

SAURASHTRA UNIVERSITY, RAJKOT



Accredited Grade “A” by NAAC (CGPA 3.05)

COURSE STRUCTURE & SYLLABUS

FOR

UNDERGRADUATE PROGRAMME

IN

BIOINFORMATICS

Semester III & IV

(Faculty of Science)

[As per Choice Based Credit System (CBCS) as recommended by UGC]

Effective from June - 2017

Annexure – “B”

SAURASHTRA UNIVERSITY
SCIENCE FACULTYSubject: **BIOINFORMATICS**

Sr. No.	Level	Semester	Course Group	Course (Paper) Title	Course (Paper) No.	Credit	Internal Marks	External Marks	Practical /Viva Marks	Total Marks	Course (Paper) Unique Code
01	UG	03	Core	Bioinformatics Databases and Sequence Analysis	BI-301	5	30	70	50	150	1603 2200 0103 0100
02	UG	03	Core	Algorithms in Bioinformatics	BI-302	5	30	70	50	150	1603 2200 0103 0200
03	UG	03	Core	Programming in C	BI-303	5	30	70	50	150	1603 2200 0103 0300
04	UG	03	Core	Immunology and Immunotechnology	BI-304	5	30	70	50	150	1603 2200 0103 0400
05	UG	03	Core	Medicinal Chemistry	BI-305	4	30	70	50	150	1603 2200 0103 0500
06	UG	04	Core	Structural & Applied Bioinformatics	BI-401	5	30	70	50	150	1603 2200 0104 0100
07	UG	04	Core	Genetic Engineering	BI-402	5	30	70	50	150	1603 2200 0104 0200
08	UG	04	Core	Web Technology	BI-403	5	30	70	50	150	1603 2200 0104 0300
09	UG	04	Core	Object oriented Programming using JAVA	BI-404	5	30	70	50	150	1603 2200 0104 0400
10	UG	04	Core	Cheminformatics	BI-405	4	30	70	50	150	1603 2200 0104 0500

**SKELETON OF COMPLETE COURSE CONTENT OF
UNDER GRADUATE BIOINFORMATICS
SEMESTER III & IV**

SEMESTER	PAPER NO. & CODE	TITLE OF THE PAPER	CREDIT
III	BI-301 (Theory)	Bioinformatics Databases and Sequence Analysis	3
	BI-301 (Practical)	-do-	2
	BI-302 (Theory)	Algorithms in Bioinformatics	3
	BI-302 (Practical)	-do-	2
	BI-303 (Theory)	Programming in C	3
	BI-303 (Practical)	-do-	2
	BI-304 (Theory)	Immunology and Immunotechnology	3
	BI-304 (Practical)	-do-	2
	BI-305 (Theory)	Medicinal Chemistry	3
	BI-305 (Practical)	-do-	1
IV	BI-401 (Theory)	Structural & Applied Bioinformatics	3
	BI-401 (Practical)	-do-	2
	BI-402 (Theory)	Genetic Engineering	3
	BI-402 (Practical)	-do-	2
	BI-403 (Theory)	Web Technology	3
	BI-403 (Practical)	-do-	2
	BI-404 (Theory)	Object oriented Programming using JAVA	3
	BI-404 (Practical)	-do-	2
	BI-405 (Theory)	Cheminformatics	3
	BI-405 (Practical)	-do-	1

FACULTY OF SCIENCE

Syllabus

Subject: **BIOINFORMATICS**

Course (Paper) Name & No.: Bioinformatics Databases and Sequence Analysis (BI-301)

Course (Paper) Unique Code: 1603 2200 0103 0100

External Exam Time Duration: 2 Hours and 30 minutes

Name of Program	Semester	Course Group	Credit	Internal Marks	External Marks	Practical /Viva Marks	Total Marks
Bachelor of Science	03	Core	5	30	70	50	150

Course Objective:

- To uncover basics of Bioinformatics databases and analysis of sequence

**COURSE STRUCTURE FOR UG PROGRAMME
BIOINFORMATICS- 301
SEMESTER- III**

Semester	Course	Title	Hours /week	Credit	Exam duration	Internal marks	External marks	Total marks
I	BI-301 (Theory)	Bioinformatics Databases and Sequence Analysis	5	3	2.5 hrs	30	70	100
I	BI-301 (Practical)	Bioinformatics Databases and Sequence Analysis	3	2	One day per batch	15	35	50
Total credits				5	Total marks			150

General instructions

1. The medium of instruction will be English for theory and practical courses
2. There will be 5 lectures / week / theory paper / semester.
3. Each lecture will be of 55 mins.
4. There will be 1 practical / week / paper / batch. Each practical will be of 3 periods
5. Each semester theory paper will be of “five” units. There will be 40 hrs. of theory teaching / paper / semester.
6. Each Theory Paper / Semester will be of 100 Marks. There will be 30 marks for internal evaluation and 70 marks for external evaluation. Each Practical Paper / Semester will be of 50 Marks with 15 marks for internal and 35 marks for external evaluation. So, Total Marks of Theory and Practical for each Paper will be 150. (100 + 50 = 150)

**SKELETON OF THEORY EXAMINATION PAPER -EXTERNAL
(SEMESTER –III)**

Total five questions. One question from each unit. Each question having equal weightage of 14 Marks		
a) Four One mark questions (All compulsory)	4 x 1= 4 Marks	14 Marks
b) Answer specifically- (attempt any one out of two)	1 x 2= 2 Marks	
c) Short Questions - (attempt any one out of two)	1 x 3= 3 Marks	
d) Answer in detail – (attempt any one out of two)	1 x 5= 5 Marks	

General Instructions

1. Time duration of each theory paper will be of two and half hours.
2. Total marks of each theory paper will be 70 marks.
3. There will be internal option for all the questions (as shown in table above)
4. All questions are compulsory

BI.301 Bioinformatics Databases & Sequence Analysis

(Theory)

Unit I: Bioinformatics database management

- Data management in Bioinformatics
- Omics Data Management and Annotation
- Data integration in biological research: an overview
- Data integration in the era of omics: current and future challenges
- Integrated Bio-Search: challenges and trends for the integration, search and comprehensive processing of biological information
- Big Biological Data: Challenges and Opportunities
- The big challenges of big data
- Big data bioinformatics
- Bioinformatics clouds for big data manipulation

Unit II: Bioinformatics databases-1 (Each category at least any one database need to be covered from the database issue of Nucleic Acids Research journals)

- The 2016 database issue of Nucleic Acids Research and an updated molecular biology database collection
- Nucleotide Sequence Databases: International Nucleotide Sequence Database Collaboration, Coding and non-coding DNA, Gene structure, introns and exons, splice sites, Transcriptional regulator sites and transcription factors
- RNA sequence databases
- Protein sequence databases: General sequence databases, Protein properties, Protein localization and targeting, Protein sequence motifs and active sites, Protein domain databases; protein classification, Databases of individual protein families
- Structure Databases: Small molecules, Carbohydrates, Nucleic acid structure, Protein structure

Unit III: Bioinformatics databases-2 (Each category at least any one database need to be covered from the database issue of Nucleic Acids Research journals)

- Genomics Databases (non-vertebrate): Genome annotation terms, ontologies and nomenclature, Taxonomy and identification, General genomics databases, Viral genome databases, Prokaryotic genome databases, Unicellular eukaryotes genome databases, Fungal genome databases, Invertebrate genome databases
- Metabolic and Signaling Pathways: Prokaryotic genome databases, Enzymes and enzyme nomenclature, Metabolic pathways, Protein-protein interactions, Signalling pathways
- Human and other Vertebrate Genomes: Model organisms, comparative genomics, Human genome databases, maps and viewers, Human ORFs

- Human Genes and Diseases: General human genetics databases, General polymorphism databases, Cancer gene databases, Gene-, system- or disease-specific databases

Unit IV: Bioinformatics databases-3 (Each category at least any one database need to be covered from the database issue of Nucleic Acids Research journals)

- Microarray Data and other Gene Expression Databases
- Proteomics Resources
- Other Molecular Biology Databases: Drugs and drug design, Molecular probes and primers
- Organelle databases: Mitochondrial genes and proteins
- Plant databases: General plant databases, Arabidopsis thaliana, Rice, Other plants
- Immunological databases
- Cell biology

Unit V: Sequence Analysis

- Pairwise sequence comparison: Dot matrix, Dynamic Programming, use of scoring matrices and gap penalties in sequence alignments, Assessing the significance of sequence alignments
- Multiple sequence alignment: Multiple sequence alignment as an extension of sequence pair alignment by dynamic programming, scoring multiple sequence alignments, Progressive methods of multiple sequence alignment, Iterative methods of multiple sequence alignment, Localized alignments in sequences
- Database Searching for Similar Sequences

BI.301 Bioinformatics Databases & Sequence Analysis

(Practical)

Based on theory syllabus

References:

- Zoe Lacroix and Terence Critchlow, Bioinformatics – Managing Scientific Data, Morgan, Kaufmann publishers, 2003
- Brandenburg, A., Gmuender, H., and Wittenberger, T.: ‘In Silico Approaches: Data Management – Bioinformatics’: ‘Predictive Toxicology’ (Wiley-VCH Verlag GmbH & Co. KGaA, 2014), pp. 33-52
- Harel A, Dalah I, Pietrokovski S, Safran M, Lancet D. Omics data management and annotation. *Methods Mol Biol.* 2011;719:71-96. doi: 10.1007/978-1-61779-027-0_3. PubMed PMID: 21370079.
- Lapatas, V., Stefanidakis, M., Jimenez, R. C., Via, A., & Schneider, M. V. (2015). Data integration in biological research: an overview. *Journal of Biological Research*, 22(1), 9. <http://doi.org/10.1186/s40709-015-0032-5>

- Gomez-Cabrero, D., Abugessaisa, I., Maier, D., Teschendorff, A., Merckenschlager, M., Gisel, A., Ballestar, E., Bongcam-Rudloff, E., Conesa, A., and Tegnér, J.: 'Data integration in the era of omics: current and future challenges', *BMC Systems Biology*, 2014, 8, (2), pp. 11
- Li Y, Chen L. Big biological data: challenges and opportunities. *Genomics Proteomics Bioinformatics*. 2014 Oct;12(5):187-9. doi: 10.1016/j.gpb.2014.10.001. PubMed PMID: 25462151; PubMed Central PMCID: PMC4411415.
- Marx V. Biology: The big challenges of big data. *Nature*. 2013 Jun 13;498(7453):255-60. doi: 10.1038/498255a. PubMed PMID: 23765498.
- Greene CS, Tan J, Ung M, Moore JH, Cheng C. Big data bioinformatics. *J Cell Physiol*. 2014 Dec;229(12):1896-900. doi: 10.1002/jcp.24662. Review. Erratum in: *J Cell Physiol*. 2016 Jan;231(1):257. PubMed PMID: 24799088.
- Dai, L., Gao, X., Guo, Y., Xiao, J., and Zhang, Z.: 'Bioinformatics clouds for big data manipulation', *Biology Direct*, 2012, 7, (1), pp. 43
- Rigden DJ, Fernández-Suárez XM, Galperin MY. The 2016 database issue of *Nucleic Acids Research* and an updated molecular biology database collection. *Nucleic Acids Res*. 2016 Jan 4;44(D1):D1-6. doi: 10.1093/nar/gkv1356. PubMed PMID: 26740669; PubMed Central PMCID: PMC4702933.
- http://www.oxfordjournals.org/our_journals/nar/database/cap/
- Arthur M. Lesk, *Introduction to Bioinformatics*, Oxford University Press, New Delhi, 2003.
- David W. Mount, *Bioinformatics – Sequence and Genome analysis*, 2nd edition, Cold Spring Harbor Laboratory Press, New York.
- Baxevanis and B.F. Ouellette. *Bioinformatics: A practical Guide to the Analysis of Genes and Proteins*, Wiley- Interscience, Hoboken, NJ, 2005.
- M.Campbell& L. J. Heyer, *Discovering Genomics, Proteomics & Bioinformatics*, CSHL Press, 2003.
- S.R. Pennington & M.J. Dunn, *Proteomics – from protein sequence to function*, BIOS Scientific Publishers, 2002.

Annexure – “C”

FACULTY OF SCIENCE

Syllabus

Subject: **BIOINFORMATICS**

Course (Paper) Name & No.: Algorithms in Bioinformatics(BI-302)

Course (Paper) Unique Code: 1603 2200 0103 0200

External Exam Time Duration: 2 Hours and 30 minutes

Name of Program	Semester	Course Group	Credit	Internal Marks	External Marks	Practical /Viva Marks	Total Marks
Bachelor of Science	03	Core	5	30	70	50	150

Course Objective:

- To understand basic Advance algorithms in Bioinformatics

**COURSE STRUCTURE FOR UG PROGRAMME
BIOINFORMATICS- 302
SEMESTER- III**

Semester	Course	Title	Hours /week	Credit	Exam duration	Internal marks	External marks	Total marks
I	BI-302 (Theory)	Algorithms in Bioinformatics	5	3	2.5 hrs	30	70	100
I	BI-302 (Practical)	Algorithms in Bioinformatics	3	2	One day per batch	15	35	50
Total credits				5	Total marks			150

General instructions

1. The medium of instruction will be English for theory and practical courses
2. There will be 5 lectures / week / theory paper / semester.
3. Each lecture will be of 55 mins.
4. There will be 1 practical / week / paper / batch. Each practical will be of 3 periods
5. Each semester theory paper will be of “five” units. There will be 50 hrs. of theory teaching / paper / semester.
6. Each Theory Paper / Semester will be of 100 Marks. There will be 30 marks for internal evaluation and 70 marks for external evaluation. Each Practical Paper / Semester will be of 50 Marks with 15 marks for internal and 35 marks for external evaluation. So, Total Marks of Theory and Practical for each Paper will be 150. (100 + 50 = 150)

SKELETON OF THEORY EXAMINATION PAPER -EXTERNAL

(SEMESTER- III)

Total five questions. One question from each unit. Each question having equal weightage of 14 Marks		
a) Four One mark questions (All compulsory)	4 x 1= 4 Marks	14 Marks
b) Answer specifically- (attempt any one out of two)	1 x 2= 2 Marks	
c) Short Questions - (attempt any one out of two)	1 x 3= 3 Marks	
d) Answer in detail – (attempt any one out of two)	1 x 5= 5 Marks	

General Instructions

1. Time duration of each theory paper will be of two and half hours.
2. Total marks of each theory paper will be 70 marks.
3. There will be internal option for all the questions (as shown in table above)
4. All questions are compulsory

BI.302 Algorithms in Bioinformatics

(Theory)

Unit-1 Basic of Algorithms and Algorithm Design

- Algorithms for basic problems
- Sorting & searching algorithm
- Algorithm analysis, Algorithm's complexity, input size, running time, memory requirements, worst-case and average-case, order of growth
- Basic concepts of string similarity and distances, distance metrics, scoring matrices, Sequence similarity, Hamming distances, Levenstein distances

Unit-2 Some basic concept and definition

- Learning, model, inference, utility
- Different kinds of models and inference
- Generalization and bias, Rule induction
- Concept learning, Version space

Unit-3 Learning sets of rules

- Neural networks
- Basic principles, Feedforward & Backward nets
- Backpropagation, Instance based learning
- Distance metrics, Nearest neighbor, Case based reasoning

Unit-4 Bayesian statistics

- Bayesian inference
- Probabilistic expert systems
- Conditional probability, Prior probability,
- Bayes theorem, Naïve Bayesian classifier

Unit-5 Rule based expert systems

- Graphical models/Markov graphs
- Inference in polytrees
- Modifying the structure of general networks
- General learning difficulties
- Algorithm for learning probabilistic networks

BI.302 Algorithms in Bioinformatics

(Practical)

Based on theory syllabus

References:

- Fundamental concepts of Bioinformatics: Dan E Krane and Michael L.Raymer- Pearson Education
- Bioinformatics A Beginners Guide: Claverie and Notredame- Wiley Dreamtech India PVT ltd 2003
- An introduction to bioinformatics algorithms: Wel C Jones and Pavel A. Pevnezer- Ane Books, New Delhi

Annexure – “C”

FACULTY OF SCIENCE

Syllabus

Subject: **BIOINFORMATICS**

Course (Paper) Name & No.: Programming in C(BI-303)

Course (Paper) Unique Code: 1603 2200 0103 0300

External Exam Time Duration: 2 Hours and 30 minutes

Name of Program	Semester	Course Group	Credit	Internal Marks	External Marks	Practical /Viva Marks	Total Marks
Bachelor of Science	03	Core	5	30	70	50	150

Course Objective:

- To understand basic of Computer Language C

**COURSE STRUCTURE FOR UG PROGRAMME
BIOINFORMATICS- 303
SEMESTER- III**

Semester	Course	Title	Hours /week	Credit	Exam duration	Internal marks	External marks	Total marks
I	BI-303 (Theory)	Programming in C	5	3	2.5 hrs	30	70	100
I	BI-303 (Practical)	Programming in C	3	2	One day per batch	15	35	50
Total credits				5	Total marks			150

General instructions

1. The medium of instruction will be English for theory and practical courses
2. There will be 5 lectures / week / theory paper / semester.
3. Each lecture will be of 55 mins.
4. There will be 1 practical / week / paper / batch. Each practical will be of 3 periods
5. Each semester theory paper will be of “five” units. There will be 50 hrs. of theory teaching / paper / semester.
6. Each Theory Paper / Semester will be of 100 Marks. There will be 30 marks for internal evaluation and 70 marks for external evaluation. Each Practical Paper / Semester will be of 50 Marks with 15 marks for internal and 35 marks for external evaluation. So, Total Marks of Theory and Practical for each Paper will be 150. (100 + 50 = 150)

SKELETON OF THEORY EXAMINATION PAPER -EXTERNAL

(SEMESTER- III)

Total five questions. One question from each unit. Each question having equal weightage of 14 Marks		
a) Four One mark questions (All compulsory)	4 x 1= 4 Marks	14 Marks
b) Answer specifically- (attempt any one out of two)	1 x 2= 2 Marks	
c) Short Questions - (attempt any one out of two)	1 x 3= 3 Marks	
d) Answer in detail – (attempt any one out of two)	1 x 5= 5 Marks	

General Instructions

1. Time duration of each theory paper will be of two and half hours.
2. Total marks of each theory paper will be 70 marks.
3. There will be internal option for all the questions (as shown in table above)
4. All questions are compulsory

BI.303 Programming in C **(Theory)**

UNIT 1

- Programming Techniques: Importance of computer programming techniques
- Programming tools: Algorithms development
- Concept of Flowcharts
- Pseudo codes

UNIT 2

- Started with C: Introduction and History
- C program Structure; Character Set, Constant, Variables and Keywords in C
- Data Types and Type Casting
- Different Operators and expressions

UNIT 3

- Control Structure: Decision – If, if-else, nested if-else, if-else if, switch..case
- Loops: For, While, Do..While, Nesting of loops
- Use of break and continue statements; Goto with label
- Function: Function Types, Function Prototype, Calling Function, Variable Scope, Arguments, Advantages of function
- External and Static Variables, Recursion

UNIT 4

- Arrays: Concept of Single and two Dimensional arrays, Initialization and working with array, sorting of numeric and string arrays
- String operations: reading a character, writing a character, character Strings, Reading and Writing String
- Structures: define a structure, accessing elements, memory allocation, array of structure, array within structure
- Union

UNIT 5

- Pointers: Pointers and Arrays
- Pointer Arithmetics
- Pointer and Function
- Files: Open Files, Closing Files, Read and Write Operations

BI.303 Programming in C **(Practical)**

Based on theory syllabus

Reference Books:

- ANSI C : E. Balaguruswamy-BPB
- Let us C: YashvantKanetkar, BPB
- C: How to Program, Deitel&Deital, Pearson Education
- Programming with ANSI C and TURBO C, Pearson Education

FACULTY OF SCIENCE

Syllabus

Subject: **BIOINFORMATICS**

Course (Paper) Name & No.: Immunology and Immunotechnology(BI-304)

Course (Paper) Unique Code: 1603 2200 0103 0400

External Exam Time Duration: 2 Hours and 30 minutes

Name of Program	Semester	Course Group	Credit	Internal Marks	External Marks	Practical /Viva Marks	Total Marks
Bachelor of Science	03	Core	5	30	70	50	150

Course Objective:

- To understand the structure, function and inter-relationships of Immunology

**COURSE STRUCTURE FOR UG PROGRAMME
BIOINFORMATICS- 304
SEMESTER- III**

Semester	Course	Title	Hours /week	Credit	Exam duration	Internal marks	External marks	Total marks
I	BI-304 (Theory)	Immunology and Immunotechnology	5	3	2.5 hrs	30	70	100
I	BI-304 (Practical)	Immunology and Immunotechnology	3	2	One day per batch	15	35	50
Total credits				5	Total marks			150

General instructions

1. The medium of instruction will be English for theory and practical courses
2. There will be 5 lectures / week / theory paper / semester.
3. Each lecture will be of 55 mins.
4. There will be 1 practical / week / paper / batch. Each practical will be of 3 periods
5. Each semester theory paper will be of “five” units. There will be 50 hrs. of theory teaching / paper / semester.
6. Each Theory Paper / Semester will be of 100 Marks. There will be 30 marks for internal evaluation and 70 marks for external evaluation. Each Practical Paper / Semester will be of 50 Marks with 15 marks for internal and 35 marks for external evaluation. So, Total Marks of Theory and Practical for each Paper will be 150. (100 + 50 = 150)

**SKELETON OF THEORY EXAMINATION PAPER -EXTERNAL
(SEMESTER- III)**

Total five questions. One question from each unit. Each question having equal weightage of 14 Marks		
a) Four One mark questions (All compulsory)	4 x 1= 4 Marks	14 Marks
b) Answer specifically- (attempt any one out of two)	1 x 2= 2 Marks	
c) Short Questions - (attempt any one out of two)	1 x 3= 3 Marks	
d) Answer in detail – (attempt any one out of two)	1 x 5= 5 Marks	

General Instructions

1. Time duration of each theory paper will be of two and half hours.
2. Total marks of each theory paper will be 70 marks.
3. There will be internal option for all the questions (as shown in table above)
4. All questions are compulsory

BI.304 Immunology and Immunotechnology
(Theory)

UNIT 1

- Types of immunity- innate, acquired, passive and active.
- Physiology of immune response- HI and CMI specificity and memory.
- Cells and Organs of Immune system

UNIT 2

- Antigen-antibody reactions.
- Antigens- types- hapten.
- Immunoglobulins - structure, distribution and function.
- Immunoregulation - helper and suppressor cells, specific factors. Idiotypic network. Immune response genes. Immunological tolerance

UNIT 3

- MHC – Classification, Structure and function .MHC-restriction
- T –cell and B – cell receptors
- T –cell maturation, Activation & differentiation
- B-cell maturation, Activation & differentiation

UNIT 4

- The complement systems- mode of activation, classical and alternate pathway, biological functions
- Transplantation immunity- organ transplantation and HLA tissue typing.
- Hypersensitivity reactions.
- Autoimmune disorders

UNIT 5

- Immunology of infectious diseases: Tuberculosis, Malaria, Amoebiasis, Rabies, Typhoid, AIDS
- Immunodiagnosis of infectious disease
- Hybridoma techniques and monoclonal antibody production
- Methods of vaccine preparation

BI.304 Immunology and Immunotechnology
(Practical)

Based on theory syllabus

Reference Books:

- Immunology by I.M. Roitt, J. Brostoff and D.K. Male (1993) Gower medical publishing, London.
- Immunology – A short course by E. Benzamini, G. Sunshine and Leskpwitz, Willy – Liss 1996..
- Janis Kubey, Immunology ,W.H.Freeman and Co.,New York, 2002

FACULTY OF SCIENCE

Syllabus

Subject: **BIOINFORMATICS**

Course (Paper) Name & No.: Medicinal Chemistry (BI-305)

Course (Paper) Unique Code: 1603 2200 0103 0500

External Exam Time Duration: 2 Hours and 30 minutes

Name of Program	Semester	Course Group	Credit	Internal Marks	External Marks	Practical /Viva Marks	Total Marks
Bachelor of Science	03	Core	4	30	70	50	150

Course Objective:

- To understand the structure, functions of small molecules & drugs

**COURSE STRUCTURE FOR UG PROGRAMME
BIOINFORMATICS- 305
SEMESTER- III**

Semester	Course	Title	Hours /week	Credit	Exam duration	Internal marks	External marks	Total marks
I	BI-305 (Theory)	Medicinal Chemistry	5	3	2.5 hrs	30	70	100
I	BI-305 (Practical)	Medicinal Chemistry	3	2	One day per batch	15	35	50
Total credits				5	Total marks			150

General instructions

1. The medium of instruction will be English for theory and practical courses
2. There will be 5 lectures / week / theory paper / semester.
3. Each lecture will be of 55 mins.
4. There will be 1 practical / week / paper / batch. Each practical will be of 3 periods
5. Each semester theory paper will be of “five” units. There will be 50 hrs. of theory teaching / paper / semester.
6. Each Theory Paper / Semester will be of 100 Marks. There will be 30 marks for internal evaluation and 70 marks for external evaluation. Each Practical Paper / Semester will be of 50 Marks with 15 marks for internal and 35 marks for external evaluation. So, Total Marks of Theory and Practical for each Paper will be 150. (100 + 50 = 150)

SKELETON OF THEORY EXAMINATION PAPER -EXTERNAL

(SEMESTER- III)

Total five questions. One question from each unit. Each question having equal weightage of 14 Marks		
a) Four One mark questions (All compulsory)	4 x 1= 4 Marks	14 Marks
b) Answer specifically- (attempt any one out of two)	1 x 2= 2 Marks	
c) Short Questions - (attempt any one out of two)	1 x 3= 3 Marks	
d) Answer in detail – (attempt any one out of two)	1 x 5= 5 Marks	

General Instructions

1. Time duration of each theory paper will be of two and half hours.
2. Total marks of each theory paper will be 70 marks.
3. There will be internal option for all the questions (as shown in table above)
4. All questions are compulsory

BL.305 Medicinal Chemistry **(Theory)**

Unit I: Drug Targets: Pharmacodynamics and pharmacokinetics

- Drugs and drug targets: an overview
- Enzymes as drug targets
- Receptors as drug targets
- Nucleic acids as drug targets
- Miscellaneous drug targets
- Pharmacokinetics and related topics

Unit II: Drug discovery, design, and development

- Drug discovery: finding a lead
- Drug design: optimizing target interactions

Unit III: Drug discovery, design, development, and tools of the trade

- Drug design: optimizing access to the target
- Getting the drug to market
- Combinatorial and parallel synthesis

Unit IV: Selected topics in medicinal chemistry-1

- Antibacterial agents
- Antiviral agents
- Anticancer agents

Unit V: Selected topics in medicinal chemistry-2

- Cholinergics, anticholinergics, and anticholinesterases
- Drugs acting on the adrenergic nervous system
- The opioid analgesics
- Anti-ulcer agents

BL.305 Medicinal Chemistry **(Practical)**

Based on theory syllabus

Reference Books:

- An Introduction to Medicinal Chemistry 5th edition 2013 by Graham L. Patrick (ISBN: 978-0-19-969739-7)
- Drugs: From discovery to approval 2nd ed by Rick NG. Wiley Blackwell (2009)
- Burger's Medicinal Chemistry and Drug discovery. Volume 2, Drug Discovery and development. 6th Edition. Ed Donald J Abraham Wiley-Interscience.
- Essentials of Medical Pharmacology, 6th Edition (Hardcover) by Tripathi Kd. Publisher: Jaypee Brothers (2008)

FACULTY OF SCIENCE

Syllabus

Subject: **BIOINFORMATICS**

Course (Paper) Name & No.: Structural & Applied Bioinformatics (BI-401)

Course (Paper) Unique Code: 161603 2200 0104 0100

External Exam Time Duration: 2 Hours and 30 minutes

Name of Program	Semester	Course Group	Credit	Internal Marks	External Marks	Practical /Viva Marks	Total Marks
Bachelor of Science	04	Core	5	30	70	50	150

Course Objective:

- To uncover structure of Biomolecules through computational approach & applied Bioinformatics

**COURSE STRUCTURE FOR UG PROGRAMME
BIOINFORMATICS- 401
SEMESTER- IV**

Semester	Course	Title	Hours /week	Credit	Exam duration	Internal marks	External marks	Total marks
I	BI-401 (Theory)	Structural & Applied Bioinformatics	5	3	2.5 hrs	30	70	100
I	BI-401 (Practical)	Structural & Applied Bioinformatics	3	2	One day per batch	15	35	50
Total credits				5	Total marks			150

General instructions

1. The medium of instruction will be English for theory and practical courses
2. There will be 5 lectures / week / theory paper / semester.
3. Each lecture will be of 55 mins.
4. There will be 1 practical / week / paper / batch. Each practical will be of 3 periods
5. Each semester theory paper will be of “five” units. There will be 40 hrs. of theory teaching / paper / semester.
6. Each Theory Paper / Semester will be of 100 Marks. There will be 30 marks for internal evaluation and 70 marks for external evaluation. Each Practical Paper / Semester will be of 50 Marks with 15 marks for internal and 35 marks for external evaluation. So, Total Marks of Theory and Practical for each Paper will be 150. (100 + 50 = 150)

**SKELETON OF THEORY EXAMINATION PAPER -EXTERNAL
(SEMESTER- IV)**

Total five questions. One question from each unit. Each question having equal weightage of 14 Marks		
a) Four One mark questions (All compulsory)	4 x 1= 4 Marks	14 Marks
b) Answer specifically- (attempt any one out of two)	1 x 2= 2 Marks	
c) Short Questions - (attempt any one out of two)	1 x 3= 3 Marks	
d) Answer in detail – (attempt any one out of two)	1 x 5= 5 Marks	

General Instructions

1. Time duration of each theory paper will be of two and half hours.
2. Total marks of each theory paper will be 70 marks.
3. There will be internal option for all the questions (as shown in table above)
4. All questions are compulsory

BL.401 Structural & Applied Bioinformatics

(Theory)

Unit I: Data collection, analysis, and visualization.

- Defining bioinformatics and structural bioinformatics
- Fundamentals of protein, DNA & RNA structure
- Computational aspects of high-throughput crystallographic macromolecular structure determination
- Macromolecular structure determination by NMR spectroscopy, electron microscopy in the context of structural systems biology
- Study of protein three-dimensional structure and dynamics using peptide amide hydrogen/ deuterium exchange mass spectrometry (DXMS) and chemical cross-linking with mass spectrometry to constrain molecular modeling
- Search and sampling in structural bioinformatics
- Molecular visualization

Unit II: Data representation, databases, data integrity and comparative features

- The PDB format, MMCIF formats, and other data formats
- The worldwide protein data bank, the nucleic acid database
- Other structure-based databases
- Structural quality assurance
- The impact of local accuracy in protein and RNA structures: validation as an active tool
- Structure comparison and alignment
- Protein structure evolution and the SCOP and CATH domain structure database

Unit III: Structural and functional assignment

- Secondary structure assignment
- Identifying structural domains in proteins
- Inferring protein function from structure
- Structural annotation of genomes
- Evolution studied using protein structure

Macromolecular interactions

- Electrostatic interactions
- Prediction of protein–nucleic acid interactions
- Prediction of protein–protein interactions from evolutionary information

Unit IV: Structure prediction

- CASP and other community-wide assessments to advance the field of structure prediction
- Prediction of protein structure in 1D: secondary structure, membrane regions, and solvent accessibility
- Homology modeling, Fold recognition methods, de novo protein structure prediction: methods and application
- RNA structural bioinformatics

Therapeutic discovery

- Structural bioinformatics in drug discovery
- B-Cell epitope prediction

Future challenges in Structural Bioinformatics

- Methods to classify and predict the structure of membrane proteins
- Protein motion: Simulation
- The significance and impacts of protein disorder and conformational variants
- Protein designability and engineering
- Structural genomics of protein superfamilies

Unit V: Applied Bioinformatics

- Commercial Bioinformatics
- Bioinformatics Companies & Research Institutes – India & International
- Genomics, Transcriptomics & Proteomics in Medicine
- Applied fields of Bioinformatics (Basic Concepts): Immunoinformatics&Neuroinformatics, Clinical Bioinformatics, Nanoinformatics
- Web Resources for Stem Cell Research
- Intellectual Property Rights(IPR) & Patents
- Biosafety & Bioethics

BI.401 Structural & Applied Bioinformatics (Practical)

Based on theory syllabus

References

- Jenny Gu (Editor), Philip E. Bourne (Editor), Structural Bioinformatics (ISBN: 978-0-470-18105-8), 2nd Edition, February 2009, Wiley-Blackwell
- Wei T, Peng X, Ye L, Wang J, Song F, Bai Z, Han G, Ji F, Lei H. Web resources for stem cell research. *Genomics Proteomics Bioinformatics*. 2015 Feb;13(1):40-5. doi: 10.1016/j.gpb.2015.01.001. Review. PubMed PMID: 25701763; PubMed Central PMCID: PMC4411488. Primrose and Twyman R.M: Principles of Genome analysis: Blackwell publication
- Backert L, Kohlbacher O. Immunoinformatics and epitope prediction in the age of genomic medicine. *Genome Med*. 2015 Nov 20;7:119. doi: 10.1186/s13073-015-0245-0. Review. PubMed PMID: 26589500; PubMed Central PMCID: PMC4654883.
- Tomar N, De RK. Immunoinformatics: a brief review. *Methods Mol Biol*. 2014;1184:23-55. doi: 10.1007/978-1-4939-1115-8_3. Review. PubMed PMID: 25048118.
- Bloom FE, Morrison JH, Young WG. Neuroinformatics: a new tool for studying the brain. *J Affect Disord*. 2006 May;92(1):133-8. Review. PubMed PMID: 16488481.
- Bellazzi, R., Masseroli, M., Murphy, S., Shabo, A., & Romano, P. (2012). Clinical Bioinformatics: challenges and opportunities. *BMC bioinformatics*, 13(Suppl 14), S1.
- Panneerselvam S, Choi S. Nanoinformatics: emerging databases and available tools. *Int J Mol Sci*. 2014 Apr 25;15(5):7158-82. doi: 10.3390/ijms15057158. Review. PubMed PMID: 24776761; PubMed Central PMCID: PMC4057665.
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- Baxevanis A.D & Ouellette B.F.F: Bioinformatics-A Practical guide to the analysis of Genes and Proteins: *John Wiley & Sons, INC. Publication*
- Andrade M.A: Bioinformatics & Genomes-Current Perspectives: *Horizon Scientific press*
- Lesk. A.M: Introduction to Bioinformatics: *Oxford Press.*
- Mount. D.W: Bioinformatics sequence and Genome Analysis: *Cold spring Harbor Laboratory Press.*
- Higgins. D and Taylor.W: Bioinformatics – Sequence, structure and databanks: *Oxford University press.*
- Nelson.D.L and Cox.M.M : Lehninger- Principles of Biochemistry: *Mac Milan Worth Publication.*
- Stryer: Biochemistry: *W.H. Fedman & co.*
- Orengo.C.A, Jones.D.T, J.M.Thornton: Bioinformatics – Genes, Proteins & Computers: *BIOS Scientific Publishers Ltd.*
- Ralph Rapley and Stuart Harbron: Molecular Analysis and Genome Discovery: *John Wiley & Sons Ltd*
- Campbell. M. K: Biochemistry, 3rd edition: *Harcourt Brace college Publishers*

FACULTY OF SCIENCE

Syllabus

Subject: **BIOINFORMATICS**

Course (Paper) Name & No.: Genetic Engineering (BI-402)

Course (Paper) Unique Code: 1603 2200 0104 0200

External Exam Time Duration: 2 Hours and 30 minutes

Name of Program	Semester	Course Group	Credit	Internal Marks	External Marks	Practical /Viva Marks	Total Marks
Bachelor of Science	04	Core	5	30	70	50	150

Course Objective:

- To understand basics of Genetic engineering techniques

**COURSE STRUCTURE FOR UG PROGRAMME
BIOINFORMATICS- 402
SEMESTER- IV**

Semester	Course	Title	Hours /week	Credit	Exam duration	Internal marks	External marks	Total marks
I	BI-402 (Theory)	Genetic Engineering	5	3	2.5 hrs	30	70	100
I	BI-402 (Practical)	Genetic Engineering	3	2	One day per batch	15	35	50
Total credits				5	Total marks			150

General instructions

1. The medium of instruction will be English for theory and practical courses
2. There will be 5 lectures / week / theory paper / semester.
3. Each lecture will be of 55 mins.
4. There will be 1 practical / week / paper / batch. Each practical will be of 3 periods
5. Each semester theory paper will be of “five” units. There will be 50 hrs. of theory teaching / paper / semester.
6. Each Theory Paper / Semester will be of 100 Marks. There will be 30 marks for internal evaluation and 70 marks for external evaluation. Each Practical Paper / Semester will be of 50 Marks with 15 marks for internal and 35 marks for external evaluation. So, Total Marks of Theory and Practical for each Paper will be 150. (100 + 50 = 150)

SKELETON OF THEORY EXAMINATION PAPER -EXTERNAL

(SEMESTER- IV)

Total five questions. One question from each unit. Each question having equal weightage of 14 Marks		
a) Four One mark questions (All compulsory)	4 x 1= 4 Marks	14 Marks
b) Answer specifically- (attempt any one out of two)	1 x 2= 2 Marks	
c) Short Questions - (attempt any one out of two)	1 x 3= 3 Marks	
d) Answer in detail – (attempt any one out of two)	1 x 5= 5 Marks	

General Instructions

1. Time duration of each theory paper will be of two and half hours.
2. Total marks of each theory paper will be 70 marks.
3. There will be internal option for all the questions (as shown in table above)
4. All questions are compulsory

BI.402 Genetic Engineering **(Theory)**

UNIT 1

- Techniques in gene manipulation – Steps involved in Genetic engineering
- Cutting and Joining DNA
- Restriction and modification enzymes
- Polymerases, Ligase, kinases and phosphatases

UNIT 2

- Isolation and purification of DNA (genomic and plasmid) and RNA
- Introduction of DNA into cells using Gene transfer techniques
- Cloning vectors – Plasmids, Phages, Cosmid, YACs, BACs Expression vectors
- Construction of genomic libraries and cDNA libraries

UNIT 3

- Analysis of recombinant DNA - Sequencing, mutagenesis
- PCR - Polymerase chain reactions: Primer design, heat stable polymerases, types of PCR and application
- Ligase chain reaction
- RFLP mapping, chromosome walking and jumping

UNIT 4

- Screening and characterization of clones Expression systems and their applications. *E.coli*, *Streptomyces*, *Yeast*, *Baculovirus* and animal cells as cloning hosts.
- Molecular Diagnostics-High throughput screening.
- Expression arrays and DNA arrays.
- Expression based screening.
- Interaction based screening: yeast two-hybrid system

UNIT 5: Web resources for Genetic Engineering

- Primer & Probe Designing tools
- SNP: Types, databases, Tools
- *In silico* molecular cloning experiments: UGENE, Serial Cloner, SnapGene, Molecular Cloning Designer Simulator, etc..
- Synthetic biology: Overview, Tools and applications

BI.402 Genetic Engineering (Practical)

Based on theory syllabus

References:

- Levin B 1994. Genes V Oxford University Press.
- RN.Old and SB. Primrose 1994. Principles of gene manipulation IV edition, Blackwell pub. Ny.
- Molecular cloning – A Laboratory manual 1993. sambrooketal.
- R-DNA – W.H. Freeman & co. NY. 1992 – by Woston JD, M. Gilman J. Witkowski and M.Zoller.
- **Gene Cloning: An Introduction.** by **T. A. BROWN**; Chapman and Hall, 1990; 2nd Edition
- <https://ugene.net/wiki/display/UUOUM15/About+UGENE>
- Serial Cloner: http://serialbasics.free.fr/Serial_Cloner.html
- SnapGene: <http://www.snapgene.com/>
- Molecular Cloning Designer Simulator: <https://mcds.codeplex.com/>
- Mathur M, Xiang JS, Smolke CD. Mammalian synthetic biology for studying the cell. J Cell Biol. 2016 Dec 8. pii: jcb.201611002. [Epub ahead of print] Review. PubMed PMID: 27932576.
- Macnaghten P, Owen R, Jackson R. Synthetic biology and the prospects for responsible innovation. Essays Biochem. 2016 Nov 30;60(4):347-355. Review. PubMed PMID: 27903822.
- MacDonald IC, Deans TL. Tools and applications in synthetic biology. Adv Drug Deliv Rev. 2016 Oct 1;105(Pt A):20-34. doi: 10.1016/j.addr.2016.08.008. Review. PubMed PMID: 27568463.

FACULTY OF SCIENCE

Syllabus

Subject: **BIOINFORMATICS**

Course (Paper) Name & No.: Web Technology (BI-403)

Course (Paper) Unique Code: 1603 2200 0104 0300

External Exam Time Duration: 2 Hours and 30 minutes

Name of Program	Semester	Course Group	Credit	Internal Marks	External Marks	Practical /Viva Marks	Total Marks
Bachelor of Science	04	Core	5	30	70	50	150

Course Objective:

- To understand basic of web designing and databases connectivity

**COURSE STRUCTURE FOR UG PROGRAMME
BIOINFORMATICS- 403
SEMESTER- IV**

Semester	Course	Title	Hours /week	Credit	Exam duration	Internal marks	External marks	Total marks
I	BI-403 (Theory)	Web Technology	5	3	2.5 hrs	30	70	100
I	BI-403 (Practical)	Web Technology	3	2	One day per batch	15	35	50
Total credits				5	Total marks			150

General instructions

1. The medium of instruction will be English for theory and practical courses
2. There will be 5 lectures / week / theory paper / semester.
3. Each lecture will be of 55 mins.
4. There will be 1 practical / week / paper / batch. Each practical will be of 3 periods
5. Each semester theory paper will be of “five” units. There will be 50 hrs. of theory teaching / paper / semester.
6. Each Theory Paper / Semester will be of 100 Marks. There will be 30 marks for internal evaluation and 70 marks for external evaluation. Each Practical Paper / Semester will be of 50 Marks with 15 marks for internal and 35 marks for external evaluation. So, Total Marks of Theory and Practical for each Paper will be 150. (100 + 50 = 150)

SKELETON OF THEORY EXAMINATION PAPER -EXTERNAL

(SEMESTER- IV)

Total five questions. One question from each unit. Each question having equal weightage of 14 Marks		
a) Four One mark questions (All compulsory)	4 x 1= 4 Marks	14 Marks
b) Answer specifically- (attempt any one out of two)	1 x 2= 2 Marks	
c) Short Questions - (attempt any one out of two)	1 x 3= 3 Marks	
d) Answer in detail – (attempt any one out of two)	1 x 5= 5 Marks	

General Instructions

1. Time duration of each theory paper will be of two and half hours.
2. Total marks of each theory paper will be 70 marks.
3. There will be internal option for all the questions (as shown in table above)
4. All questions are compulsory

BI.403 Web Technology **(Theory)**

Unit I: Introduction to WWW (World Wide Web) and Internet

- HTML (Hyper Text Markup Language)
- DHTML (Dynamic HTML)
- More Programming Power to HTML, Clickable maps, MPEG and other formats
- Client - Server Technology, Server Side Applications
- Basic of XML

Unit II: Introduction to PHP

- PHP configuration in IIS and Apache web server
- Web protocol: HTTP, PHP variable, static and global, Form processing, get and post methods, PHP operator

Decision Making

- Conditional structure, looping structure, Arrays, Functions: user defined Functions, variable length argument function, Variable function
- Array function, String function, Math function, Date function, File handling function, Miscellaneous functions.

Unit III: Introduction to Database Systems

- Definition, Concepts of various types of databases,
- Characteristics of database approach
- Advantages of Using a DBMS

Database System Concepts and Architecture

- Schemas, and Instances, Entity Types, Entity Sets, Attributes, and Keys
- DBMS Architecture and Data Independence

Data Modeling Using the Entity-Relationship Model

- The Database System Environment, Data Models, Types of Databases and Relationships, Constraints, Using High-Level Conceptual Data Models for Database Design

Unit IV: SQL - Queries

- Introduction to SQL, SQL commands and data types, Operators and Expression
- **Managing tables and data:** Select statements, creating and altering tables (including constraints), data manipulations statements, data control statements, built in functions, Grouping Data.

Unit V: Introduction to MYSQL and Interfacing with Databases through PHP

- Working with MYSQL data, Connecting to MYSQL with PHP
- Creating, viewing, Modifying, Fetching, data from tables and displaying in proper format.

BI.403 Web Technology
(Practical)

Based on theory syllabus

References:

- RamezElmasri, Shamkant B. Navathe, Fundamentals of database systems, third edition
- Raghu Ramakrishnan, Johannes Gehrke, *Database Management System*, McGraw Hill, 3rd Edition 2003
- Ivan Bayross, SQL.PL/SQL The programming – Language of Oracle, BPB Publications.
- VikramVaswani, The Complete Reference MySQL, Tata McGraw-Hill, New Delhi, 2002
- Mastering HTML 4: Ray & Ray- BPB
- Advances Programming in Web Design: V. K Jain-Cyber Tech Publications
- PHP Bible, second edition, Tim Converse, Joyce Park
- PHP manual

Annexure – “C”

FACULTY OF SCIENCE

Syllabus

Subject: **BIOINFORMATICS**

Course (Paper) Name & No.: Object oriented Programming using JAVA (BI-404)

Course (Paper) Unique Code: 1603 2200 0104 0400

External Exam Time Duration: 2 Hours and 30 minutes

Name of Program	Semester	Course Group	Credit	Internal Marks	External Marks	Practical /Viva Marks	Total Marks
Bachelor of Science	04	Core	5	30	70	50	150

Course Objective:

- To understand basic JAVA & develop program using JAVA

COURSE STRUCTURE FOR UG PROGRAMME
BIOINFORMATICS- 404
SEMESTER- IV

Semester	Course	Title	Hours /week	Credit	Exam duration	Internal marks	External marks	Total marks
I	BI-404 (Theory)	Object oriented Programming using JAVA	5	3	2.5 hrs	30	70	100
I	BI-404 (Practical)	Object oriented Programming using JAVA	3	2	One day per batch	15	35	50
Total credits				5	Total marks			150

General instructions

1. The medium of instruction will be English for theory and practical courses
2. There will be 5 lectures / week / theory paper / semester.
3. Each lecture will be of 55 mins.
4. There will be 1 practical / week / paper / batch. Each practical will be of 3 periods
5. Each semester theory paper will be of “five” units. There will be 50 hrs. of theory teaching / paper / semester.
6. Each Theory Paper / Semester will be of 100 Marks. There will be 30 marks for internal evaluation and 70 marks for external evaluation. Each Practical Paper / Semester will be of 50 Marks with 15 marks for internal and 35 marks for external evaluation. So, Total Marks of Theory and Practical for each Paper will be 150. (100 + 50 = 150)

**SKELETON OF THEORY EXAMINATION PAPER -EXTERNAL
(SEMESTER- IV)**

Total five questions. One question from each unit. Each question having equal weightage of 14 Marks		
a) Four One mark questions (All compulsory)	4 x 1= 4 Marks	14 Marks
b) Answer specifically- (attempt any one out of two)	1 x 2= 2 Marks	
c) Short Questions - (attempt any one out of two)	1 x 3= 3 Marks	
d) Answer in detail – (attempt any one out of two)	1 x 5= 5 Marks	

General Instructions

1. Time duration of each theory paper will be of two and half hours.
2. Total marks of each theory paper will be 70 marks.
3. There will be internal option for all the questions (as shown in table above)
4. All questions are compulsory

BI.404: Object oriented Programming using JAVA **(Theory)**

UNIT 1: Basics

- Introduction to Java Programming Language: History and features, JDK and its components, byte code and JVM
- Data types and Operators
- Selection Statement: IF, IF...ELSE, ELSE IF LADDER, SWITCH...CASE
- Loop statements: while, do...while, for, labeled for
- Jumping statements: break, continue

UNIT 2: Class Fundamentals

- Defining classes, Creating objects
- Constructor
- Inheritance
- Polymorphism
- overloading and overriding of methods
- visibility control and modifier

UNIT 3: Packages, Multithreading and Exception handling

- Java API packages, Creating and using packages
- Applications of packages
- Multithreading programming
- Applications of threads, synchronization, dead lock
- Handling exceptions: try...catch, try...multiple catch, finally, throw, throws
- Creating user defined exception

UNIT 4: Input and Output

- Concept of Streams
- Difference between Character streams and Byte streams
- Character Streams
- (Reader,Writer,BufferedReader,InputStreamReader, OutputStreamReader,FileReader, FileWriter,Bufferwriter,PrintWriter)
- ByteStreams
- OtherClasses

UNIT 5: Applet & Swing

Applet:

- Introduction to Applet, life cycle
- Applet context class, passing parameters to applet
- Graphics class and various methods in an applet

- Event handling, AWT controls

Swing:

- Introduction to Swing
- Swing vs AWT, container class
- Swing components (JApplet, JButton, JCheckbox, Jcheckboxgroup, JChoice, JTextfield, JTextarea, Jlist, JScrollbar, Jpanel, JFrame, Jmenu, Jmenubar, JMenuItem, Jpasswordfield, JRadiobutton)
- Application development using Swing

BI.404: Object oriented Programming using JAVA
(Practical)

Based on theory syllabus

Reference Books:

- Programming with Java: E. Balaguruswamy- TMH Publications
- The Complete reference Java 2 – Herbert Schildt and Patrick Naughton
- Teach Yourself Java: Joseph O' Neil, TMH publications

Annexure – “C”

FACULTY OF SCIENCE

Syllabus

Subject: **BIOINFORMATICS**

Course (Paper) Name & No.: Cheminformatics (BI-405)

Course (Paper) Unique Code: 1603 2200 0104 0500

External Exam Time Duration: 2 Hours and 30 minutes

Name of Program	Semester	Course Group	Credit	Internal Marks	External Marks	Practical /Viva Marks	Total Marks
Bachelor of Science	04	Core	4	30	70	50	150

Course Objective:

- To understand Cheminformatics and drug designing

COURSE STRUCTURE FOR UG PROGRAMME
BIOINFORMATICS- 405
SEMESTER- IV

Semester	Course	Title	Hours /week	Credit	Exam duration	Internal marks	External marks	Total marks
I	BI-405 (Theory)	Cheminformatics	5	3	2.5 hrs	30	70	100
I	BI-405 (Practical)	Cheminformatics	3	2	One day per batch	15	35	50
Total credits				5	Total marks			150

General instructions

1. The medium of instruction will be English for theory and practical courses
2. There will be 5 lectures / week / theory paper / semester.
3. Each lecture will be of 55 mins.
4. There will be 1 practical / week / paper / batch. Each practical will be of 3 periods
5. Each semester theory paper will be of “five” units. There will be 50 hrs. of theory teaching / paper / semester.
6. Each Theory Paper / Semester will be of 100 Marks. There will be 30 marks for internal evaluation and 70 marks for external evaluation. Each Practical Paper / Semester will be of 50 Marks with 15 marks for internal and 35 marks for external evaluation. So, Total Marks of Theory and Practical for each Paper will be 150. (100 + 50 = 150)

SKELETON OF THEORY EXAMINATION PAPER -EXTERNAL

(SEMESTER- IV)

Total five questions. One question from each unit. Each question having equal weightage of 14 Marks		
a) Four One mark questions (All compulsory)	4 x 1= 4 Marks	14 Marks
b) Answer specifically- (attempt any one out of two)	1 x 2= 2 Marks	
c) Short Questions - (attempt any one out of two)	1 x 3= 3 Marks	
d) Answer in detail – (attempt any one out of two)	1 x 5= 5 Marks	

General Instructions

1. Time duration of each theory paper will be of two and half hours.
2. Total marks of each theory paper will be 70 marks.
3. There will be internal option for all the questions (as shown in table above)
4. All questions are compulsory

BL.405 Cheminformatics **(Theory)**

UNIT I: Introduction to Cheminformatics

- Introduction to Cheminformatics - History and evolution of Cheminformatics
- Chemical representation - Sequence, 2D, 3D structure
- Types of chemical representation - linear notation, tabular storage, graphical representation
- Chemical data management - Chemical markup languages.

UNIT II: Chemical Databases

- Chemical Databases: Examples- CHEMDB, KEGG LIGAND, CSD, CAS REGISTRY, BIOMETA DB, National Cancer Institute Database(NCI) , PubChem, chEMBL, DrugBank, etc.
- Chemical searching methods - exact searching, sub structure searching, similarity searching, reaction searching.

UNIT III: Combinatorial Library Design

- Combinatorial library design - Rational principles of compound selection for combinatorial library design and optimization approach, Descriptor Analysis, Modeling toxicity
- Computer Assisted Synthesis design and structure based library design.

UNIT IV: Application of Cheminformatics-1

- Application of Cheminformatics in Drug Design
- QSAR & QSPR
- Novel Drug Target Identification
- Target Fishing for Chemical Compounds

UNIT V: Application of Cheminformatics-2

- Structure Based Drug Discovery: Target identification and Validation, lead finding and optimization
- Ligand Based drug Discovery
- Pharmacophore-Based Drug Design

BI.405 Cheminformatics
(Practical)

Based on theory syllabus

Reference Books:

- Andrew Leach, Molecular Modelling: Principles and Applications (2nd Edition), Addison Wesley Longman, Essex, England, 1996.
- Johann Gasteiger, Dr. Thomas Engel, "Cheminformatics", Wiley-VCH Press
- Alan Hinchliffe, Modelling Molecular Structures, 2nd Edition, John-Wiley, 2000.
- Alan Hinchliffe, Molecular Modelling for Beginners, John-Wiley, 2003.
- N. Cohen (Ed.), Guide Book on Molecular Modeling in Drug Design, Academic Press, San Diego, 1996.
- D. Frenkel and B. Smith, Understanding Molecular Simulations. From Algorithms to Applications, Academic Press, San Diego, California, 1996.
- C. Rauter and K. Horn, X-ray crystallography and drug design, Elsevier, 1984.
- M. Kalos and P. A. Whitlock, Monte Carlo Methods. John Wiley & Sons, New York, 1986.
- J.A. McCammon and S.C. Harvey. Dynamics of Proteins and Nucleic Acids. Cambridge University Press, Cambridge, 1987.