Resolution Number: AC/II(23-24).2.RUS1

S. P. Mandali's

Ramnarain Ruia Autonomous College

(Affiliated to University of Mumbai)



Syllabus For:

Program: Integrated M.Sc. in Bioanalytical Sciences

(T.Y. B.Sc. Sem V Syllabus)

Program Code: RUSBAS

(Credit Based Semester and Grading System for the academic year 2024-25)

GRADUATE ATTRIBUTES

GA	GA Description		
	A student completing Bachelor's Degree in Science program		
	will be able to:		
GA 1	Recall and explain acquired scientific knowledge in a		
	comprehensive manner and apply the skills acquired in their		
	chosen discipline. Interpret scientific ideas and relate its		
	interconnectedness to various fields in science.		
GA 2	Evaluate scientific ideas critically, analyse problems, explore		
	options for practical demonstrations, illustrate work plans and		
	execute them, organise data and draw inferences.		
GA 3	Explore and evaluate digital information and use it for knowledge		
un 3	upgradation. Apply relevant information so gathered for analysis		
	and communication using appropriate digital tools.		
	and communication using appropriate digital tools.		
GA 4	Ask relevant questions, understand scientific relevance,		
	hypothesize a scientific problem, construct and execute a project		
	plan and analyse results.		
GA 5	Take complex challenges, work responsibly and independently, as		
	well as in cohesion with a team for completion of a task.		
	Communicate effectively, convincingly and in an articulate manner.		
GA 6	Apply scientific information with sensitivity to values of differen		
	cultural groups. Disseminate scientific knowledge effectively for		
	upliftment of the society.		
GA 7	Follow ethical practices at work place and be unbiased and critical		
	in interpretation of scientific data. Understand the environmental		
	issues and explore sustainable solutions for it.		
GA 8	Keep abreast with current scientific developments in the specific		
	discipline and adapt to technological advancements for better		
	application of scientific knowledge as a lifelong learner.		

Program Outcomes (PO)

PO	Description		
	A student completing Bachelor's Degree in Science program in the subject of Bioanalytical Sciences will be able to:		
PO 1	Gain high quality science education in a vibrant academic ambience with the faculty of distinguished teachers and scientists.		
PO 2	Take up the challenge of doing quality research and teaching and also contribute to industrial production and R & D in the fields of Bioanalysis, Bioinformatics and Nutraceutical Sciences.		
PO 3	Amalgamate classical analytical chemical techniques with modern genomic and proteomic technologies of manufacturing and analysis to better characterize the products useful as medicines as well as nutraceuticals.		

Course Title: Entrepreneurship Skills

Academic Year 2024-25

T.Y.B.Sc.

COURSE	DESCRIPTION	
OUTCOME	90	
CO 1	Encouraged to start their own enterprise after getting the insights from	
	the course.	
CO2	Prepare for the required skill set of an entrepreneur and also realize	
	the challenges in this area.	

Paper Code	Semester V	Lectures
RUSBAS501	ENTREPRENEURSHIP SKILLS	40
501.1 The Ent	epreneur	10
1. Entrepreneu	rial motivation – dynamics of motivation.	
2. Developing E	ntrepreneurial competencies - requirements and understanding	
the process of	f entrepreneurship development, self-awareness, interpersonal	
skills, creativ	ity, assertiveness, achievement, factors affecting entrepreneur's	
role.		
3. Case study of	Successful Entrepreneurs from India.	
501.2 Concept	ual Frame Work	10
_	d and process in entrepreneurship development.	
	e Global Business Environment in post Reform Time, LPG Reforms	
in India.		
7 -	erprise – Merits and Demerits	
	policies and schemes for enterprise development	
5. Mudra Yojan		
501.3 Business		10
	ysis, concept & types of demand, law of demand	
	to Cost & Revenue, its types	
	ation (Various types of Cost Concepts)	
, ,	tation / targeting / positioning)	
5. P's of Market		
	ons and Agreements with Reference to TRIPS, TRIMS and GATS.	
	an Start Ups, case study approach	
501.4 Knowled		10
1. Introduct		
2. History at		
	Knowledge Management ignificance Technology & Knowledge Management.	
	iccess Factors of KM	
6. Case Stud		
o. Jase blad	100	

RUSBASP501 PRACTICALS

- 1. Case Study/Assignment/Project Report/Industrial Visit
- 2. Work management tools Google sheets
- 3. Preparing Project plan/ Project management

Entrepreneurship Skills	Eric Ries: The Lean StartupKimiz Dalkir: Knowledge Management in theory and
	Practice • Jugaad Innovation: Radjou, Prabhu, Ahuja

Course Title: Biological Sciences V

Academic Year 2024-25

T.Y.B.Sc.

COURSE OUTCOMES:

COURSE	DESCRIPTION
OUTCOME	30
CO 1	Understand and design basic cloning experiments to obtain genetically modified organisms. They should be sensitized regarding ethical guidelines of cloning.
CO2	To identify the importance of phytochemicals as possible drug candidates and learn the techniques to extract phytochemicals from plants

Paper Code	Semester V	Lectures
RUSBAS502	Biological Sciences V	45
502.1: Recomb	inant DNA Technology	15
Restriction Enzy Plants and Anima	ression vectors (Plasmids, Phages, Cosmids, YACs, BACs, etc.), mes, process of generating recombinant DNA, Transgenic Bacteria, als: Commercial applications with suitable examples (Any Two), ransposonsas genetic tools, Cloning- current Status, Regulations,	
metabolites, Fun Terpenoids, Alka	nemistry condary metabolites from plants, Classification of Plant Secondary ctions of Plant Secondary Metabolites, Chemistry of Phenolics, lloids, Key factors affecting synthesis of secondary metabolites, as Drugs, Commercial applications	15
Extraction of pl modern methods Steam Distillatio	on Technologies for Phytochemicals nytoconstituents, Choice of solvent for extraction, classical and s of extraction, Percolation & Maceration, Soxhlet extraction, in & Rotary vacuum evaporator, Liquid-Liquid & Solid Phase sonication, Microwave Assisted Extraction, Supercritical Fluid	15

RUSBASP502 PRACTICALS

- 1. Extraction of phytoconstituents by maceration, percolation, steam distillation and using Soxhlet extractor
- 2. Qualitative tests for Phytoconstituents
- 3. Study of antimicrobial activity of phytoconstituents
- 4. Extraction of Genomic DNA from suitable plant or microbial material
- 5. Microscopic evaluation of plants
- 6. Problems on Restriction enzyme digestion

Biological	Molecular Biotechnology: Glick
Sciences V	Biotechnology and Genetic Engineering: Kathy Wilson
	Gene Cloning : T.A.Brown
	 Text book of Pharmacognosy: G.E.Trease, W.C. Evans
	 Herbal Drug Technology: Agrawal, Paridhavi

Course Title: Chemical Sciences V

Academic Year 2024-25

T.Y.B.Sc.

COURSE OUTCOME	DESCRIPTION
CO 1	To get acquainted with the basic concepts of atomic and molecular spectroscopy and their applications in bioanalysis also to choose the correct method for analysis based on chemical property of analyte and objective of analysis.
CO2	Introduction to concepts of Raman Spectroscopy and applications of the same.

Paper Code	Semester V	Lectures
RUSBAS503	Chemical Sciences V	45
Flame Photomet Spectroscopy, Op 3. Quantitative application calibration curve me	roscopy rumentation	15
method. 503.2 Molecular Spectro		15
Molecular Fluorescence and Theory, instrumentation as polarization of a bond, born structure. Rotational Spectrigid rotor, moment of inexpectrum, determination of Vibrational spectrum: (In Vibrational motion, degree spectrum of a diatomic motion and the spectrum of a diatomic motion, nature of spectrum. Vibrational-Rotational spectrum. Vibrational-Rotational spectrum of spectrum. Vibrational-Rotational spectrum. Vibrational-Rotational spectrum of spectrum. Vibrational-Rotational spectrum. Vibrational-Rotational spectrum of spectrum. Vibrational-Rotational spectrum of spectrum. Vibrational-Rotational spectrum of spectrum.	and Phosphorescence Spectroscopy: nd applications, Dipole moment: Dipole moment, nd moment, dipole moment and molecular trum:Rotational spectrum of a diatomic molecule, rtia, energy levels, selection rule, nature of of inter nuclear distance and isotopic shift.	13

503.3 Raman Spectroscopy & IR Spectroscopy

Raman Spectroscopy: Scattering of electromagnetic radiation, Rayleigh scattering, Raman scattering, nature of Raman spectrum, Stoke's lines, Anti-Stoke's lines, Raman shift, quantum theory of Raman spectrum, comparative study of IR and Raman spectra, rule of mutual exclusion. (Example of CO_2 molecule)

Infrared spectroscopy: Diatomic Molecules, Polyatomic Molecules, Characteristic Vibration Frequencies, Factors Affecting Group Frequencies. Qualitative Analysis –Identification of Structural Features, Quantitative Analysis, Sampling Procedures, Near Infrared Spectrometry, Applications of Infrared Spectroscopy

15

Reference Books:

Chemical Sciences V

- Principles of instrumental analysis: Douglas a. Skoog
- Introduction to Spectroscopy: Donald L. Pavia
- Organic Spectroscopy: William Kemp
- Introduction to Molecular Spectroscopy: Gordon M. Barrow
- Molecular Luminescence Spectroscopy Methods and Applications John Wiley and sons
- Concept Instrumentation and techniques in Atomic Absorption Spectroscopy: Perkin Elmer

Course Title: Chemical Sciences VI

Academic Year 2024-25

T.Y.B.Sc.

COURSE OUTCOME	DESCRIPTION		
CO 1	Learn to interpret simple NMR spectra. Introduction to basic		
	concepts of hyphenated techniques which will be useful in		
	studying advanced instrumentation.		
CO2	Understand the importance of safe handling of biomatrices.		
	Should be familiar with routine diagnostic tests and advanced		
	instrumentation in pathological testing.		

Paper Code	Semester V	Lectures
RUSBAS504	Chemical Sciences VI	45
504.1 Nucle	ar Magnetic Spectroscopy	15
Chemical shif	t, Shielding and deshielding of protons, low resolution N.M.R.	
spectrum of m	nethanol and ethanol.	
PMR Spectros	copy: Basic theory of NMR, Nature of PMR spectrum, Chemical	
shift (∂ unit),	Standard for PMR, Solvents used, Factors affecting Chemical	
Shift: Inductiv	we effect, Anisotropic effect (with reference to C=C, $C\equiv C$, C=O	
and benzene	ring), Spin-spin coupling and coupling constant. Proton	
exchange app	lication of deuterium exchange, Application of PMR in structure	
determination	1.	
504.2 Bioch	emical methods of Analysis	15
Electrophoresis	s: PAGE, SDS-PAGE, Western Blotting, 2D gel electrophoresis, AGE,	
ELISA, Microar	ray	
504.3 Bioan	alysis	15
Introduction	to Bioanalysis, Different sample matrices and special	
precautions to	be taken while handling clinical samples	
Biochemical a	nalysis of clinical samples: Glucose, calcium,	
kidney test, liv	ver test, electrolytes, proteins, complete blood count.	
Advanced in	strumentation in Bioanalysis: Flowcytometer, blood gas	
analyzer, auto	omatic haematology analyzer, blood glucose analyzer, alcohol	
breath analyz	er	

RUSBASP503 PRACTICALS

- 1. Gravimetric estimation of Nickel as Ni-DMG
- 2. Antioxidant activity of any one sample
- 3. **Flame photometric determination-** Flame photometric determination of Li/Na/K by Calibration Curve and Standard addition methods
- 4. Spectroscopic Techniques:
 - i. Atomic absorption spectroscopy (AAS)- Sample preparation only
 - ii. Infrared (IR) analysis (Glucose and Glycine)
 - iii. Nuclear Magnetic Resonance (Demo)
- 5. Handling of a biofluid (e.g. Plasma)

Chemical	Principles of instrumental analysis: Douglas a. Skoog
Sciences VI	 Introduction to Spectroscopy: Donald L. Pavia
	Organic Spectroscopy: William Kemp
	 Introduction to hyphenated techniques and applications in
	pharmacy: Patel
	 Principle and practice of Bioanalysis: Richard F. Venn

Course Title: Computational Sciences V

Academic Year 2024-25

T.Y.B.Sc.

COURSE	DESCRIPTION	
OUTCOME	1/8%	
CO 1	Comprehend the logic behind dynamic programming algorithms.	
CO2	Effectively use bioinformatics algorithms like BLAST and FASTA for	
	sequence alignment and phylogenetic studies.	

Pa	Paper Code Semester V		Lectures
RU	RUSBAS505 Computational Sciences V		30
50	5.1 Dyna	mic Programming Algorithm	10
1.	Needleman	& Wunch, Smith & Waterman algorithms for Pairwise	
	alignment		
2.	Use of pai	rwise alignments for analysis of Nucleic acid and Protein	
	Sequences	and interpretation of results.	
3.	Overview of	of BLAST, its variants & working, BLAST algorithm	
4.	PSI BLAST	and PHI BLAST: Working and interpretation of result	
50	5.2 Multi	iple sequence alignment	10
1.	Concept of	multiple sequence alignment (MSA)	
2.	Algorithm	in MSA and its application	
3.	3. Multiple sequence alignment methods		
4.	PSSM		
_	5. MSA Tool: Clustal Omega- Working		
50	5.3 Mole	cular Phylogenetics	10
1.	Phylogenet	tic analysis	
2.	Basic conce	epts in taxonomy and phylogeny.	
3.	Definition	and description of Phylogenetic trees and various methods	
4.	_	method –UPGMA & NJ	
5.	Cladistic m	ethod – Maximum Parsimony	
6.	Phylogenet	tic Analysis software Phylip/PAUP	

RUSBASP504 PRACTICALS

- 1. Working with BLAST
- 2. Basic BLAST
 - i. Proteins
 - ii. Nucleotides
- 3. Advanced BLAST
 - i. PHI BLAST
 - ii. PSI BLAST
- 4. Working with FASTA
 - i. Proteins
 - ii. Nucleotides
- 5. Working of Clustal Omega
- 6. Phylogenetic Tree construction & Visualization
- 7. Basics of PHYLIP
- 8. Basics of PAUP

Computational	 Algorithms and Data structure: Niklaus Wirth
Sciences V	 The Art of Computer Programming: Donald E. Knuth
	 Multiple Sequence Alignment Methods: Russell and
	Springer
	 Molecular Evolution and Phylogenetics: Masatoshi Nei and
	Sudhir Kumar



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S. P. Mandali's Ramnarain Ruia Autonomous College

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Syllabus For:

Program: Integrated M.Sc. in Bioanalytical Sciences

(T.Y. B.Sc. Sem VI Syllabus)
Program Code: RUSBAS

(Credit Based Semester and Grading System for the academic year 2024-25)

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CAR		
GA 3	Explore and evaluate digital information and use it for knowledge	
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200	cultural groups. Disseminate scientific knowledge effectively for	
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0,9,		
GA 7	Follow ethical practices at work place and be unbiased and critical	
	in interpretation of scientific data. Understand the environmental	
	issues and explore sustainable solutions for it.	
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	discipline and adapt to technological advancements for better	
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Course Title: Entrepreneurship Skills

Academic Year 2024-25

T.Y.B.Sc.

COURSE	DESCRIPTION	
OUTCOME	1/6,0	
CO 1	To develop innovative ideas which may be commercially viable.	
CO 2	Start building knowledge base and skill set which will be useful to	
	start a new enterprise in future.	

Paper Code		Semester VI	Lectures
R	RUSBAS601 ENTREPRENEURSHIP SKILLS		40
60	1.1 Launc	hing and Organizing An Enterprise	10
1.	Environmen problems.	nt scanning – Information, sources, schemes of assistance,	
2. 3.	Enterprise s SWOT Analy	selection, market assessment, enterprise feasibility study ysis.	
4.	Resource m	obilisation – How to Manage Finance, Sources of Finance, , Raw material Planning.	
5.		trol and Quality Norms.	
60	1.2 Growt	h Strategies, Networking & Innovation	10
	Future Grov strategies	versification wth – Techniques of expansion and diversification, vision	
3. 4. 5.	Human Res	siness Organisations (Joint Stock, Co-operative, MNCs) ource Management and Start Ups (Training Methods) of Successful Indian Brands.	
60	1.3 Princi	ples of Corporate Management	10
1.	Principles o	f Management	
2.	Functions o Coordinatin	f management (Planning, Organizing, Directing, Controlling,	
3.	Quality Circ Managemen	les nt by Wandering Around (MBW)	

1. Introduction 2. Principle 1 Seek Opportunity in adversity 3. Principle 2 Do more with less 4. Principle 3 Think & act flexibly 5. Principle 4 Keep it simple 6. Principle 5 Include the margin 7. Principle 6 Follow your Heart RUSBASP601 PRACTICALS 1. Case Study/Assignment/Project Report/Industrial Visit 2. Preparing Project plan/ Project management

Entrepreneurship Skills	 Jugaad Innovation: Radjou,Prabhu,Ahuja 	
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Course Title: Biological Sciences V

Academic Year 2024-25

T.Y.B.Sc.

COURSE OUTCOME	DESCRIPTION	
CO 1	Study Phytochemistry with an emphasis on its applications in	
	pharmaceuticals and bioanalysis. To perform and interpret qualitative	
	tests for phytochemicals.	
CO 2	To interpret results of molecular biology experiments like PCR and	
	RFLP.	
CO 3	Investigate the various aspects and applications of	
	biopharmaceuticals as an upcoming branch in pharmaceuticals.	

Paper Code	Semester VI	Lectures
RUSBAS602	Biological Sciences V	45
602.1: Herba	l Analysis	15
Classical metho	ds of analysis (Gravimetric & Titrimetric),	
Chromatograph	nic & Spectroscopic analysis of phytoconstituents	
Chromatograph	nic fingerprints, Isolation and characterisation of	
phytoconstituents, Analysis of herbal formulation, Bioactivity guided natural		
drug discovery		
602.2: Techn	iques in Recombinant DNA Technology	15
RFLP, AFLP, PC	R, RAPD, Nucleic acid probes, Southern Blotting, Northern	
	Vaccines, Biosensors and Biochips	
602.3: Introd	uction to Biopharmaceuticals & Biosimilars	15
Introduction to Biopharmaceuticals, Sources of Biopharmaceuticals (E. Coli,		
Animal cells, Ac	lditional systems), Upstream & Downstream processing, Product	
Analysis, Therapeutic Hormones, Recombinant Blood Products & Therapeutic		
Enzymes, Produ	uction of antibodies, Vaccines & adjuvants	

RUSBASP602 PRACTICALS

- 1. Standardization of a solvent for extraction of phytoconstituents
- 2. Estimation of alkaloids by gravimetry
- 3. Quantitation of tannins by colorimetry
- 4. Paper chromatography for Separation of Plant Pigments (Spinach)/ Separation of Amino acids
- 5. Thin Layer Chromatography of Alkaloids
- 6. Demonstration of SDS-PAGE
- 7. Sterility testing of biopharmaceuticals
- 8. Analysis of Biosimilars by Bradford's method & UV-Visible Spectrophotometer.
- 9. Study of Chromatographic fingerprint for raw material by: i) HPLTC ii) HPLC iii) GC

Biological Sciences V	The Medicinal Plant Industry: Wojesekera
	 Pharmaceutical Chemistry: H.J.Roth,A.Kleemann
	 Pharmacognosy: Tyler, Brody, Robbers
	 Molecular Biotechnology: Mukesh Pasupuleti
	 Biosimilars: Regulatory, Clinical and Biopharmaceutical
	development:Springer

Course Title: Chemical Sciences V

Academic Year 2024-25

T.Y.B.Sc.

COURSE	DESCRIPTION
OUTCOME	
CO 1	Get associated to the theory and instrumentation of HPLC and GC.
CO 2	To be able to analyze and interpret simple chromatograms.
CO 3	To introduce basics of LC-MS and GC-MS as hyphenated techniques.

Paper Code	Semester VI	Lectures
RUSBAS603	Chemical Sciences V	45
603.1 Liqui	d chromatography	15
HPLC Instrun	atography and its development to HPLC and its applications nentation, Pumps, solvent delivery system, isocratic and gradient modes, Sample introduction system, Columns, Detectors. Reversed mal phase chromatography.	
603.2 Gas cl	hromatography	15
applications Gas Chromato	ography, Gas Solid and Gas liquid Chromatography and its ography Instrumentation, Carrier gas supply, Injectors, Columns, capillary columns, Column oven and temperature programming, ctors.	
603.3 Mass	spectrometry & Hyphenated techniques	15

Introduction to mass spectroscopy: Concept of mass to charge ratio, study of ionization techniques(electron ionization, chemical ionization, electrospray ionization, atmospheric pressure ionization techniques, thermospray ionization), Components of mass spectrograph.

Hyphenation: Need of hyphenation, Interfacing devices

Applications of Liquid Chromatography-Mass Spectrometry and Gas

chromatography-Mass spectrometry

Chemical	Principles and Practice of Chromatography:B.Ravindranath
Sciences V	 High performance liquid chromatography in biotechnology; William S.
	Hancook
	Principle and practice of Bioanalysis:Richard F. Venn
	 Principles and Techniques of Biochemistry and Molecular Biology by
	Wilson and Walker
	Biochemical methods ;S.Sadasivam,A. Manickam

Course Title: Chemical Sciences VI

Academic Year 2024-25

T.Y.B.Sc.

COURSE	DESCRIPTION	
OUTCOME		
CO 1	To be introduced to basic concepts of drug development and action	
	and understand the importance of a bioanalyst in pharmaceutical	
	industry.	
CO 2	Realize the problems involved in analyzing trace elements and complex	
	matrices and learn to choose the suitable bioanalytical method for	
	their analysis.	
CO 3	Apply techniques learned in bioanalysis for characterization of	
	nutritional value of a food sample.	

Paper Code	Semester VI	Lectures
RUSBAS604	Chemical Sciences VI	45
604.1 Drug	development	15
Definition of	the following medicinal terms: Pharmacon, Pharmacophore, Drug	
Formulations	Receptors, Drug-receptor interaction, Drug Potency, Drug toxicity,	
Drug efficienc	y, Pharmacopoeia.	
Routes of drug administration with advantages and disadvantages		
Different dosa	ge forms (emphasis on sustained release formulations)	
Introduction t	o Drug Discovery, Design and Development,	
Discovery of a observation	Lead compound: Screening, drug metabolism studies and clinical	
Classification:	Anti-infective agents, Anti-cancer agents, CNS agents	
Development	of drug: Pharmacophore identification, modification of structure or	
functional gro	up.	
Different type	s of chemical transformation of drugs with specific examples.	
Structure and	therapeutic use of Diclofenac sodium (DFS), Aceclofenac,	
Paracetamol, l	Phenytoin, Aspirin, Atenolol, Laevodopa, Ciprofloxacin,	
Metronidazole	e, Dapsone, Ethambutol	

604.2 Micro analysis and Surface analysis

15

Microanalysis:

Problems associated with trace analysis, Special extraction procedures for separating analyte/s from the complex matrix, Extraction of organic/inorganic analyte from organic/inorganic matrix.

Special techniques and care to be taken during micro analysis

Surface analysis:

Surface chemistry, Phenomenon of adsorption, Adsorption isotherms Surface area by BET method, Pore size distribution, Particle size analysis Catalysis, Heterogeneous and homogenous catalysis

604.3 General Metabolism and Nutrition

15

Overview of mineral metabolism and abnormalities of mineral metabolism with respect to calcium, iron, iodine, fluoride, manganese, selenium

Energy metabolism and nutrition: Concepts of calorific value, Respiratory quotient, BMR, RDA, Nutritional indices, proximate principles of diet, protein energy malnutrition, obesity, BMI, diseases related to obesity, glycemic index.

Free radicals and anti-oxidants: reactive oxygen species- generation and damage, free radical scavenger systems, inflammation, respiratory, skin and age related diseases, atherosclerosis, lipid per oxidation, preventive and chain breaking anti-oxidants

RUSBASP603 PRACTICALS

Separation of Organic mixtures:-

- 1. Volatile liquid + Non-volatile liquid (Liquid + Liquid) by fractional distillation method
- 2. Volatile liquid + Water insoluble solid (Liquid + Solid) by distillation method.

Separation Techniques: -

- 1. Column Chromatography of Separation of mixture of dyes/Separation of Plant Pigments (Spinach)
- 2. Ion Exchange Chromatography of Estimation of sodium using cation exchanger/Estimation of Mg using anion exchange resin column
- 3. **High Performance Thin Layer Chromatography –** Menthol and Paracetamol
- 4. **High Performance Liquid Chromatography –** Separation of modern drug (Diclofenac sodium) from their combination formulation.
- 5. **Gas Chromatography -** Separation of solvent mixtures (Toluene and n-Hexane)

Chemical	Pharmaceutical Analysis: David Lee
Sciences VI	 Excipients and Delivery Systems of Pharmaceutical formulations:
	Karsa, Stephenson
	Microanalysis of solids: Yacobi, Holt, Kazmerski
	 Surface Analysis Methods in Material Science: Brett Sexton, R. C.
	Smart
	 Introduction to nutrition and Metabolism: David A. Bender

Course Code: RUSBAS605

Course Title: Computational Sciences V

Academic Year 2024-25

T.Y.B.Sc.

COURSE	DESCRIPTION	
OUTCOME		
CO 1	Comprehend the programming logic for protein structure prediction, Cheminformatics and drug design.	
CO 2	Learn to effectively use bioinformatics tools like Modeller, Marvin Sketch and iGem Dock for basic structural characterization.	

Paper Code	Semester VI	Lectures	
RUSBAS605	Computational Sciences V	30	
605.1 Protein structure prediction		10	
1. Protein stru	acture basics		
2. Computation	2. Computational prediction methods		
3. Homology r			
4. Protein thre	eading		
5. Fold recogn			
6. Tools used:	•		
605.2 Chemin	nformatics	10	
1. Cheminforn	1. Cheminformatics Introduction		
2. Chemical structure storage formats			
3. Cheminforn	natics tools		
4. Application			
605.3 Compu	itational Drug designing	10	

- 1. Introduction to drugs
- 2. Steps in drug discovery & development
- 3. Computational Drug designing
- 4. Structure based drug designing
- 5. Virtual Screening
- 6. Novel drug Targets



RUSBASP604 PRACTICALS

- 1. Introduction to homology modelling using Modeller (demonstration)
- 2. Automated modelling using Swiss Model
- 3. Validation of predicted structures
 - a. ProSA
 - b. Verify 3D
 - c. SAVES
- 4. Chemical structure designing- Marvin Sketch/ Marvin View
- 5. Virtual Screening- Docking using various online tools (iGemDock, CB Dock)

Computational Sciences	Cheminformatics: Johann Gastieger
V	Bioinformatics and drug Discovery: Richard S. Larson