</b>	04					
Cos :							
<ol> <li>Have the k</li> <li>Understand common C</li> <li>Understand</li> </ol>	nowledge of the basic ligand/structure base d the basic algorithms used in the establishe ADD project. d the importance of proper use of various pa	ed approaches. ed software to carry out the most arameters in cheminformatics					
application	i programs.	for computer aided drug design					
including 2	2D/3D structural database.	ior computer alded drug design					
Unit-I : (Introduction to Chemo- informatics)	<ul> <li>Chemo-informatics: Introduction, scope and application, Basics of Chemo-informatics, Current Chemo-informatics resources for synthetic polymers, pigments. Primary, secondary and tertiary sources of chemical information, Databases: Chemical Structure Databases (PubChem, Binding database, Drugbank), Database search methods: chemical indexing, proximity searching, 2D and 3D structure and substructure searching. Drawing the Chemical Structure: 2D &amp; 3D drawing tools (ACD Chemsketch) Structure ontimization</li> </ul>						
Unit-II :	Introduction to quantum methods, combi	natorial chemistry (library design,					
(Introduction to	synthesis), spectroscopic methods and analytical techniques, Representation						
Cnemo- informatics)	SMILES Coding, Structure of Mol files and Sd files (Molecular converter)						
mormatics	SMILES Translator). Similarity search of the molecule (Zinc Database).						
Unit-III :	Analysis and use of chemical reaction	information, chemical property					
(Introduction to	information, spectroscopic information,	analytical chemistry information,					
Chemo-	chemical safety information, QSAR- Data Analysis, Structure-Activity						
mormatics)	OSAR, Lead Identification, Molecular De	escriptor Analysis.					
Unit-IV :	Target Identification: Molecular Mode	eling and Structure Elucidation:					
(Introduction to	Homology Modelling (Modeller 9v7,	PROCHECK), Visualization and					
Chemo-	validation of the Molecule (Rasmol, Pyme	ol Discovery studio), Applications					
miormatics)	Screening, Prediction of Pharmacological	Properties					
Unit-V :	Drug Discovery: Structure based drug de	esigning, Docking Studies (Target					
(Introduction to	Selection, Active site analysis, Ligand	preparation and conformational					
Chemo-	analysis, Rigid and flexible docking,	Structure based design of lead					
informatics)	Compounds, Library docking), Pharma Pharmacophore Modeling (Identification	on of pharmacophore features					
	Building 2D/3D pharmacophore hy	ypothesis), Toxicity Analysis-					
	Pharmacological Properties (Absorption,	Distribution and Toxicity), Global					
	Properties (Oral Bioavailability and Drug	-Likeness) (ADME, OSIRIS, and					
	WULINSPIKATION) Suggested Reading:						
1. Bai	orath J (2004), "Chemoinformatics: Conce	pts, Methods and Tools for Drug					
Dis	covery" Humana Press						
2. Lea	ach A, Gillet V, "An Introduction to Che	emoinformatics" Revised edition,					
Spr	Springer						

2	Container I. Er col T. "A touth only of Champinformation" Wiley, VOU Contribute						
5.	Gastelger J. Engel 1. A textbook of Chemoinformatics whey- vCH Ginon &						
	Co. KGaA						
4.	Bunin B. Siesel B. Guillermo M. "Chemoinformatics: Theory, practice &						
	nroducts" Springer						
5	Lavine B (2005) "Chemometrics and chemoinformatics" American Chemical						
5.	Lavine D. (2005), Chemometries and chemomormatics American Chemical						
	Society						
6.	Casteiger J. and Engel T (2003) "Chemoinformatics" Wiley-VCH						
7.	Bunin Barry A. SieselBrian, MoralesGuillermo, Bajorath Jürgen.						
	Chemoinformatics: Theory, Practice, & Products Publisher: New York, Springer.						
	2006 ISBN: 1402050003						
8	Gasteiger Johann Engel Thomas Chemoinformatics: A Textbook Publisher:						
0.	Witz-Well, 1st s litistr. 2002. IGDN: 252720(911						
	wiley VCH; 1st edition. 2003. ISBN: 352/306811.						
9.	Leach Andrew R., Valerie J. Gillet. An introduction to chemoinformatics.						
	Publisher: Kluwer academic, 2003. ISBN: 1402013477.						
10.	Gasteiger Johann, Handbook of Chemoinformatics: From Data to Knowledge (4						
	Volumes), 2003, Publisher: Wiley-VCH, ISBN: 3527306803.						
Learning Out	come:						
Loui ing out	• To import knowledge on chemical detabases verious educated						
	• To impart knowledge on chemical databases, various advanced						
	techniques and tools like docking, QSAR studies etc employed in						
	computational drug discovery						
	<ul> <li>Introduction about the basic concepts of cheminformatics</li> </ul>						
	• Explain about various approaches used in the design of pharmacophores						
	<ul> <li>Explain about various approaches used in the design of pharmacophores</li> <li>D '1 1 4 4</li> <li>CAD &amp; OCAD</li> </ul>						
	• Describe about the concepts of SAR & QSAR						

- •
- Explain various techniques used in virtual screening Describe about various techniques used in Structure Based Drug Design •

Part B					
Syllabus Prescribed for 2022	Year P	PG. Programme			
Programme	Μ	I.Sc. Bioinformatics			
Semester IV					
Code of the Course Subject	Title of the Course/ Subject	No. of periods/			
week					
DSC XIII Molecular Modelin	g and Drug Design	04			
<ul> <li>15. A Molecular Modeling a biophysical aspects of n</li> <li>16. A working knowledge o models that facilitate the 17. The skills required for v the areas of molecular s</li> <li>Unit-I : (Concepts in Molecular Modeling)</li> </ul>	and Drug Design is structure-based nacromolecule and small molecule of the molecular modeling tools and e understanding of macromolecula vorking in the pharmaceutical indu- tructure and interaction. Introduction; Coordinate Syster molecular graphics; Compute Mathematical concepts – introdu & quantum mechanics	d drug design and the interactions. d databases used to produce ar interactions. ustry and for further study in m; potential energy surfaces r hardware and software; uction of molecular mechanics			
Unit-II : (Molecular Mechanics)	Features of molecular mechanics and bending angles – electrosta bonded interactions, hydroge mechanics; Derivatives of m function; Calculating thermodyn field; Transferability of force fit delocalized pi system; Force fit systems – Application of energy	s, force fields; Bond structure atic, Vander Waals and non- en bonding in molecular nolecular mechanics energy namic properties using force ield parameters, treatment of eld for metals and inorganic minimization			
Unit-III : (Molecular Dynamics Simulation Methods)	Molecular Dynamics using Dynamics with continuous p temperature and pressure; Time- effects in Molecular Dynamics; O	simple models; Molecular potentials and at constant dependent properties; Solvent Conformational changes from			

	Molecular Dynamics simulation. Introduction, Newton's		
equation of motion. equilibrium point. radial distribution			
	function, pair correlation functions, MD methodology, periodic		
	hox algorithm for time dependence: leanfrog algorithm Verlet		
	algorithm Boltzman velocity time steps duration of the MD		
	run Ligand protein interactions using Gromacs		
Unit-IV · (Molecular	Deriving and using 3D pharmacophore: Molecular Docking:		
Modeling in Drug	Structure based methods to identify lead compounds: de novo		
Discovery)	ligand design: Applications of 3D Database Searching and		
Discovery	Docking Finding new drug targets to treat diseases –		
	Pharmaconhore identification - Structure based drug design -		
	Molecular Simulations		
Unit-V · (Structure	OSARs and OSPRs OSAR Methodology Various Descriptors		
Activity Relationshin)	used in OSARs: Electronic: Topology: Quantum Chemical		
	based Descriptors. Use of Genetic Algorithms. Neural		
	Networks and Principle Components Analysis in the OSAR		
	equations		
	Suggested Reading:		
21. Andrew R. Leac	h (2001) "Molecular Modeling – Principles and Applications";		
Second Edition,	Prentice Hall, USA		
22. Fenniri, H. (200	0) "Combinatorial Chemistry – A practical approach", Oxford		
University Press	, UK.		
23. Gordon, E.M. ar	d Kerwin, J.F. (1998) "Combinatorial chemistry and molecular		
diversity in drug discovery"; Wiley-Liss Publishers			
24. Lednicer, D. (1	998) "Strategies for Organic Drug Discovery Synthesis and		
Design"; Wiley	Design"; Wiley International Publishers		
25. Swatz, M.E. (20	00) "Analytical techniques in Combinatorial Chemistry"; Marcel		
Dekker Publishers			
Learning Outcome:			
This course will be able to demonstrate:			
1. An understanding of the general concepts of macromolecule interactions.			
2. A solid grounding in the mathematics that underpin the methods used.			
3. A working knowledge of the methods and tools used in molecular modelling.			
4. Knowledge of the experimental techniques that support molecular models.			
5. Strong skills in the critical analysis and synthesis of scientific information.			
6. The ability t	o conduct independent research, place findings in context and		
suggest new	research ideas.		
7. How to conduct an independent research project and how to report research			
data in forma	ats suitable for publication.		

Part B			
Syllabus Prescribed for 2022	2 Year PG.	Programme	
Programme	M.S	M.Sc. Bioinformatics	
Semester IV			
Code of the Course Subject	Title of the Course/ Subject	No. of periods/	
week			
DSC XIV	Research Methodology, IPR and B	ioethics 04	
Cos :			
<ol> <li>13. Identify an appropriate</li> <li>14. Understand ethical iss</li> <li>15. Understand the Prepare</li> <li>16. Understand the law of</li> </ol>	e research problem in their interesting ues Understand the Preparation of a res ration of a research project thesis repor- patent and copyrights.	domain. search project thesis report. t	
17. Understand the Adequ	ate knowledge on IPR		

Unit I. (Dessauch	Bassarch and Tashnical Writing: What is research? The		
Unit 1: (Research	Research and Technical Writing: What is research? The		
wiethodology)	process of research – various types of research – research		
	methodology – rypoinesis – research writing – basic		
	principles; publication process – peer review - Journal impact		
	tactors – popular journals in Computational Biology &		
	Bioinformatics (brief overview of their scope),		
	Professional Societies in the field – their role in research and		
	knowledge dissemination, Open Access Publications, Concept		
	of ethics – its application in Scientific Research and		
	Academics, Solving ethical conflicts, moral reasoning &		
	ethical theories, responsibilities and rights.		
Unit II : (Intellectual	General principles of Intellectual property rights (IPR); Patents		
Property Rights)	and methods; application of patents; Legal implications;		
	International treaties for protection of IP – Bern, Paris, TRIPS,		
	WIPO treaties, Biodiversity convention, etc		
Unit III : (Intellectual	Nature of Intellectual Property: Patents, Designs, Trademarks		
Property Rights)	and Copyright. Process of Patenting and Development:		
	technological research, innovation, patenting, development;		
	International cooperation on Intellectual Property, Procedure		
	for grants of patents, Patenting under PCT; Scope of Patent		
	Rights: Licensing and transfer of technology. Patent		
	information and databases. Geographical Indications		
Unit IV : (Bioethics)	The legal and socioeconomic impacts of biotechnology: public		
	education of the process of the processes of biotechnology		
	involved in generating new forms of life for informed decision		
	making; Biosafety regulation and national and international		
	guidelines; rDNA guidelines; Experimental protocol approval:		
	levels of containment		
Unit V : (Bioethics)	Environmental aspects of biotechnology applications: Use of		
	genetically modified organisms and their release in		
	environment: Special procedures for rDNA-based product		
	production: Biodiversity and farmers rights: Beneficial		
	applications and development of research focus to the need of		
	the poor: Identification of directions for yield effect in		
agriculture aquaculture etc: Rioremediation			
Suggested Reading:			
15. Sasson, A. (1988) "Biotechnologies and Development". UNESCO Publications			
16. Sasson, A. (1993) "Biotechnologies in developing countries present and			
future"; UNESCO Publishers			
17. Singh, K. "Intellectual Property Rights on Biotechnology"; BCIL, New Delhi			
18. Halbert, (2007) "Resisting Intellectual Property" Taylor & Francis Ltd			
19. Ramappa T., "Intellectual Property Rights Under WTO", S. Chand			
Learning Outcome:			
1. Understand the research	n problem and research process.		
2. Understand research ethics .			
3. Prepare a well-structured research paper and scientific presentations			

Explore on various IPR components and process of filing.
 Understand the adequate knowledge on patent and rights.

Part B		
Syllabus Prescribed for 2022	Year I	PG. Programme
Programme	Ν	<b>1.Sc. Bioinformatics</b>
Semester IV		
Code of the Course Subject	Title of the Course/ Subject	No. of periods/
week		
SEC II	Python	01
Cos :		
1. Identify/characterize/de	fine a problem	
2. Design a program to sol	ve the problem	
3. Create executable code		
4. Read most Python code	1	r <b>r • .1 1•</b>
Olife IGeneral Intrand developGitHub, Bastructure, scexpressionsSequences:methods anComprehensinheritance,and General	Strings, Tuples, Lists, Iteration, lo difference of formatting, Dictionaries, Sets sions, Advanced Argument Properties, Special methods, Em- tors, Decorators, Context Manage	oping and control flow. String and Mutability. List and Dict passing, Lambda, Multiple ulating built-in types, Iterators rs, Regular expression.
	Suggested Reading:	
<ol> <li>Jake VanderPlas, "Pyth Data", 1st Edition, O'Re</li> <li>AurelienGeron, "Hands Concepts, Tools, and To Media, 2019. ISBN – 13</li> <li>Wesley, J. Chun, "Corr</li> </ol>	on Data Science Handbook: Esse silly Media, 2016. ISBN-13: 978- s-On Machine Learning with S echniques to Build Intelligent Sy 8: 978-9352139057.	ential Tools for Working with 1491912058 cikit-Learn and TensorFlow: stems", 2nd Edition, O'Reilly ming" 3rd Edition Pearson
Education India 2015 I	SBN-13. 978-9332555365	ning, 510 Euron, realson
11. Miguel Grinberg, "Fla Python", 2nd Edition, O	sk Web Development: Develop 'Reilly Media, 2018. ISBN-13: 9'	ping Web Applications with 78-1491991732.
Learning Outcome:		

Problem solving and programming capability.

Part B			
Syllabus Prescribed	Syllabus Prescribed for 2022 Year PG. Programme		Programme
Programme		M.Sc. Bioinformatics	
Semester IV			
Code of the Course	Subject Title of the	Course/ Subject	No. of periods/ week
OEC II	Language	for Bioinformatics	04
Cos :			
3. Able to apply design principles to develop web based applications specially for biological data analysis Familiarity CO-2			
4. To understand working on world wide web through implementations Familiarity and Assessment CO-3			
5. Use various methods from computational biology to implement their programmatic versions			
Assessment CO-4			
6. Able to design new web pages and web sites Assessment and Usage CO-5			
7. Able to developed programs to describe and analyze problems in biology			
Unit-I: (Language)	<ul> <li>Introduction to Internet and World Wide Web. An overview of scripting languages</li> <li>with applications towards biological data and sequence analysis. Complexity on DNA problems and their computational implications and applications. Introduction</li> </ul>		
	Di al problemb una men	compatational implied	and approximations. Introduction

to HTML, DHTML, XML. accessing different objects of the HTML page,			
Dynamic page generation, Cascading Style Sheets (CSS).			
Unit-II: JAVASCRIPT: Document object model, Elements of the document object mod			
(Language) basic principles of JS, object based programming using JavaScript; data types a			
	structures, array and string handling, function implementations, XML: DTD, XML		
	schemas, XML document structure, retrieving data from database in XML format;		
	various bio based versions of XML.		
Unit III:	PHP: PHP beginning to advanced level, data types, array and string handling,		
(Language)	mathematical expressions and functions in PHP, PHP programming		
	(implementation of object model), Database connectivity using PHP.		
Unit-VI	Programming basics, Sequences and Strings: Storing a DNA sequence,		
:(Language)	Concatenation, Transcription, Translation, Arrays and Scalar list, Strings to Array,		
	Operations on Strings, Subroutines and Command line arguments		
Unit-V	Calling modules, Hashes, Data Structures in Perl, Reading files and writing output		
:(Language)	formats, Regular expressions and Perl Operations, Parsing genbank, PDB, BLAST,		
	and other file formats, Object-oriented programming, Complex Data Structures,		
	Relational Databases.		
	Suggested Reading:		
4. Beginning l	Perl for Bioinformatics By James Tisdall, O'Reilly Media (2001)		
5. Mastering I	Perl for Bioinformatics By James Tisdall, O'Reilly Media (2003)		
6. Python For	Bioinformatics By Sebastian Bassi, Chapman and Hall (2010)		
7. HTML the complete reference, 2004, TMH.			
8. Beginning	8. Beginning PHP and Professional PHP, 2009, Wrox, Wiley Dreamtech.		
9. JavaScript:	The complete Reference, 2004, TMH.		
Learning Outcome			
1. Students will demonstrate the ability to identify, formulate and solve computer			
systemsengineering problems.			
2. Students will demonstrate the ability to design and experiment both in hardware			
andsoftware, analyze and interpret data.			
3. Students will demonstrate an ability to analyze the given problems and design			
solutions, as per the needs and specifications.			
4. Students will develop confidence for self education and ability for lifelong learning			

	Sant Gadge Baba Amravati Unive	ersity, Amravati	
Syllabus Prescribed for 202 Programme: M. Sc. Bioinfor	2 Year PG I rmatics	• PG Programme	
Semester 1 Code of the Course/Subject	<b>Title of the Course/Subject</b> (Laboratory/Practical/practicu m/hands-on/Activity)	(No. of Periods/Week)	
Practical VII	Practical Based on DSC XI, XII, XIII & XIV	12	

CO:

- 1. To develop logical understanding of the subject.
- 2. To create the ability to model, solve and interpret Molecular Modelling, Drug Design, Chemo-informatics, Bio-Programming and Research Methodology, IPR and Bioethics problems.
- 3. To provide an overview of functions of complex variable which helps in solvingmany biological problems

## \* List of Practical/Laboratory Experiments/Activities etc.

# Molecular Modeling, Drug Design, Chemo-informatics, Bio-Programming –II and Research Methodology, IPR and Bioethics

1	Binding site identification
2	Pharmacophore identification
3	Rigid body docking using Autodock and ADT
4	Molecular dynamics simulations using Gromacs
5	Visual Molecular Dynamics (VMD)
6	Advance Visualization with (Discovery Studio)
7	Receptor and Ligand Optimization

8	Conformational Analysis	
9	Chemo-informatics Software	
a.	AMBER	
b.	ArgusLab 3.0	
c.	BABEL	
d.	Chemos	
e.	VEGA	
f.	PubChem	
g.	ChemSketch	
10	Chemo-informatics databases	
11	Chemical structure representation	
12	Smiles - Simplified Molecular Input Line Entry System	
10	Molecular Dimension Limited (MDL) file format for chemical	
13	connectivity	
14	Chemical Structure similarity	
15	Fingerprints and search for substructure similarity using expasy	
16	Generation of 3D structures from 2D representations	
1/	3D structure similarity	
18	Elements of molecular descriptors	
19	Writing Pseudo Codes	
20	Creating Classes and Annlingting in Loops	
21	Creating Classes and Applications in Java	
22	Creating User Interfaces with AWT Modifiers	
23	Packages and Interfaces Exception Multithreading	
25	Streams and I/O Using Native Methods and Libraries	
26	Java Programming Tools. Working with Data Structures	
27	Sequence Analysis Packages - EMBOSS, NCBI Tool Kit	
28	Analysis of Biological Sequences	
a.	Basic Blast	
b.	Specialized Blast	
Learning	Outcome:	
1. R	esearch, inquiry and analytical thinking abilities	
2. T	he capability and motivation for intellectual development	
3. E	thical, social and professional understanding	
4. E	frective research communication	
5. 1 6 h	e able to describe the process of drug discovery and development	
0. 0 7 h	e able to discuss the challenges faced in each step of the drug	
,. d	iscoveryprocess	
8. ł	nave gained a basic knowledge of computational methods used in	
drugdiscovery		

# Sant Gadge Baba Amravati University, Amravati

Syllabus Prescribed for 2022 Programme: M. Sc. Bioinfor	Year PG I matics	PG Programme	
Semester 1 Code of the Course/Subject	<b>Title of the Course/Subject</b> (Laboratory/Practical/practicu m/hands-on/Activity)	(No. of Periods/Week)	
Practical VII	Practical Based on Project Work	06	

- CO:
  - 1. Identify and discuss the role and importance of research in the bioinformatics.
  - 2. Identify and discuss the issues and concepts salient to the research process.
  - 3. Identify and discuss the complex issues inherent in selecting a research problem, selecting an appropriate research design, and implementing a research project.
  - 4. Identify and discuss the concepts and procedures of sampling, data collection, analysis and reporting.

### Learning Outcome:

- 1. Explain key research concepts and issues
- 2. Read, comprehend, and explain research articles in their academic discipline.
- 3. Able to formulate new research problem.