

# M.Sc. Pharmaceutical and analytical Chemistry

Curriculum and Syllabus (Based on Choice based credit system) Effective from the Academic Year

2018 – 2019

**Department of Chemistry** 

**School of Basic Sciences** 

## **PROGRAM EDUCATIONAL OBJECTIVES(PEO)**

PEO 1	Postgraduate will have significant opportunities in various service
	domains at National and International level, and can work as
	scientist, analyst, quality controller, academics, research
	organizations and set chemical testing labs.

- PEO 2 On the basis of specialized knowledge and experience, postgraduate students will be able to do synthesis, separation, analysis, computational design and development of new products.
- PEO 3 Post-graduate have leadership quality to handle all kind of circumstances in diversities by providing interdisciplinary and multidisciplinary learning environment.
- PEO 4 To encourage leadership qualities in graduates with strong communication skills, mold them as good team players and managers so that they have the competence to function effectively in multi disciplinary orientation teams.
- PEO 5 Postgraduate will be able to formulate, investigate and analyze scientifically real life problems along with ethical attitude which works in multidisciplinary team

## **PROGRAM OUTCOME (PO)**

- PO1 **Problem analyze:** Identify, formulate, review research literature and analyze the chemical problems reaching substantiated conclusions using basics concepts of mathematics, physics and biology.
- PO2 **Design and development of solutions:** Design solutions for complex chemical problems and design systems, components or processes that meet specified needs with appropriate consideration for public health and safety, cultural, societal, and environmental considerations.
- PO3 Conduct investigations of complex problems: Use research based knowledge and including design of experiments, analysis and interpretation of data, and synthesis of information to provide valid conclusions.

## **PROGRAM SPECIFIC OUTCOME**

PSO1	Global level research opportunities to pursue Ph.D programme and targeted approach of CSIR –NET examination.
PSO2	To execute new ideas in the field of research and to develop principles and techniques of science through seminars and the project work.

#### **BOARD OF STUDIES**

S. No	NAME	AFFILIATION	ROLE
1.	Dr . G.Nithya	Associate Professor & HoD, Department of Chemistry, Vels Institute of Science, Technology and Advanced Studies, Pallavaram, Chennai - 600 117.	Chair Person
2.	Dr. Narasimhan Srinivasan	Chairman and Managing Director, Asthagiri Herbal Research Foundation, Perungudi.	External Expert
3.	Mr.V. Neelakantan	Managing Director, Kousikh Therapeutics Private Limited, Gerugambakkam	External Expert
4.	Ms. M. Vidhya lakshmi	Chemist, Instrumentation department, ABC Techno labs India Private Limited.	Alumini Member
5.	Dr. R. A. Kalaivani	Professor & Director, School of Basic Sciences, Vels Institute of Science, Technology and Advanced Studies, Pallavaram,Chennai - 600 117.	Internal member
6.	Dr. T. Somanathan	Associate Professor, Department of Chemistry, School of Basic Sciences, Vels Institute of Science, Technology and Advanced Studies, Pallavaram.Chennai - 600 117.	Internal member
7.	Dr.M. Revathy	Associate Professor, Department of Chemistry, School of Basic Sciences, Vels Institute of Science, Technology and Advanced Studies, Pallavaram,Chennai - 600 117.	Internal member
8.	Mr.V.Sriraman	Assistant Professor, Department of Chemistry, School of Basic Sciences, Vels Institute of Science, Technology and Advanced Studies, Pallavaram,Chennai - 600 117.	Internal member
9.	Dr.R.Sudha	Assistant Professor, Department of Chemistry, School of Basic Sciences, Vels Institute of Science, Technology and Advanced Studies, Pallavaram,Chennai - 600 117.	Internal member

## VELS INSTITUTE OF SCIENCE, TECHNOLOGY AND ADVANCED STUDIES (VISTAS)

#### CHENNAI - 600 117

#### **REGULATIONS 2018**

## MASTER OF SCIENCE IN PHARMACEUTICAL AND ANALYTICAL CHEMISTRY

#### **1. DURATION OF THE PROGRAMME**

1.1. Two years (four semesters)

1.2. Each academic year shall be divided into two semesters. The odd semesters shall consist of the period from July to November of each year and the even semesters from January to May of each year.

1.3 There shall be not less than 90 working days for each semester.

#### 2. ELIGIBILITY FOR ADMISSION

2.1. Candidates for admission to the first year of the degree of Master of Science courses shall be required to have passed the undergraduate Examinations in any basic science / life science degree with chemistry as a paper conducted by the Government of Tamil Nadu or an Examination accepted as equivalent thereof by the Syndicate of the Vels Institute of Science, Technology & Advanced studies.

#### 3. CREDIT REQUIRMENTS AND ELIGIBILITY FOR AWARD OF DEGREE

3.1. A Candidate shall be eligible for the award of the Degree only if he/she has undergone the prescribed course of study in a College affiliated to the University for a period of not less than two academic years and passed the examinations of all the four Semesters prescribed earning a minimum of 90 credits and also fulfilled such other conditions as have been prescribed thereof.

#### 4. COURSE OF STUDY, CREDITS AND SCHEME OF EXAMINATION

4.1. The Course Components and Credit Distribution shall consist

(Minimum number of Credits to be obtained)

Credit Assignment Each course is assigned certain number of credits based on the following: Contact period per week CREDITS

1 Lecture Period - 1 Credit

1 Tutorial Period - 1 Credit

2 Practical Periods - 1 Credit

(Laboratory / Seminar / Project Work / etc.)

#### 5. REQUIREMENTS FOR PROCEEDING TO SUBSEQUENT SEMESTER

5.1. **Eligibility:** Students shall be eligible to go to subsequent semester only if they earn sufficient attendance as prescribed thereof by the Board of Management from time to time.

5.2. Attendance: All Students must earn 75% and above of attendance for appearing for the University Examination. (Theory/Practical)

5.3. **Condonation of shortage of attendance:** If a Student fails to earn the minimum attendance (Percentage stipulated), the HODs shall condone the shortage of attendance up to a maximum limit of 10% (i.e. between 65% and above and less than 75%) after collecting the prescribed fee towards the condonation of shortage of attendance. Such fees collected and should be remitted to the University.

5.4. Non-eligibility for condonation of shortage of attendance: Students who have secured less than 65 % but more than 50 % of attendance are NOT ELIGIBLE for condonation of shortage of attendance and such Students will not be permitted to appear for the regular examination, but will be allowed to proceed to the next year/next semester of the program

5.5. **Detained students for want of attendance:** Students who have earned less than 50% of attendance shall be permitted to proceed to the next semester and to complete the Program of study. Such Students shall have to repeat the semester, which they have missed by rejoining after completion of final semester of the course, by paying the fee for the break of study as prescribed by the University from time to time.

5.6. Condonation of shortage of attendance for married women students: In respect of married women students undergoing UG programs, the minimum attendance for condonation (Theory/Practical) shall be relaxed and prescribed as 55% instead of 65% if they conceive

during their academic career. Medical certificate from the Doctor together with the attendance details shall be forwarded to the university to consider the condonation of attendance mentioning the category.

5.7. **Zero Percent (0%) Attendance:** The Students, who have earned 0% of attendance, have to repeat the program (by rejoining) without proceeding to succeeding semester and they have to obtain prior permission from the University immediately to rejoin the program.

5.8. **Transfer of Students and Credits:** The strength of the credits system is that it permits inter Institutional transfer of students. By providing mobility, it enables individual students to develop their capabilities fully by permitting them to move from one Institution to another in accordance with their aptitude and abilities.

5.8.1. Transfer of Students is permitted from one Institution to another Institution for the same program with same nomenclature. Provided, there is a vacancy in the respective program of Study in the Institution where the transfer is requested. Provided the Student should have passed all the courses in the Institution from where the transfer is requested.

5.8.2. The marks obtained in the courses will be converted and grades will be assigned as per the University norms.

5.8.3. The transfer students are not eligible for classification.

5.8.4. The transfer students are not eligible for Ranking, Prizes and Medals.

5.8.5. Students who want to go to foreign Universities upto two semesters or Project Work with the prior approval of the Departmental / College Committee are allowed to get transfer of credits and marks which will be converted into Grades as per the University norms and are eligible to get CGPA and Classification; they are not eligible for Ranking, Prizes and Medals.

#### 6. EXAMINATION AND EVALUATION

6.1. Register for all subjects: Students shall be permitted to proceed from the First Semester up to Final Semester irrespective of their failure in any of the Semester Examination. For this purpose, Students shall register for all the arrear subjects of earlier semesters along with the current (subsequent) Semester Subjects.

6.2. Marks for Internal and End Semester Examinations.

6.2.1 There shall be no passing minimum for Internal.

6.2.2 For external examination, passing minimum shall be 50% [Fifty Percentage] of the maximum marks prescribed for the paper for each Paper/Practical/Project and Viva-Voce.

6.2.3 In the aggregate [External/Internal] the passing minimum shall be of 50%.

6.2.4. He / She shall be declared to have passed the whole examination, if he/she passes in all the papers and practical wherever prescribed as per the scheme of the examinations by earning 90 CREDITS.

## 7. MAXIMUM PERIOD FOR COMPLETION OF THE PROGRAMS TO QUALIFY FOR A DEGREE

7.1. A Student who for whatever reasons is not able to complete the programs within the normal period (N) or the Minimum duration prescribed for the programme, may be allowed two years period beyond the normal period to clear the backlog to be qualified for the degree. (Time Span = N + 2 years for the completion of programme)

#### 8. REVISION OF REGULATIONS, CURRICULUM AND SYLLABI

The University may from time to time revise, amend or change the Regulations, Curriculum, Syllabus and Scheme of examinations through the Academic Council with the approval of the Board of Management.

## M.Sc. PHARMACEUTICAL AND ANALYTICAL CHEMISTRY CURRICULUM

### Total number of credits: 90

Category	Code	Course	Hours/Week			
			Lecture	Tutorial	Practical	Credits
SEMESTE	R I					
Core	18 CMSP11	Medicinal Chemistry	4	0	0	4
Core	18 CMSP12	Fundamentals of Pharmaceutical	4	0	0	4
		Chemistry				
Core	18 CMSP13	Advanced Organic Chemistry	4	0	0	4
DSE		Discipline Specific Elective – I	3	0	0	3
DSE		Discipline Specific Elective – II	3	0	0	3
GE		Generic Elective – I	1	0	2	2
Core	18PMSP11	Organic Synthesis - Practical I	0	0	6	3
			19	0	8	23
SEMESTER	RII					
Core	18 CMSP21	Advanced Pharmaceutical Chemistry	4	0	0	4
Core	18 CMSP 22	QA & QC in Drugs and Pharmaceuticals	4	0	0	4
Core	18CMSP23	Analytical Techniques in Chemistry	4	0	0	4
DSE		Discipline Specific Elective – III	3	0	0	3
Core	18PMSP21	Pharmaceutical and Drug	0	0	6	3
Cole	101 101 21	Analysis - Practical II	0	0	0	5
Core	18PMSP22	Phyto Chemistry - Practical III	0	0	6	3
Core	18IMSP21	Internship	0	0	30	2
			15	0	42	23
SEMESTER	RIII		1		1	
Core	18 CMSP31	Pharmaceutical Formulation Technology – I	4	0	0	4
Core	18 CMSP32	Advanced Chromatographic 4 0		0	4	
Core	18 CMSP33	Chemical and Instrumental	4	0	0	4
DSE		Discipline Specific Elective – IV	3	0	0	3
DSE		Discipline Specific Elective – V	3	0	0	3
GE		Generic Elective – II	2	0	0	2
Core	18PMSP31	Medicinal Chemistry - Practical	0	0	6	3
			20	0	6	23
SEMESTER			-•	v	Ŭ	-0
Core	18 CMSP41	Pharmaceutical Formulation	5	0	0	5
DSE		Discipling Specific Elective VI	Λ	0	0	1
Core	18DMCD/1	Project work	4	0	24	4
	101/101/101/41		0	0	24	12 <b>71</b>
		Over all Total	63	0	80	<u>-21</u> 90

S.No.	Subject code	Subject title	
1		Fundamentals of Biochemistry	
2		Organic Chemistry – I	
3		Thermodynamics and Chemical Kinetics	
4		Synthesis of APIs and Their Manufacture	
5		Organic Name Reactions and Synthesis of	
		Reagents	
6		Macromolecular Chemistry	
7		Separation Techniques	
8		Organic Chemistry- II	
9		Analytical Techniques	
10		Chemistry of Natural Products	
11		Enzyme Technology and Related	
		Entrepreneureal Skills	
12		Nuclear and Photochemistry	
13		Novel Materials and Green Industrial Catalysis	
14		Organic Chemistry- III	
15		Strategic Management of Pharma Industry	
16		Stereochemistry and Reaction Mechanism	
17		Pharmaceutical Chemistry	
18		Organic Spectroscopy	
19		Inorganic Chemistry	
20		Electrochemistry and spectroscopy	

## List of Discipline Specific Elective Courses

## List of Generic Elective Courses

S.No.	Subject code	Subject title	
		Soft Skill - I	
		Soft Skill - II	
		Green Chemistry	
		Cheminformatics	
		Food Chemistry and Adulteration	

# Syllabus Core Courses

#### **18CMSP11**

#### MEDICINAL CHEMISTRY

#### **Course Objective**

To learn about physicochemical properties of drugs, general pathways of drug metabolism, significance of drug metabolism, basic concepts of prodrugs. To learn about medicinal properties of the given drugs.

#### Unit IPhysicochemical properties in relation to biological action12

Ionization, Drug distribution and pKa values of specified APIs such as hydrogen bonding, protein binding, chelation, isosterism, stereoisomerism, steric effect, redox potential and surface activity,

#### Unit II Drug metabolism

General pathways of drug metabolism (different types of reaction in phase-I and phase-II with example), factors affecting drug metabolism,

#### Unit III Significance of drug metabolism

Significance of drug metabolism in medicinal chemistry. The role of liver in drug metabolism. Preclinical experimental models of drug metabolism.

#### Unit IV Basic concepts of prodrugs

Basic concepts of prodrugs need for prodrugs, specific prodrugs such as methodology of prodrug design. Applications of prodrugs.

#### Unit VMedicinal chemistry of the following group of drugs12

a) Antivirals for HIV infection -Indinavir CAS Reg. No. [150378-17-9] synthesis and pharmacology

b) Antineoplastics- Etoposide CAS Reg. No. [33419-42-0] synthesis and pharmacology.

c) Diuretics-Indapamide CAS Reg. No. [26807-65-8] and Isosorbide CAS Reg, No. [652-67-5] Synthesis, and pharmacology.

d) Antidiabetics - Liraglutide CAS Reg. No. [204656-20-2](harmone analog) and Gliclazide CAS Reg. No. [21187-98-4] (sulfonylurea) Synthesis and pharmacol.

#### Total: 60 h

#### **Course Outcomes:**

- To understand the importance of different bondings and their relation in biological action
- To know the importance of isosterism, redox potential and surface activity
- To familiarize the factors affecting drug metabolism

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- To understand complete knowledge of the role of the lever
- To know pre-clinical experiment models

## **Text Book**

AshutoshKar. Medicinal Chemistry, New Age International Ltd. Third Edison, 2006.

### **Reference Books**

- 1. William O. Foye, Principles of medicinal chemistry, Fourth Edition, 1996
- 2. Graham L. Patrick, An introduction to medicinal chemistry, 4<sup>th</sup> edition, Oxford University press.

#### FUNDAMENTALS OF PHARMACEUTICAL CHEMISTRY 4004 **18CMSP12**

#### **Course Objective**

To learn about molecular basis of drug action and receptor concept and to know about drug receptor concept.To learn about the drug molecules from lead molecules.To know about the basic concept of enzyme and their catalytic activity.

#### Unit I Molecular basis of drug action

Receptor: Types of Receptors, Drug- Receptor Interaction including signal transduction mechanism. Basic ligand concept, Agonist, antagonist, partial Agonist, and inverse Agonist.Receptor theories – Occupancy, Rate and Activation theories.

#### Unit II **Receptor concept**

Receptor complex and Allosteric modulation, Second and Third messenger system, Receptor dynamics, Molecular biology of receptors, Receptor Models, Receptor Binding assays, Autoradiography. (Above concepts with special reference to opioid, histaminergic, adrenergic and GABA-ergic receptors)

#### Unit III New drugs from lead molecules

Lead molecule choice and modification for API, Bioisosteric replacement, rigid analogs, alteration of chain branching, changes in ring size, ring position isomers, design of stereoisomers and geometric isomers, fragments of lead molecule.

#### Unit IV Enzymes

Enzymes structure – primary, secondary, tertiary and quaternary. Enzyme kinetics, Enzyme inhibitors, irreversible and reversible inhibitions, Kcat inhibitors. Transition - State analogues.

#### Unit V **Enzyme inhibitor – drugs**

Enzyme Inhibitors as drugs like cytochrome P450 inhibitors, Aromatase, lipoxygenases. Protein and peptide drugs - insulin, somatostatin, Relaxin, DNAse interferon, inteleukin, Growth stimulating factors and urokinase enzymes.

#### Total: 60 h

#### **Course Outcomes:**

- To understand agonist, anti agonist, partial agonist and inverse agonist •
- To gain the knowledge of various receptor theories
- To understand the role of receptors and auto radiography
- To learn various receptors like GABA and familiar adriginic receptors.
- To learn lead molecules choice and API modification.

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#### **Text Books**

- 1. Purich& Allison, A Comprehensive Guidebook to Enzyme Nomenclature, Reactions, and Methods, The Enzyme Reference, 1st Edition, Allison Academic Press, 2002.
- 2. Lednicer, Organic Chemistry of Drug Synthesis, Wiley Interscience, 1977.
- 3. Wilson & Gisvold, Medicinal Chemistry, 10<sup>th</sup> Edition, 1998.

#### **Reference Books**

- 1. William Foye, Medicinal Chemistry, 4<sup>th</sup> Edition, 1995.
- 2. Burger, Medicinal Chemistry, 5th Edition, 1995.

#### **18CMSP13**

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#### **Course Objective**

To learn about simple reactions such as substitution, addition and elimination reactions of organic chemistry. To learn about basics of stereo chemistry, heterocyclic chemistry and some naming reactions

#### Unit I Substitution and Addition reactions

Mechanism of aliphatic substitution reaction – SN1, SN2, SNi mechanism – Neighboring group participation. Stereo specific and stereo selective synthesis. Concepts of hard, soft acids and bases. Role of crown ethers, PTCs in nucleophilic substitution mechanism. Mechanism of esterification and ester hydrolysis – aromatic electrophilic and nucleophilic substitution. Electrophilic and nucleophilic addition. Addition of halogens, Hydrogen halide,  $H_2$  and water to carbon-carbon double bonds. Nucleophilic addition to carbonyl group

#### **Unit II Elimination and Rearrangement**

E1, E2 and E1CB mechanisms.Orientation of a double bond. Hoffmann and Saytzeff rule. Reactivity – the effect of changes in the substrate, base, leaving group and medium on overall reactivity – acyclic & cyclic system. Carbocation rearrangement.Wagner-Meerwein, Favorski, Baeyer-villiger, Schmidt, Curtius, Claisen, Pinacol-Pinacolone and cope rearrangement.

#### Unit III Stereochemistry

Molecular symmetry and chirality, classification of chiral molecules – Chemical resolutionillustration by specific example; principles of symmetry – illustrations of homotopic, enantiotopic and diastereotopic hydrogen and prochiral carbons with suitable examples. R – S notation -illustration of erythro and threo nomenclature. Asymmetric synthesis – Cram's rule. E, Z notation of simple olefins. Determination of absolute configuration .Mechanism and stereochemistry of chemical reaction.Conformational analysis – alkane, cyclohexane and disubstituted cyclohexane.

#### Unit IV Naming Reactions

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Aldol reaction, Mukaiyama reaction, Acyloin, Barbier -weiland degradation reaction, Arndteistert reaction, Wittig, Wittig-Horner, Tebbe reactions, Micheal reaction and Robinson annulations reactions.

#### UnitV Heterocyclic chemistry

Synthesis, reactions and structure of Isothiazole, Isooxazole, Quinoline, Isoquinoline, Purines.Azoles – Imidazoles, Oxazoles, Thiazoles and Pyrazoles.Pyrmidines and quinazolines, phenothiazines

#### Total: 60 h

#### **Outcomes:**

- To learn about the Substitution and elimaination reactions of molecules
- To learn about the electrophilic and nucleophilic addition of halogens.
- To learn about the rearrangement Wagner-Meerwein, Favorski, Baeyer-villiger, Schmidt, Curtius, Claisen, Pinacol-Pinacolone and cope rearrangement.
- To learn how to work out synthetic strategies for complex organic molecules.
- To learn the principles and terminology used in retrosynthetic analysis

#### **Text Books**

- 1. Raj K.Bansal, Heterocyclic Chemistry, 3<sup>rd</sup> Edition, New Age International Publisher, 1999.
- 2. P.S. Kalsi, Organic Reactions and their Mechanisms, New Age International Publishers, 2<sup>nd</sup> Edition, 2000.
- 3. Francies, A Carey and Richard J. Sundberg, Advanced Organic Chemistry, Part A and Part B, 4<sup>th</sup> Edition, 2000.

#### **Reference Books**

- E.H. Eliel, Stereo chemistry of carbon compounds, Tat Mc Graw-Hill Publishing Company Ltd., 1998..
- 2. I.L. Finar, Organic Chemistry, Vol. I and Vol. II, ELBS, 6<sup>th</sup> Edition 2003.

#### 18PMSP11ORGANIC SYNTHESIS - PRACTICAL I0063

#### **Course Objective**

To learn about Good Laboratory Practice(GLP) in chemistry lab.To learn about the synthetic techniques and crystallization techniques of following organic compounds.

#### **Lists of Experiments**

- 1. Oxidation of anthracene to anthraquinone oxidation process.
- 2. Terephthalic acid from p-xylene oxidation process.
- 3. Preparation of benzhydrol from benzophenone reduction process.
- 4. Preparation of p-bromo acetanilide from acetanilide bromination process.
- 5. Preparation of 1,2,3,4 tetra hydro carbazole from cyclohexanone Fischer indolization process.
- 6. Preparation of p-nitro benzoic acid from p-nitro toluene.
- 7. Preparation of methyl orange from sulphanilic acid coupling diazotization process.
- 8. Preparation of benzophenoneoxime from benzophenone molecular rearrangement.
- 9. Methyl salicylate from salicylic acid esterification process.
- 10. Picric acid from phenol nitration process.
- 11. O-benzoylbenzioc acid from phthalic anhydride electrophilic substitution & Friedel-Crafts acylation.
- 12. Benzilic acid from benzoin elimination addition process.
- 13.  $\beta$  naphthol from naphthlene-(by sulphonation & hydrolysis)

#### Total: 90 h

#### **Outcomes:**

- To learn the common experimental techniques of synthesis of organic molecules.
- To know the preparation involving molecular rearrangement.
- To learn the preparation involving oxidation, nitration.
- To learn the preparation involving halogenations, reduction, elimination.
- To learn esterification, sulphonation, hydrolysis.

#### **Text Book**

1. A.A. Siddiqui, S. Siddiqui, Natural Products Chemistry Practical Manual, CBS Publishers & Distributors, 2008.

#### **Reference Books**

- 1. Gnanprakasam, Ramamurthy, Organic Chemistry Lab Manual, S. Wisvanathan Printers & bPublishers Pvt. Ltd, 2010.
- 2. Vogel, Arthur I. Vogel, Text Book of Practical Organic Chemistry, 5<sup>th</sup> Edition, Pearson Education, Prentice Hall, 1996.

#### 18CMSP21ADVANCED PHARMACEUTICAL CHEMISTRY4004

#### **Course Objective**

To know about basic concepts of pharmaceutical chemistry. To learn about Introduction, classification, concept and mechanism of actionand synthesis of drugs.

#### Unit I Anti-infective agents

Introduction, classification, concept and mechanism of action, Structure Activity Relationship(SAR) and synthesis of representative members of the following class of drugs – sulphonamides, non-steroidal anti-inflammatory analgesics, antibiotics, antifungal, anti-mycobacterium agents, Antiviral agents.

Hantsch equation, Craig plot, Topliss decision tree approach, Bio-isosterism.

#### Unit II Chemotherapy

Chemotherapy of Malaria, AIDS, Cancer, Hepatitis as illustrative.

#### Unit III CNS Drugs

Introduction, Classification, Mechanism of Action, SAR and Synthesis of following CNS Drugs. Drugs acting on CNS – Hypnotics & Sedatives, Antianxiety drugs, anticonvulsive drugs, Antidepressant and antipsychotic drugs. Drugs used for neurodegenerative disorders like Dementia, Alzheimer's and Parkinson's disease.

#### Unit IV CVS and ANS Drugs

Drugs acting on CVS- Anti-hypertensive, Anti-arrhythimic, Vasopressor, Anti-Anginal agents, cardiacglycosides.Drugs acting on Adrenergic and Cholinergic systems.Drugs acting on kidneys, Analgesics (NSAIDS, Opioids), Anti-Ulcers and coagulant and anti-coagulants.

#### Unit V QSAR

Introduction, quantitative models, Hantsch-analysis, Free-Wilson models, Non-linear method, mixed method and other QSAR methods. Application of above methods, statistical methods in QSAR.

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#### **Course Outcomes:**

- To understand the concept, structural activity relationship (SAR)
- To understand the concept chemotherapy
- To understand various anti infective agents
- To understand what is CNS drugs, their types, mechanism of action and the importance of their role
- To understand what is CVS and ANS drugs

#### **Text Book**

1. Burger's Medicinal Chemistry & Drug Discovery, Vol.1-5, 5<sup>th</sup> Edition, 1995.

#### **Reference Books**

- 1. Wilson and Gisvold"s, Text book of medicinal chemistry, 2006.
- 2. SurendraNathPandeya, Text book of medicinal chemistry, vol –I & II, 5<sup>th</sup> edition, SG publisher, 2003.

## 18CMSP22QUALITY ASSURANCE AND QUALITY CONTROL4004IN DRUGS AND PHARMACEUTICALS

#### **Course Objective**

To learn about the concept and philosophy of quality assurance and quality control in drugs. To learn about the regulatory aspects of pharmaceuticals. To learn about quality control of packaging materials and microbiological assay.

#### Unit I Concept and philosophy

TQM, GLP, GMP, Quality audit, SOP, ICH, ISO-9000.

#### Unit II Regulatory aspects of pharmaceuticals

Validation of Personnel, Equipment and cleaning methods, In-process quality control on various dosage forms, (Sterile and non-sterile).

Unit III	Quality control of finished products	12

Factor affecting stability of formulations, shelf-life prediction.

#### Unit IVQuality control of packaging materials12

Types of plastics, primary and secondary packaging materials, glass, closures, cartons, blister and their control.

#### Unit V Microbiological assay 12

Microbiological assay- antibiotics and vitamins.

Total: 60 h

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#### **Outcomes:**

- To learn about the importance of TQM, GLP and GMP
- To learn about the importance of Quality audit, SOP, ICH and ISO-9000
- To understand the validation of Personnel, Equipment and cleaning methods.
- To learn about the In-process quality control on various dosage forms.
- To understand the quality control of finished products.

#### **Text Books**

- 1. Liberman&Lachman, Theory & Practice of Industrial Pharmacy, 3<sup>rd</sup> Edition, 1986.
- 2. Ira R. Berry, A. Robert, Nash Pharmaceutical process validation 2<sup>nd</sup> Edition,

## **Reference Books**

- 1. WHO, Quality assurance of pharamaceuticals,vol-I & II, Geneva, A.I.T.B.S Publishers india, 2007.
- 2. Leon Lachman, Herbert A liberman, The theory and practice of industrial pharmacy, special indian edition, 2009.

#### 18CMSP23 ANALYTICAL TECHNIQUES IN CHEMISTRY 4004

#### **Course Objective**

To learn about the basic concepts and instrumentation of various analytical instruments such as potentiometry, conductometry, biamperometry, nephelometry, fluorimetry, polarimetry, refractometry, radio analytical techniques and thermal methods.

#### Unit I Instrumentation-I

Potentiometry, Conductometry, Biamperometry –Theory, Instrumentation and Applications.

#### Unit II Instrumentation-II

Nephelometry, Fluorimetry, Polarimetry, Refractometry - Theory, Instrumentation and Applications.

#### Unit IIIInstrumentation – III12

Flame Photometry, and Atomic Absorption Spectroscopy - Theory, Instrumentation and Applications.

#### Unit IV Instrumentation-IV

Radio analytical Techniques, Isotope dilution analysis, Radioimmunoassasy, Radiochromatography and Radio electrophoresis, Activation analysis.

#### Unit V Instrumentation-V

Thermal methods - Thermogravimetric and differential thermal analysis, thermometric titrations, differential scanning calorimetry – basic instrumentation and applications.

Total: 60 h

#### **Course Outcomes:**

- To learn the various instrumental methods, potentiometry, conductometric, biamperometry
- To learn what is nephelometry, fluorimetry, polarimetry, refractometry
- To understand what is flame photometry and atomic absorption spectroscopy
- To learn what is radio analytical techniques

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• To learn the concept, what is thermal methods and their types

### **Text Book**

1. D.A. Skoog and D.M. West, Fundamental of Analytical Chemistry, International Edition, 7<sup>th</sup>Edition, Saunders College Publishing, Philadelphia, Holt, London, 1996.

#### **Reference Books**

- 1. Willard, Merritt, Dean and Settle, Instrumental methods of analysis, 2004.
- Gurdeep R. Chatwal, Sham K. Anand, Instrumental methods of chemical analysis, Himalaya publishing house, 2007.

#### 18CMSP21 PHARMACEUTICAL AND DRUG ANALYSIS - PRACTICAL II 0063

#### **Course Objective**

To learn about the synthetic techniques of active pharmaceutical drugs. To know about the monographs of drugs and to learn about the basic concepts of drug analysis.

#### List of Experiments

#### Synthesis of active pharmaceutical ingredients

- 1. Synthesis of Sulphacetamide
- 2. Synthesis of Aspirin
- 3. Synthesis of Methyl Orange
- 4. Synthesis of 5,5-Diphenylhydantoin
- 5. Synthesis of Chlorbutol
- 6. Synthesis of Paracetamol

#### IP Monograph of the following drugs

- 7. Aspirin
- 8. Paracetamol
- 9. Sulphacetamide
- 10. Chlorbutol

#### **Drug analysis**

- 11. Assay of Metronidazole
- 12. Assay of Calcium Gluconate
- 13. Assay of Sulphacetamide
- 14. Assay of Chlorobutol
- 15. Disintegration Test
- 16. Hardness Test

#### **Course Outcomes:**

- To learn about the synthesis of sulphaacetamides and Aspirin
- To learn about the preparation of methylorange
- To learn about the preparation of 5,5-Diphenylhydantoin
- To learn about the IP monograph of Aspirin and Paraacetamol
- To learn about the drug analysis

#### Total: 90 h

#### **Text Book**

1. A.A. Siddiqui, S. Siddiqui, Natural Products Chemistry Practical Manual, CBS Publishers & Distributors, 2008.

#### **Reference Book**

1. Gnanprakasam, Ramamurthy, Organic Chemistry Lab Manual, S. Wisvanathan Printers & bPublishers Pvt. Ltd, 2010.

#### 18PMSP22 PHYTO CHEMISTRY- PRACTICAL III

#### **Course Objective**

To learn about the separation techniques of various natural products from natural sources. To learn about the experimental techniques and solvent extraction techniques involved in the extraction of the following natural products.

#### **Lists of Experiments**

- 1. Isolation of caffeine from tea leaves.
- 2. Extraction of piperine from black pepper.
- 3. Extraction of hesperidin from orange peel.
- 4. Extraction of pectin from orange peels.
- 5. Extraction of nicotine picrate from tobacco.
- 6. Extraction of Curcumin from turmeric.
- 7. Isolation of lycopene.
- 8. Extraction beta carotene from plant leaves.
- 9. Extraction of flavonoids.
- 10. Extraction of naringin.
- 11. Isolation of Ascorbic Acid from lemon.
- 12. Isolation of Tartaric Acid from grape

Total: 90 h

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#### **Course Outcomes:**

- To learn about Isolation of caffeine from tea leaves
- To learn about Extraction of pectin from orange peels
- To learn about Extraction of nicotine picrate from tobacco
- To learn about Isolation of lycopene
- To learn about Extraction of flavonoids.

#### **Text Book**

1. A.A. Siddiqui, S. Siddiqui, Natural Products Chemistry Practical Manual, CBS Publishers & Distributors, 2008.

#### **Reference Book**

1. Gnanprakasam, Ramamurthy, Organic Chemistry Lab Manual, S. Wisvanathan Printers & Publishers Pvt. Ltd, 2010.

#### **18IMSP21**

#### **INTERNSHIP**

#### **Course Objective**

- > To gain practical experience by working in a well-established research environment.
- To demonstrate an ability to work independently and utilize principles of doing research.

#### Requirements

- Students wishing to receive credit for internship are required to find, apply for, and be selected for a chemistry or materials related internship position with an organization of their choice. They will then need to seek permission from the Department Chair to register for the appropriate internship course.
- The student must complete at least 90 h of work during the semester for each hour of academic credit awarded, and these work hours must be completed during the term (odd or even semester vacation) in which the student is registered for the internship course.
- After the student has completed the internship, the student must submit the final evaluation report of the internship experience and 20 minute presentation to department at conclusion of semester. The Department Chair and class instructor will allot the marks for the internship evaluation report.

#### **Course Outcomes:**

- To know the various types of industries.
- To learn the procedure of identifying, approaching, applying and getting approval of internship from a leading industry.
- To witness the entire work area of the industry.
- To understand the nature of job involved in the various sector of the industry.
- To adapt with the working people.

#### 18CMSP31 PHARMACEUTICAL FORMULATION TECHNOLOGY I 4004

#### **Course Objective**

To learn about the basic concepts of pharmaceutical formulations. To learn about the physicochemical principles, pharmaceutical operations, profile of pharmaceutical formulations.

#### Unit IIntroduction to pharmaceutical formulations12

Need for formulation; History of formulation; Challenges in early formulations; Drug substance to Drug product with reference to formulating for the patient; Physical and chemical properties of Formulation.

#### Unit II Physicochemical Principles I

Solutions; pH, EMF and redox potentials ; physicochemical properties evolving into in vivo bioavailability; Absorption, Dissolution, Permeability, Distribution, Metabolism, Excretion.

#### Unit III Physicochemical Principles II

Complexation; Modifies release dosage forms; profile of common formulations; colloidal systems, Rheology; Drug stability and ICH Guidelines for stability testing.

#### Unit IV Pharmaceutical operations

Extraction; Drying; Evaporation; Distillation; Filtration/Centrifugation; Size reduction and handling of solids in the powder form; Anti-solvent and reactive crystallization; Melting approaches to particle size; Wet milling and dry milling; packaging.

#### Unit V Profile of formulations

Tablets, capsules, solution and suspension formulation; Modified release formulation; Parenteral Formulation; Inhaled formulations/aerosols, Topicals.

Total: 60 h

12

12

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#### **Course Outcomes:**

- To learn about the introduction of pharmaceutical formulation
- To learn about the important properties of physical and chemical properties.
- To understand the pH, EMF and redox potentials
- To learn about the physicochemical properties

• To understand the drug stability and ICH Guidelines for stability testing

#### **Text Book**

1. S.K.Jain and V.Soni, Bentley's Textbook of Pharmaceutics, An Adaptation, Elsevier, 2012.

## **Reference Book**

1. C.B.Gupta and S. S. Khanka, Sultan Chand & Sons, Entrepreneurship and Small Business Management- New Delhi, 2012.

#### **18PMSP32 ADVANCED CHROMATOGRAPHIC TECHNIQUES** 4004

#### **Course Objective**

To learn about the basic concepts of chromatographic techniques. To learn about the basics, instrumentation and application of TLC, HPTLC, GC, HPLC, GPC and IEC techniques.

#### Unit I Introduction to chromatography

Adsorption and partition chromatography, definition of terms, techniques and chemical concepts of TLC, HPTLC and Paper chromatography followed by Gas and liquid chromatographic analysis and Sophisticated techniques in chromatography.

#### Unit II **TLC and HPTLC**

TLC - Principles and applications, HPTLC - Theory, principle, instrumentation and application.

Size exclusion Supercritical fluid chromatography – principle, theory, instrumentation and application.

Ion-exchange chromatography, hydrophobic interaction chromatography, affinity chromatography – principle and theory.

Capillary electrophoresis :principle, techniques and application.

#### Unit III Gas chromatography

Theory of gas chromatography, principle of gas chromatography, instrumentation and application of gas chromatography.

#### Unit IV High performance liquid chromatography

High performance liquid chromatography – principles, theories, stationary phases, Instrumentation for HPLC. Factors affecting resolution, tailing, selectivity, gradient elution, reversed phase chromatography.

Preparative HPLC, separation of enantiomers - chiral mobile phases - chiral solid stationary phases - Indirect separation of enantiomers.

Special techniques in HPLC – Micro and capillary HPLC, High speed and super speed HPLC – Hyphenated techniques.

#### Unit V Sophisticated techniques in chromatography 12

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Separation of proteins: Gel filtration, gel electrophoresis – PAGP – (Polyacrylamide gel electrophoresis). Immino electrophoresis – Methods of purifying proteins – Ion-exchange chromatography, hydroprobic interaction, chromatography, affinity chromatography – Analysis of blood sample – components of blood (serum, plasma, protein-free fraction) – Methods of analysis.

#### Total: 60 h

#### **Course Outcomes**:

- To learn about the Adsorption and partition chromatography
- To learn about the techniques and principle, instrumentation, applications of TLC, HPTLC and Paper chromatography.
- To understand the Size exclusion Supercritical fluid chromatography
- To learn about the physicochemical properties
- To understand the principle and theory Ion-exchange chromatography, hydrophobic interaction chromatography and affinity chromatography

#### **Text Book**

1. Beckett &Stenlake, Practical Pharmaceutical chemistry, Vol. I and II, 4<sup>th</sup> edition, The Athlone Press, London, 2002.

#### **Reference Books**

- 1. D.C.Garrett, Quantitative Analysis of Drugs, 3<sup>rd</sup> Edition, Springer, 2002.
- 2. Lloyd R.Snyder, Joseph J.Kirkland & Joseph L.Glajch , Practical HPLC Method

Development, 2<sup>nd</sup> Edition, Wiley Interscience, 2001.

# 18CMSP33 CHEMICAL AND INSTRUMENTAL METHODS 4004 OF DRUG ANALYSIS

#### **Course Objective**

To understand the basic principles, instrumentation and applications in drug analysis using IR, UV-Visible, NMR and Mass spectrometry.

#### Unit IUV-visible spectrophotometry12

Theory – Beer Lambert's law – limitations of the law, Design and working of single beam and double beam spectrophotometry. Applications of UV absorption spectrometry in qualitative analysis and quantitative analysis.

#### Unit II Thermometry and XRD

Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC). Polymorphism/XRD – analysis.

#### Unit III IR-spectrometry

Theory - Molecular vibration, instrumentation and mechanics of measurement – sample preparation –IR Spectrometry,. FTIR and use in structural elucidation .

#### Unit IV NMR-spectrometry

Theory, spin-spin coupling, chemical shift, magnetic equivalence – spin-spin decoupling – shift reagents instrumentation. Applications of NMR spectrometry in characterization of chemical structure using spectra of simple organic compound as examples. Principles, Instruments and applications of  $^{13}$ C NMR.

#### Unit V Mass spectrometry

Theory, fragmentation pattern, ionization techniques; electron bombardment, chemical ionization, field desorption, fast atom bombardment. Different analyzers, Interpretation of mass spectra, Determination of molecular weight and molecular formula and applications of mass spectrometry

Total: 60 h

35

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#### **Course Outcomes:**

- To learn about the theory and beer Lambert's law
- To learn about the working of single beam, double beam spectrophotometry and pplications of UV absorption spectrometry
- To understand the DTA, DSC and XRD.
- To learn about the theory, instrumentation and application of IR spectroscopy.
- To understand the spin-spin coupling, chemical shift and decoupling

# **Text Book**

 Y.R.Sharma, Elementary Organic Absorption Spectroscopy, S.Chand & Co., 2<sup>nd</sup> edition New Delhi. 1996.

#### **Reference Books**

- 1. A.H.Beckett and J.B.stenlake, Practical Pharmaceutical Chemistry, Part-I and II, the Athlone Press, London, 4<sup>th</sup> Edition, CBS Publisher, Delhi, 1998.
- 2. H.H.Willard, L.L.Meritt, J.A.Dean and F.A.Settle, Instrumental Methods of Analysis, Wadsworth, New York, 7thedition, 1986.
- 3. John R.Dyer, Applications of absorption spectroscopy of Organic Compounds, PrenticeHall, London, 1987.
- 4. Robert M.Silverstein, ClaydonBassler and Terence C.Morril, Spectrophotometric

Identification of Organic Compounds, 6<sup>th</sup> Edition, John Wiley & Sons, New York, 2002.

#### 18PMSP31MEDICINAL CHEMISTRY - PRACTICAL IV0063

#### **Course Objective**

To learn about the basic concepts of assay of some important dugs. To learn about various analytical techniques used for drug assay and to know about the basic calculations involved in the drug assay.

#### List of Experiments

- 1. Assay of Paracetamol.
- 2. Determination of Isoniazid.
- 3. Estimation of Aspirin by Colorimetry.
- 4. Estimation of Caffeine.
- 5. Estimation of Aspirin by UV-VIS Spectrophotometry.
- 6. Estimation of Ibuprofen.
- 7. Thin Layer Chromatography.
- 8. Determination of water content by Karl Fisher method.
- 9. Test for identity of selected drugs.
- 10. Determination of strength of strong acid by potentiometry.
- 11. Determination of quinine sulphate by fluorimetry.
- 12. Conductometric titration of mixture of acids.
- 13. Determination of pKa of a weak acid using Henderson equation.

Total: 90 h

#### **Course Outcomes:**

- To learn about the assay of paracetamol
- To learn about estimation of Aspirin by colorimetry
- To learn about Estimation of Aspirin by UV-VIS Spectrophotometry
- To learn about Thin Layer Chromatography
- To learn about Test for identity of selected drugs.

## **Text Book**

1. A.A. Siddiqui, S. Siddiqui, Natural Products Chemistry Practical Manual, CBS Publishers & Distributors, 2008.

#### **Reference Books**

- 1. Gnaprakasam, Ramamurthy, Organic Chemistry Lab Manual, S. Viswanathan Printers & Publishers Pvt. Ltd, 2010.
- 2. Kenneth A. Connors, Textbook of Pharmaceutical Analysis, 3ed., Wiley, 2010.

#### **18CMSP41** PHARMACEUTICAL FORMULATION TECHNOLOGY – II 5005

#### **Course Objective**

To learn about basic principles of Pharmaceutical Formulation Technology. To learn about the standard pharmaceutical practice, role of microbiology in formulations, pilot plant manufacturing and entrepreneurial aspects.

#### Unit I Standard pharmaceutical practice

Pharmacopoeias; Formularies; Pharmaceutical calculations and prescriptions; Preparations-oral, external, ocular; New drug delivery system; Radio isotopes.

#### Unit II **Role of microbiology in formulations**

Principles; Disinfection; Sterilization, microbial contamination and control; Sterility testing; Antibiotics; Blood products and plasma substitutes.

#### Unit III **Pilot plant manufacturing**

Pilot plant techniques and objectives; Personnel requirement; GMP perspectives; Analytical method transfer to quality assurance; Mixing/Blending; Drug uniformity; Excipient uniformity;

#### Unit IV **Manufacturing Techniques**

Wet granulation, binder addition, drying and milling, dry blending and compression, milling and tablet compression; Coating techniques; Contract manufacture;

#### Unit V **Entrepreneurial aspects**

Concept of entrepreneurship; Competency and functions of entrepreneur; Women entrepreneurs; Entrepreneurship vis-à-vis Intrapreneurship; Small business management; Role of entrepreneurship in economic development.

#### Total: 75 h

#### **Course Outcomes:**

- To learn about the Pharmacopoeias and formularies
- To learn about the New drug delivery system and radio isotopes.
- understand the Principles; Disinfection; То Sterilization, microbial contamination and control
- To learn about the Antibiotics; Blood products and plasma substitutes

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• To understand the Pilot plant techniques

# **Text Book**

1. S.K.Jain and V.Soni, Bentley's Textbook of Pharmaceutics, An Adaptation-Elsevier, 2012.

#### **Reference Book**

1. C.B.Gupta and S.S.Khanka, Sultan Chand & Sons, Entrepreneurship and Small Business Management- NewDelhi, 2012.

#### **18RMSP41**

#### **Project work**

#### **Course Objective**

To learn about the concept of project work. To know about designing new experiments and carry out the experiments. To know about the various characterization techniques used to characterize the synthesized compounds. To know about the necessities of literature survey and to learn about writing dissertation of project work.

#### NOTE:

The project work may be carried in pharmaceutical industries / National laboratories/R&D centers/ Academic institutions/ National and International Universities in the field of Pharma or Analytical chemistry with emphasis on the academics or applied fields. In-house project may be carried out.

#### Total: 24 h

#### **Course Outcomes:**

- To identify the topic with the consideration feasibility.
- To learn the procedure of literature survey of the concered topic.
- To derive a plan for executing the work in the stipulated time with maximum efficiency and success.
- The intensive exposure to industry as a first time experience.
- Understanding different sectors of an industry and the functionaries of each sector.

# Syllabus Discipline Specific Elective Courses

#### FUNDAMENTALS OF BIOCHEMISTRY 3003

#### **Course Objective**

To study the metabolism of carbohydrates, aminoacids, proteins and lipids. To understand the functions of DNA and RNA - To know about vitamins.

#### Unit I **Chemistry And Metabolism Of Carbohydrates**

Definition, Classification and biological role of carbohydrates. Monosaccharides Linear and ring structures (Haworth formula) of ribose, glucose, fructose and mannose (structural determination not required) physical and chemical properties of glucose and fructose.

Disaccharides: Ring structures (Haworth formula) - occurrence, physical and chemical properties of maltose, lactose and sucrose. Glycolysis of carbohydrates.

#### Unit II **Chemistry And Metabolism Of Amino Acids And Proteins**

Amino acids: Various classification, essential amino acids, physical properties (amphoteric nature and isoelectric point) reactions.

Proteins: Classifications (based on shape, composition and solubility), physical properties.

Primary structure - End group analysis (N - terminal analysis - Edman's method, dansyl chloride method; C – terminal analysis – hydrazinolysis and bio-chemical mehods)

Biological functions of proteins, Deamination, transamination reactions, Urea cycle.

#### Unit III **Chemistry and Metabolism of Lipids**

Definition, classification - simple lipids (fatty acids), compound lipids and derived lipids, Properties: saponification number, Acetyl number.

Cholesterol (structure not needed), biological importance and chemical properties.Bile acids - functions.Biological functions of lipids.

#### Unit IV **Nucleic Acids**

Purine and pyrimidine bases, nucleosides, nucleotides, polynucleotides, DNA structure various types, RNA structure - various types. Biological functions of DNA and RNA, Genetic code.

#### **Unit V Vitamins**

Vitamins: Definition, classification – water – soluble vitamins  $(B_1, B_2, B_3, B_6, B_{12})$  and vitamin - C) and fat- soluble vitamins (A,D,E and K) - occurrence, structure, deficiency diseases, biochemical rules and daily requirements.

#### Total: 45 h

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#### **Course Outcomes:**

- To learn about the definition, Classification and biological role of carbohydrates
- To learn about the monosaccharides and disaccharides
- To understand the types and properties of Amino acids
- To learn about the types and properties of proteins
- To understand the structure and biological functions of proteins

#### **Text Book**

 J.L. Jain, Sunjay Jain, Nitin Jain, Fundamentals of biochemistry,6<sup>th</sup> edition, S.Chand and company Ltd, 2005.

# **Reference Books**

- Charlotte W. Pratt, Kathleen Cornely, Essential Biochemistry, 2<sup>nd</sup> Edition, John Wiley & Sons, 2001.
- 2. C. B. Powar and G. R Chatwal, Biochemistry-5<sup>th</sup> edition, Himalaya publishing house, 2006.

#### **ORGANIC CHEMISTRY – I**

#### **Course Objective**

To learn about the salient features of optical activity and geometrical isomers of organic compounds. To study the mechanism of substitution reactions in aliphatic and aromatic systems.

#### Unit I Stereochemistry

Optical activity and chirality.Classification of chiral molecules as asymmetric and dissymmetric.A brief study of dissymmetry of allenes, biphenyls, spiro compounds, trans-cyclooctene and cyclononene and molecules with helical structures.Absolute configuration – R, S notation of biphenyls and allenes.Fischer projection. Inter conversion of Sawhorse, Newman and Fischer projections. Molecules with more than one asymmetric center (restricted to five carbons) E.g. Erythro andthreo compounds. Asymmetric synthesis, Crams's rule.

Geometrical isomerism.E, Z nomenclature of olefins, Geometrical and optical isomerism (if shown) of disubstitutedcyclopropane, cyclobutane and cyclopentanes. Identification of enantiotopic, homotopic, diaestereotopic hydrogens and prochiral carbons in compounds containing up to ten carbons only, stereo specific and stereo selective reactions.

#### Unit II Aliphatic nucleophilic substitution reactions

Kinetic and non-kinetic methods of determining organic reaction mechanisms.Hammett and Taft equations- Simple problems.

 $SN_1$ ,  $SN_2$  and  $SN_i$  mechanisms –Neighboring group participation –reactivity, Bredl's rule structural and solvent effects- substitution in norbornyl and bridgehead systems – substitution at allylic and vinylic carbons substitution by ambident nucleophiles-substitution at carbon doubly bonded to oxygen and nitrogen-alkylation and acylation of amines, halogen exchange. Von-Braun reaction, alkylation and acylation of active methylene carbon compounds, hydrolysis of esters, Claissen and Dieckmann condensations.

#### Unit III Aromaticity

Aromaticity of benzenoid, heterocyclic and non-benzenoid compounds, Huckel's rule-Aromatic systems with pi electron numbers other than six-non-aromatic

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(cyclooctatetraene) and anti-aromatic systems (cyclo butadiene ) –systems with more than 10pi electrons –Annulenes up to  $C_{18}$  (synthesis of all these compounds is not expected).

#### Unit IV Nucleophilic substitution reactions

Method for the generation of benzyne intermediate and reactions of aryne intermediate-Nucleophilic substitution involving diazonium ions. Aromatic Nucleophilic substitutions of activated halides. Ziegler alkylation. Chichibabin reaction. Sand Meyers reagent.

#### Unit V Aromatic electrophilic substitutions

The arenium ion mechanism –Orientation and reactivity (ortho, meta and para directing groups), Hammett equations. Typical reactions –nitration, halogenation, alkylation, acylation and diazonium coupling.Formylation reactions-Gatterman, Gatterman-Koch, Vilsmeyer-Hack and Reimer –Tieman reaction. Synthesis of di and tri substituted benzenes (symmetrical tribromo benzene, 2-amino 5-methylphenol, 3-nitro - 4-bromobenzoic acid, 3,4-dibromonitrobenzene, 1,2,3trimethylbenzene) starting from benzene or any monosubstituted benzene. Electrophilic substitution of pyridine and pyridine -N-oxide, Naphthalene &Anthracene .hypso reactions

#### Total: 45 h

#### **Course Outcomes:**

- To learn about the Optical activity and chirality of molecules
- To learn about the Absolute configuration R, S notation of biphenyls and allenes
- To understand the Fischer projection. Inter conversion of Sawhorse, Newman and Fischer projections.
- To learn about the Asymmetric synthesis, Crams's rule
- To understand the Geometrical isomerism.E, Z nomenclature

# **Text Books**

- 1. Jerry march, Advanced organic chemistry, 4<sup>th</sup> edition, John Wiley student edition 2004.
- 2. John Mc Murry, Organic chemistry, 5<sup>th</sup> edition, Asian books Pvt Ltd, 2000.

# ReferenceBooks

- F. A. Carey, Richard J.Sundberg, Advanced organic chemistry, 5<sup>th</sup> edition, springer, 2007.
- P.S. Kalsi, Organic reactions stereochemistry and mechanism, 4<sup>th</sup> edition, New Age International Publishers, 2006.

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#### **Course Objective**

To understand the fundamental aspects of classical thermodynamics and chemical potential. To learn the important aspects of statistical thermodynamics and chemical potential. To study the simultaneous reaction, fast reaction, reactional in solution and the effect of temperature on reaction rate.

#### Unit I Classical thermodynamics

Definition - Fugacity : Determination of Fugacity- Variation of Fugacity with temperature and pressure. Fugacity of solids and liquids.Mixture of ideal gases.Maxwell's relationships, spontaneity, equilibria-Temperature, pressure dependence of thermodynamic quantities, Lechatlier principle.The concepts of activity and activity coefficients and determination of activity coefficient.

#### Unit II Chemical potential

Partial molar properties -Partial molar free energy –Partial molar volume and partial molar heat content –their significance and determination of these quantities. Equilibrium in heterogeneous system.Variation of chemical potential with temperature and pressure.Alternative definition of chemical potential.

#### Unit III Statistical thermodynamics

Concept of thermodynamic probability – distribution of distinguishable and nondistinguishable particles.

Maxwell – Boltzmann, Fermi – Dirac and Bohr's Einstein statistics- Comparison and applications – modes of contribution to energy- Partition function – evaluation of translational, vibrational and rotational, nuclear and electronic partition functions for mono, di atomic and poly atomic ideal gases-thermodynamic functions in terms of partition functions to heat capacities of ideal gases – Law of equipartition energy- heat capacity of solids (Einstein and Debye models).

#### Unit IV Chemical kinetics-I

Simultaneous reaction- A detail study of reversible reaction-First order opposed first order, first order opposed second order reactions-.Kinetics of complex/composite reactions, reversible reactions, consecutive reactions, parallel reactions, chain reactions, general treatment of chain reactions – chain length - Rice Herzfeld mechanism – explosion limits.

Study of fast reaction – relaxation methods – temperature and pressure jump method – stopped flow and flash photolysis methods.

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#### Unit V Chemical kinetics-II

Effect of temperature on reaction rate – Collision theory of reaction rates- Molecular beams – Collision cross sections- Effectiveness of collisions-Probability factor – Potential energysurfaces. Langmuir and BET absorption isotherms – study of kinetics of surface reaction – catalysis by metals semiconductor oxides – Mechanism of heterogeneous catalytic reaction – Absorption coefficient and its significance. Partition functions and activated complex. Eyring equation Estimation of free energy, enthalpy and entropy of activation and their significances.

Reactions in solutions – Effect of pressure, dielectric constant and ionic strength on reactions in solutions – Kinetic isotope effects – Linear free energy relationships – Hammett and Taft equations – Acid base catalysis – Mechanism of acid base catalyzed reactions – Bronsted catalysis law.

#### Total: 45 h

#### **Course Outcomes:**

- To learn about the Fugacity and determination of Fugacity
- To learn about the variation of Fugacity with temperature and pressure
- To understand the Maxwell's relationships
- To learn about the Lechatlier principle
- To understand the Partial molar properties

#### **Text Book**

1. K.L. Kapoor, Physical chemistry, 1st edition, Macmillan Publisher, 2004.

#### **Reference Books**

- 1. K.L. Kapoor, Physical chemistry, 1<sup>st</sup> Edition, Macmillan Publisher, 2004.
- Kuriacose, Rajaram, Thermodynamics, 3rd edition, ShohanLalNagil Chand & co, 1999.
- 3. Keith J. Laidler, Chemical Kinetics, 3rd edition, Pearson Education, 2008.
- M. C Gupta, Statistical thermodynamics, 2nd edition, New Age International Publishers, 2006.

#### SYNTHESIS OF API AND THEIR MANUFACTURE 3003

#### **Course Objective**

To understand the process chemistry, combinatorial chemistry, phase transfer catalysis and asymmetric synthesis and strategy of process research.

# Unit IProcess chemistry in pharmaceutical industry – An overview09Introduction, top 200 prescription drugs by worldwide sales ; Top ten drugs in the USmarket constituting 10% of world wide sales – Premarin, Synthroid, Lipitor, Prilosec,

Hydrocone, Albuterol, Norvasc, Claritin, Timox and Prozac (\$ one billion). Background of process chemistry – role of process chemistry

# Unit IIStrategy of process research & development in pharma industry09ProcessresearchanddevelopmentofPenicillinGCASReg.No.[61-33-6](antibacterial);fosinopril CASReg.No.[98048-97-6](antihypertensive);RabeprazoleCASReg.No.[117976-89-3] (antiulcerative)Time based competition – portfolio management –stages of process research and development.

# Unit III Combinatorial chemistry

Introduction – Drug Optimization – Drug discovery – Solid Phase Technique – parallel synthesis – Mixed Combinatorial Synthesis – Deconvolution – Structure Determination and limitations – Drug design / Drug discovery.

#### Unit IVPhase transfer catalysis and asymmetric synthesis09

Application of phase transfer catalysts in pharmaceutical industry for drug synthesis – enantioselective synthesis of chiral 2-hydroxycarboxylic acids and esters – asymmetric catalysis – eg. Asymmetric hydrogenation – L-Dopa process ;Sharpless asymmetric epoxidationseg. Synthesis of Fluoxetine enantiomers

#### Unit V Polymorphism and process safety in drug synthesis

Polymorphism – solid state – crystallization – recrystallization of drug molecules eg. Isolation techniques and characterization of polymorphs of Venlafaxine hydrochloride[99300-78-4] Clopidogrelbisulphate [135046-48-9] and Lorazepam[ 846-49-1] (any two)

Chemical Process safety – Principles and Practice-guidelines and norms-Green chemistry.

Total: 45 h

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#### **Course Outcomes:**

- To learn about the Premarin, Synthroid, Lipitor, Prilosec, Hydrocone, Albuterol, Norvasc, Claritin, Timox and Prozac
- To learn about the role of process chemistry
- To understand the Process research and development of PenicillinG CAS
- To learn about the Rabeprazole CAS
- To understand the drug optimization and drug discovery

# **Text Books**

- 1. R. Hilfiker, Polymorphism in Pharmaceutical industry, Wiley-VCH, 2006.
- 2. H. G.Brittain, Polymorphism in Pharmaceutical solids II<sup>nd</sup> edition, CRC Press, 1998.

#### **Reference Book**

 C. Starks, C. Liotta, M. Halpern, "Phase-Transfer Catalysis: Fundamentals, Applications and Industrial Perspectives," Chapter 16, Chapman & Hall, New York,1994.

#### ORGANIC NAME REACTIONS AND SYNTHESIS OF REAGENTS 3003

#### **Course Objective**

To study condensation reaction oxidation and reduction reaction. To know the synthesis and application of important reagent.

#### Unit I **Condensation reactions**

Condensation reactions following; Aldol of the condensation, Claisen ester condensations.

#### Unit II Naming reactions

Cannizzaro reaction, Dieckmann cyclisation, Reformatsky reaction, Dakin reaction, Etard reaction, HVZ reaction, Umpolungsynthesis and Stephen reaction.

#### **Unit III Oxidation and addition reactions**

Examples of oxidation reactions: Barton reaction, Jones oxidation, Oppenauer oxidation. Addition reaction: Michael addition.

#### Unit IV **Reduction reactions**

Examples of reduction reactions:mBirch reduction, Clemmenson reduction, Meerwin P.V reduction, rosenmund reduction,

#### Unit V Synthesis of useful reagents

Synthesis and applications of the following reagents: 9-BBN, n-butyl lithium, ceric ammonium nitrate(CAN), DDQ, DCC, Grignard reagent, LDA, Gilman reagent, NBS and PCC.

#### **Course Outcomes:**

- To learn about the aldol condensation
- TolearnabouttheClaisenester condensations. •
- To understand the Cannizzaro reaction, Dieckmann cyclisation ٠
- To learn about the Reformatsky reaction, Dakin reaction. •
- To understand the Etard reaction, HVZ reaction, Umpolungsynthesis and Stephen • reaction.

#### Total: 45 h

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# **Text Books**

- R.O.C. Norman, Principles of Organic Synthesis by, Chapman and Hall, London 1980.
- 2. Francis A. Carey and Richard J. Sundberg, Advanced Organic Chemistry-Part B, 3<sup>rd</sup> Edition, 1990.

# **Reference Book**

1. S.M. Mukherji and S.P. Singh, Organic Reaction Mechanism, Macmillan India Ltd. 1990.

# MACROMOLECULAR CHEMISTRY

#### **Course Objective**

To study the types of polymerization, polymerization techniques, crystallinity in polymers, applications of polymer, polymer degradation and additives for polymers.

#### UNIT I **Basic Concepts of Polymers**

Monomer, Repeating unit, degree of polymerization. Classification of polymers, Stereochemistry of polymer, nomenclature of stereo regular polymers. Types of polymerization - Chain polymerization, free radical polymerization; ionic polymerization; Coordination polymerization and Ziegler Natta catalyst.

#### UNIT-II **Types of Polymerisation**

Step polymerization, ring opening polymerization. Co polymerization, random, block and graft co polymers- preparation. Plastics - Types of plastics - Rubber - Natural and synthetic rubber - Vulcanisation of rubber.

Polymerisation techniques; bulk, solution, suspension and emulsion polymerization.

#### UNIT-III **Molecular Weight and Glass Transition Temperature**

Measurement of molecular weight and size; number average and weight average molecular weights. Glass transition temperature, concepts of glass transition temperature and associated properties.

#### **UNIT-IV Glassy Solids and Polymer Crystallization**

Glassy solids and glass transition, factors influencing glass transition temperature (Tg).

Crystallinity in polymers; Polymer crystallization, structural and other factors affecting crystallisability, effect of crystallinity on the properties of polymers.

#### UNIT –V **Types of Polymers and Polymer Degradation**

Synthetic resins and plastics; Manufacture and applications of polyethylene, PVC, Teflon, poly styrene, polymethylmethacrylate, poly urethane, phenol - formaldehyde resins, ureaformaldehyde resins and epoxy polymers.

Polymer degradation: Types of degradation- thermal, mechanical, photo, hydrolytic and oxidative degradations. Additives for polymers: Fillers, plasticizers, thermal stabilizers, photo stabilizers, anti oxidants and colourants.

#### TOTAL: 45h

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#### **Course Outcomes:**

- To learn about the Basic concepts of polymers, monomer, degree of polymerization
- To learn about the Classification of polymers, Stereochemistry of polymer, nomenclature of stereo regular polymers
- To understand the types of polymerisation .
- To learn about the Polymerisation techniques
- To understand the Measurement of molecular weight and size

#### **TEXT BOOKS:**

1. Fred. W. Billmeyer, Text Book of Polymer Science, John Wiley & Sons, 3<sup>rd</sup> Edition, 2007.

2. R. V. Gowariker, Polymer Science, New Age International Publication, 2006.

# **REFERENCE BOOKS:**

1. R. J. Young and P. A. Powell, Introduction to Polymers, CRC Press, 3<sup>rd</sup> Edition, 1991.

2. A. Ravve, Principles of Polymer Chemistry, Springer New York, 3<sup>rd</sup> Edition, 2012.

#### SEPARATION TECHNIQUES

# 3003

#### **Course Objective**

To study the salient features of thermal methods and atomic absorption spectroscopy.

To study the general features of chromatography and their Basic principles.

To understand HPLC Ion exchange and gel permeation chromatography.

#### Unit I Introduction to chromatography 09

Adsorption and partition chromatography, definition of terms, techniques and chemical concept of column, paper, TLC and HPTLC.

#### Unit II GLC

Gas-Liquid Chromatography, Principles, Retention Volumes, Instrumentation, Carrier Gas, Columns, Stationary Phase, Detectors, Thermal Conductivity, Flame Ionization, Electron Capture, Application of G.L.C.

#### Unit III HPLC

High Performance Liquid chromatography: Scope, Column efficiency, Instrumentation, Pumping Systems, Columns, Column packing, Detectors, Applications.

# Unit IV IEC 09

Basic principle of ion exchange chromatography (IEC), instrumentation and application of Ion-Exchange chromatography (IEC).

Unit V GPC 09

Basic principle, instrumentation and application of Gel Permeation chromatography (GPC).Standard deviation and correlation coefficient.

Total: 45 h

#### **Course Outcomes:**

- To learn about the Adsorption and partition chromatography
- To learn about the techniques and chemical concept of column, paper, TLC and HPTLC.
- To understand the principle, theory and applications of gas-liquid chromatography

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- To learn about the principle, theory and applications of High Performance Liquid chromatography
- To understand the principle, theory and applications of ion exchange chromatography (IEC)

# **Text Book**

1. E. Heftmann, Chromatography-6<sup>th</sup> Edition, Vol-69A, Elsevier Publisher, 2004.

# **Reference Book**

1. Kevin Robards, Charles, P. Jackson, Paul Haddad, Principles and Practice of Modern

Chromatographic Methods, Academic Press, Elsevier Publisher, 2015.

# Addition to carbon - carbon and carbon-hetero multiple bonds

Electrophilic, nucleophilic addition reaction and neighbouring group participation, mechanism - Addition of halogen and nitrosyl chloride to olefins. Hydration of olefins and acetylenes.Hydro boration, Syn& Anti stereochemistry.Hydroxylations, Michael addition, Diels Alder reaction, 1,3-dipolar additions.

To learn about the addition reaction involving carbon to carbon and carbon to hetero multiple bonds.To learn about some important oxidation and reduction reactions and elimination

#### Unit II Naming reactions

**Course Objective** 

reactions.

Unit I

Carbenes and their addition to double bonds-SimmonSmith reaction, Mannich, Stobbe, Darzen, Wittig, Wittig – Horner and Benzoin reactions,  $C \equiv N$  with Grignard reagent. Stereo chemical aspects to be studied wherever applicable. Nitrene: methods for generating nitrenes and their reactions.

#### UnitIII Elimination reactions

 $E_1$ ,  $E_2$  and  $E_1cB$  mechanism-  $E_1$ ,  $E_2$  and  $E_1CB$  Spectrum-orientation of the double bond –Hofmann and Saytzeff rule - competition between elimination and substitution.Typical elimination reactions – dehydration, dehydrohalogenation and dehalogenation. Stereochemistry of  $E_2$  eliminations in cyclohexane systems (Menthyl,Neomenthyl). Mechanism of pyrolytic elimination.Chugaev and Cope eliminations.

#### UnitIV Coupling Reactions

Heck Coupling-Suzki coupling-Tin Coupling-Transition metal catalyzed coupling reactions.

#### UnitV Oxidation and reduction

Mechanisms – study of the following oxidation reactions – oxidation of alcohols-use of DMSO in combination with DCC or acetic anhydride in oxidizing alcohols- oxidation of methylene to carbonyl- oxidation of aryl methanes – allylic oxidation of olefins. Reductions : selectivity in reduction of 4-T- Butyl cyclohexanone using selectrides hydride reductions -LAH, NaBH<sub>4</sub>, DIBAL, Super hydride, Lithium hydride, Sodium hydride – synthetic importance of Clemmenson and Wolff- Kishner reductions- modifications of Wolff-Kishner reduction – Birch reduction, MPV reduction.

#### Total: 45 h

#### ORGANIC CHEMISTRY- II

3003

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#### **Course Outcomes:**

- To learn about the electrophilic, nucleophilic addition reaction
- To learn about the Hydro boration, Syn& Anti stereochemistry
- To understand the Hydroxylations, Michael addition, Diels Alder reaction, 1,3-dipolar additions.
- To learn about the Carbenes and their addition to double bonds
- To understand the methods for generating nitrenes and their reactions.

# **Text Books**

- 1. R.O.C. Norman, Principles of Organic Synthesis, Chapman and Hall, London 1980.
- 2. Francis A. Carey and Richard J. Sundberg, Advanced Organic Chemistry-Part B, 3<sup>rd</sup> Edition, 1990.

#### **Reference Book**

 S.M. Mukherji and S.P. Singh, Organic Reaction Mechanism, Macmillan India Ltd. 1990

#### **ANALYTICAL TECHNIQUES**

**Course Objective** 

Unit I

Colourimetric analysis and UV- Visible spectroscopy: Beer Lambert's law, Principles of single and double beam instruments - applications for analysis of inorganic and organic samples. Infrared spectrophotometric analysis - principle and instrumentation and molecular structure determination.

To learn about several methods of analytical techniques. To learn about basic concepts of UV,

Raman Spectra – principle, basic instrumentation – structural analysis.

**UV-Visible, IR and Raman spectroscopy** 

#### Unit II NMR and mass spectroscopy

IR, NMR and mass spectrum and their applications.

Nuclear Magnetic Resonance - Principle, instrumentation, structure determination, NMR of <sup>1</sup>H, <sup>13</sup>C, <sup>31</sup>P, <sup>19</sup>F.

Electron Spin Resonance - Principle, instrumentation, applications to coordination compounds.

#### **Unit III** Mass spectroscopy

Mass Spectrometry - Principle, basic instrumentation, fragmentation patterns organic molecular structural determination.

#### **UnitIV Thermal analysis**

Thermo gravimetric and differential thermal analysis, DSC thermometric titrations, differential scanning colourimetry – basic instrumentation and applications.

#### Unit V AAS and photoelectron spectroscopy

Atomic absorption spectroscopy: Theory, Atomizers, Flame and Electro thermal. Radiation sources, Instrumentation, spectral and chemical interferences, application.

Photoelectron spectroscopy (UV and X-Ray) -photo electron spectra Koopman's theorm, fine structure in PES, chemical shift and correlation with electronic charges.

#### **Course Outcomes:**

- To learn about the Colourimetric analysis and UV- Visible spectroscopy
- To learn about the principle, instrumentation, structure determination raman spectra
- To understand the principle, instrumentation, structure determination of nuclear magnetic resonance

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Total: 45 h

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- To learn about the Principle, instrumentation, structure determination of electron spin resonance
- To understand the principle, instrumentation, structure determination of Mass Spectrometry

#### **Text Books**

- Willard Merrit, Dean and Settle, Instrumental methods of analysis, 6<sup>th</sup> Edition, CBS Publisher, 1986.
- 2. A.I.Vogel, 1976, Textbook of Qualitative Inorganic Analysis, 3<sup>rd</sup> Edition, ELBS.

# **Reference Book**

 D.A.Skoog and D.M.West, Fundamentals of Analytical Chemistry, 4<sup>th</sup>Edition, oldReinhord& Winston, Publication, 1982.

#### **Course Objective**

To study the general aspects of alkaloids, steroids, camphor, Acetic acid, carbohydrates and polysaccharides.

#### Unit I Natural pigments

Anthocyanins – general methods of determining structure and synthesis – cyanin and hirsutin chlorides.Flavones and flavanols – general method of determining structure and synthesis – Quercetin – Isoflavones – daidzein.

Carbohydrates: Structural aspects of starch and cellulose and biosynthesis of

carbohydrates

#### Unit II Terpenes

Classification, structural elucidation by chemical degradation and synthesis of pinene, camphor, zingiberene, santonin,  $\beta$ -carotene. biosynthesis of terpenes

Steroids: Structure and synthetic aspects of cholesterol, ergosterol, estrone and

progesterone. Biosynthesis of steroids.

#### Unit III Alkaloids

Classification, structural elucidation by chemical degradation and synthesis of papaverine, quinine, morphine and reserpine. Biosynthesis of alkaloids

#### Unit IV Antibiotics

Structure and synthesis of chloramphenicol, penicillins and streptomycin.

#### Unit V Synthetic methodology

Protection of functional groups (hydroxyl, amino, carboxyl, and carbonyl groups). Illustration of protection and deprotection in synthesis – synthetic analysis and planning – synthesis of target molecules based on disconnection and synthon approach. Control of stereochemistry – synthesis using simple chiral molecules.

#### **Course Outcomes:**

- To learn about the Anthocyanins
- To learn about the cyanin and hirsutin chlorides
- To understand the flavones and flavanols
- To learn about the Quercetin, Isoflavones and daidzein
- To understand the structural aspects of starch and cellulose

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# Total : 45 h

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# **Text Books**

- 1. I. L. Finar, Organic chemistry, vol.2, 5<sup>th</sup> edition, Pearson Education, 2003.
- 2. AshutoshKar, Chemistry of natural Products, Vol–I, I<sup>st</sup> edition, CBS Publisher, 2010.

#### **Reference Book**

1. Sujatha V. Bhat, B.A Nagasampagi, S. Meenakshi, Natural Products, Narosa Publishing House, 2009.

#### ENZYME TECHNOLOGY AND RELATED 3003

#### ENTREPRENEUREAL SKILLS

#### **Course Objective**

To learn biological aspects, metalloenzyms, oxygen carriers, nitrogen fixation, photosynthesis and cytochrome, and bioanalytical aspects.

#### Unit IIntroduction to biochemistry, function and applications09

Nature and functions of enzyme, Coenzyme/ Cofactor.Classification of enzyme. Assay methods and units. Examples of applications of enzymes in industry, analytical techniques, medicine and Pharmaceuticals.

#### Unit IIKinetics and mechanism of enzyme catalysis09

Enzyme catalysis and controlling factors. Kinetics of enzyme catalyzed reactions in solution. Immobilized enzyme reaction kinetics.Effect of mass transfer resistance.

#### Unit IIIEnzyme production on large scale technology09

Isolation and purification of enzymes, protein fractionation methods.

#### Unit IV Immobilization technology and development

Immobilization techniques for enzymes. Characteristics and uses for immobilized enzyme systems

# Unit VIndustrial bioreactors utilizing isolated enzymes and biosensors<br/>development and applications09

Reactor design and analysis for immobilized enzyme reactors. Applications in biosensors.Some modern developments for enzymes in organic synthesis.

#### Total: 45 h

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#### **Course Outcomes:**

- To learn about the Nature and functions, classification of enzyme, Coenzyme and Cofactor
- To learn about the applications of enzymes in industry, analytical techniques, medicine and Pharmaceuticals
- To understand the enzyme catalysis and controlling factors
- To learn about the kinetics of enzyme catalyzed reactions in solution
- To understand the immobilized enzyme reaction kinetics

# Text Book

1. J. L Jain, S. Jain , N. Jain, Fundamentals of Biochemistry, 6<sup>th</sup> Edition S.Chand & Company, 2009.

# **Reference Books**

- 1. A.Wiseman, "Handbook of Enzyme Biotechnology", Ellis Horwood, 1983.
- 2. T. Devasena, Enzymology,1<sup>st</sup> edition, Oxford University Press, 2010.

# NUCLEAR AND PHOTOCHEMISTRY 3003

#### **Course Objective**

To learn the determination of Radio activity, application of tracers and Inorganic

Photochemistry.

#### UnitI Nuclear transition and activity

Orbital electron capture: nuclear isomerism, internal conversion, detection and determination of activity by cloud chamber, nuclear emulsion, bubble chamber, G.M., Scintillation and Cherenkov counters.

#### Unit II Nuclear reactions

Nuclear fission and fusion reactions as energy sources: direct reactions, photonuclear and thermo nuclear reactions

#### Unit III Nuclear reactors

Components of nuclear reactors – the breeder reactor – nuclear reactors in India.

#### Unit IV Activation analyses

Applications of tracer in study of reaction mechanism and in analytical chemistry – neutron activation analysis – isotope dilution analysis –Carbon dating- radio active tracer in the diagnosis and treatment in field of medicine.

#### Unit V Inorganic photochemistry

Photo redox reactions and photo substitution reactions in coordination chemistry - photovoltaic and photo galvanic cells. Photo electro chemistry, Aspects of solar energy conversion.

#### **Course Outcomes:**

- To learn about the orbital electron capture
- To learn about the determination of activity by cloud chamber, nuclear emulsion, bubble chamber, G.M., Scintillation and Cherenkov counters.
- To understand the nuclear fission and fusion reactions
- To learn about the direct reactions, photonuclear and thermo nuclear reactions
- To understand the Components of nuclear reactors and the breeder reactor

#### **Text Book**

1. H.J. Arnikar, Nuclear Chemistry, Wiley Eastern Co. II Edition, 1987.

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# Total: 45 h

# **Reference Book**

1. N.N. Greenwood and Earnshaw, Chemistry of the Elements, Pergamon Press New York, 1984.

## NOVEL MATERIALS AND GREEN INDUSTRIAL CATALYSIS 4004

#### **Course Objective**

To learn about some important functional materials and nanomaterials. To learn about properties of metallic clusters and characterization techniques of functional and nanomaterials.

#### UnitIIntroduction to functional and nanomaterials12

An overview-, materials, molecular materials, functional materials, nanomaterial's classification /properties and industrial applications.

#### Unit II Properties of Metallic clusters

Supported metallic clusters, Catalysts preparation method, physical and chemical properties. Catalysis mechanism uses and synthetic applications

#### Unit III Characterization

Tools for Structural Characterization of novel materials by UV-Visible spectroscopy, Infrared spectroscopy, Nuclear magnetic resonance spectroscopy and mass spectrum

# UnitIII Metal oxides 12

Metal oxides, Supported metal oxides, Industrial catalysis (Synthesis Gas and Hydrogen).

#### UnitIVCatalysts in chemical transformation12

Ammonia Synthesis, Methanol and Fischer – Tropsch Synthesis, Hydrocarbon Transformations, Environmental Catalysis

Total : 60 h

12

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#### **Course Outcomes**:

- To learn about the nanomaterial's classification, properties and industrial applications.
- To learn about the preparation, properties of supported metallic clusters
- To understand the metal oxides and supported metal oxides
- To learn about the industrial catalysis
- To understand the ammonia Synthesis

# **Text Book**

 Harry R. Allcock, Introduction to Materials Chemistry, Wiley Interscience Publisher, 2000.

# **Reference Book**

1. Bradley D. Fahlman, Materials Chemistry, 2<sup>nd</sup> ed. Springer Publisher, 2011.

#### **Course Objective**

To study the structure elucidation of organic molecules using NMR, Maps spectroscopy and IR spectroscopy. To know about the general aspects of organic photochemistry. To learn about Heterocycles, terpenoids, steroids and cholesterol.

#### Unit IPhysical Methods Of Structure Determination0

Principle and applications of ultraviolet Woodward Fisher Rule (only application) and infra-red spectroscopy in organic structure determination.

Nuclear magnetic resonance spectroscopy.Proton chemical shift, spin-spin coupling, coupling constants and applications to organic structures <sup>13</sup>C resonance spectroscopy (elementary treatment).

#### Unit II Mass spectroscopy

Mass spectrometry and its applications Optical rotatory dispersion and its applications. Cotton effect, axial haloketone rule and octant rule. Problem solving using spectral data. (for molecules with a maximum number of  $C_{10}$ )

#### Unit III Organic photochemistry

Photochemical excitation-rate of the excited molecules –Jablonski diagram-study of photochemistry of ketone- photo reduction-photo cyclo addition-Paterno-Buchi reaction-dipi-methane rearrangement.

Unit IV Pericyclic reactions 09 classification –orbital symmetry-Woodward Hoffman rules-Analysis of electrocyclic, inter conversion of hexatrienes to cyclohexadienes. Cyclo addition and sigmatropic reactionscorrelations diagram for butadiene-cyclobutene system. Structure of butylene, a fluxional molecule –Cope and Claissen rearrangements.

# Unit VHeterocycles, terpenoids and steroids synthesis of the following09

Imidazole, oxazole, thiazole, flavones, isoflavones, anthocyanins, pyrimidines (cytocine and uracil only) and purines (adenine, guanine only). Synthesis of parent and simple (alkyl or aryl substituted derivatives are expected). Synthesis of vitamin A1 (Reformatsky and Wittig reaction methods only) Conversion of Cholesterol to progesterone, estrone and testosterone.Elucidation of structure of cholesterol (by chemical degradation)

# Total: 45 h

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#### **Course Outcomes:**

- To learn about the Principle and applications of ultraviolet Woodward Fisher Rule
- To learn about the infra-red spectroscopy in organic structure determination.
- To understand the Nuclear magnetic resonance spectroscopy
- To learn about the <sup>13</sup>C resonance spectroscopy
- To understand the mass spectrometry and its applications

#### **Text Book**

1. J.Dyer, Application of absorption spectroscopy of organic compounds,

Prentice-Hall of India Pvt.New Delhi, 2001.

#### **Reference Books**

- R.M. Silverstein, G.C. Bassler and Monsil, Spectrometric identification of Organic compounds by John Wiley and Sons, New York, 2005.
- 2. I.L. Finar, Organic Chemistry, Vol II, 5<sup>th</sup> Edition ELBS Publication, Longman, 1964.

#### **Course Objective**

To know about pharma industry, technology opportunity for innovation, project evaluation, intellectual property protective and business strategy.

#### Unit I Introduction and technology evolution

Pharma industry-Specifics, Importance and role in health sector; the Global scenario and Positioning of Indian Pharma industry; Specific challenges of the Pharma industry versus the general industrial matrix; Understanding technological change; Need for technology strategy as step towards innovation and competitive advantage; Defining technological innovation and benefits.

Technology S-curves and management; Number of firms in the industry, Process obsolescence and Reverse Engineering; Innovative synthetic routes and atom economy dovetailing aspects of Green chemistry; Technology adoption and diffusion; Forecasting demand and confronting substitution.

#### Unit II Opportunity for Innovation

Technological, Political and Regulatory changes, Diversification, Demographic changes; Research and Development (R&D); Investment in R&D and return on investment – a profit centre; Linking of Research and Development for leverage; Cost reduction exercises.

#### Unit III Project evaluation

Managing uncertainty, Analytical hierarchy process, Net Present Value(NPV), Internal Rate of Return(IRR), scenario analysis and decision tree; Portfolio Management, customer-friendly solutions; Product pricing ; Market segmentation and market research.

#### Unit IV Intellectual Property Protection

Role of IP protection in knowledge era; Patents- process and Product and the patenting process; Lead molecule development and cost; ANDA; Patent litigation; Non-disclosure agreement; Expiry of patents and generic drugs marketing and issues in IP.

#### Unit V Business strategy

Networking; Joint venturing; Licensing; Contract manufacturing; Outsourcing; Human resource management of technical professionals- R&D personnel, Product Development team, Cross-Functional team, Internal communication, Organization structure-decentralizing R&D, acquisitions.

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#### **Course Outcome:**

- To learn about the pharma industry-specifics
- To learn about the specific challenges of the Pharma industry versus the general industrial matrix.
- To understand the defining technological innovation and benefits.
- To learn about the technology S-curves and management
- To understand the innovative synthetic routes and atom economy dovetailing aspects of green chemistry

## **Text Book**

1. Scott Shane, Technology Strategy For Managers And Entrepreneurs, Dorling Kindersley India Pvt. Ltd, 2009.

## **Reference Book**

1. C.B.Gupta and S.S.Khanka, Entrepreneurship and Small Business Management, Sultan Chand & Sons, New Delhi, 2012.

## STEREOCHEMISTRY AND REACTION MECHANISM 3003

#### **Course Objective**

To understand the stereochemistry of organic compounds and the basic principle and terminology of retrosynthesis. To know about non-conventional techniques in inorganic synthesis.

#### Unit I Stereochemistry

- a) General consideration of molecular asymmetry and dissymmetry. b) Configuration absolute and relative methods of determination
- c) Chemical transformation ii) asymmetric synthesis; Chiral auxiliaries, chiral reagents and catalysts, Enantiomeric excess iii) Quasiracemates d) Atropisomerism of biphenyls.

#### Unit II Conformational analysis

Conformation – conformational analysis based on physical properties and chemical reactivity, shape of six membered ring, conformation and reactivity in cyclo hexanes and decalins.

#### Unit III Rearrangements- I

Sommelet – Hauser, Favorski, Fries and benzilic acid rearrangements. Hoffmann – Loffler- Freytag reaction, Barton reaction and Shapiro reaction.

#### Unit IV Rearrangements- II

A detailed study with suitable examples of the mechanism of the following rearrangements: Pinacol-pinacolone(Barton and Shapiro)-Wagner-Meerwein, Demjanov, dienone – phenol, Favorski, Baeyer – Villiger, Wolf, Stevens (in cyclic systems) and Von Richter rearrangements.

#### UNIT V Non-conventional techniques

Non-conventional Techniques in organic synthesis-Green chemistry-Microwave assisted reaction-Un Catalyzed reaction. Reaction in ionic organic liquids-Solid state melts reaction.

#### **Course Outcomes:**

- To learn about the general consideration of molecular asymmetry and dissymmetry
- To learn about the configuration, absolute and relative methods of determination

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Total: 45 h

- To understand the Chemical transformation ii) asymmetric synthesis; Chiral ٠ auxiliaries, chiral reagents and catalysts
- To learn about the enantiomeric excess, Quasiracemates, atropisomerism of • biphenyls.
- To understand the Conformation conformational analysis based on physical • properties and chemical reactivity

## **TEXT BOOK**

1. E.S. Gould, Mechanism & structure in organic Chemistry, Holt, Rinehart &

Winston, New Delhi, 1963.

- Morrison and Boyd, Organic Chemistry, Pearson Education Inc, 6<sup>th</sup> Edition, 1992.
  I.L. Finar, Organic Chemistry, Longmans Green & Co., 3<sup>rd</sup> Edition, 1964.

#### PHARMACEUTICAL CHEMISTRY 3003

#### **Course Objective**

To study the anesthetics, sedatives, hypnotics, analgesics, antibiotics, enzymes, coenzymes, vitamin and photo transfer catalysis.

#### Unit I Classification of drugs

Classification of drugs- general and local anesthetics.Sedatives and hypnotics.Narcotics and analgesics.

#### Unit II Antibiotics

Antibiotics – structure and synthesis; Chloromphenicol, pencillins and streptomycin.

#### Unit III Enzyme concept

Enzymes, co-enzymes, theory. Michaelis-Menten's equation and verification by graphical methods-Eadieplot and Lineweaver-Burk plot. Enzyme catalysis, Enzyme specificity, Enzyme mechanism.Enzyme Inhibition- Competitive inhibition, Un-competitive inhibition and Non-competitive inhibition.

#### Unit IV Phase transfer catalysis

Phase transfer catalysis, ionic liquids. Miscellaneous catalysis.Use of crown ethers.

#### Unit V Vitamins

Introduction , water soluble and fat soluble vitamins. Details of vitamin A, C, B<sub>1</sub>, B<sub>2</sub>, B<sub>6</sub>,

#### Total: 45 h

#### **Course Outcomes:**

- To learn about the classification of drugs
- To learn about the general and local anesthetics, sedatives and hypnotics
- To understand the Narcotics and analgesics.
- To learn about the Antibiotics
- To understand the structure and synthesis of chloromphenicol, pencillins and streptomycin To understand the Enzymes, co-enzymes

#### **Text Book**

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1. William Foye, Medicinal Chemistry, 4<sup>th</sup> Edition, 1995.

# **Reference Books**

- 1. Wilson & Gisvold, Medicinal Chemistry, 10<sup>th</sup> Edition, 1998.
- 2. Burger, Medicinal Chemistry, 5<sup>th</sup> Edition, 1995.

To understand the salient features of UV, visible, mass, infrared spectroscopy.To understand the salient features of <sup>13</sup>C-NMR and <sup>1</sup>H-NMR spectroscopy.To learn about the applications of

# Unit I UV-Visible spectroscopy

various spectral techniques in characterizing organic compounds.

**Course Objective** 

Introduction – the energy of excitation. The absorption laws, measurement of the spectrum – choice of solvent – selection rules and intensity – Chromospheres – solvent effects – Conjugated dienes, polyenes, ketones and aldehydes. $\pi - \pi^*$  transitions,  $n - \pi^*$  transition,  $\infty,\beta$ - unsaturated ketones, acids, esters, nitriles, amides. The benzene ring, the substituted benzene ring – polycyclic aromatic hydrocarbons the effect of steric hindrance to co planarity.

## Unit II Mass spectroscopy

Introduction – Instrumentation – High resolution and low resolution mass spectra – Determination of molecular formula – Molecular peaks rule.  $M^+$  ion. Natural isotope abundance analysis – fragmentation process – nitrogen rule, metastable ions, metastable peaks, retro Diels – Alder fragmentation – McLafferty rearrangement, loss of odd electron, neutral fragments from molecular ions – Factors which influence fragment abundance – Mass spectra of various functional groups containing compounds to be studied: aromatic, aliphatic hydrocarbons, ketones, acids, esters, amides, ethers, alcohols, amine and nitriles.

## Unit III Infrared spectra

Introduction – Preparation of samples and examination in an infrared spectrometer – The infrared spectrum – the use of the table of characteristic group frequencies – correlation charts. Absorption frequencies of triple bond and cumulative double bonds – the aromatic overtone and combination – Region  $2000 - 1200 \text{ cm}^{-1}$ . Absorption frequencies' of the double bond region – Groups absorbing in the finger print region – identification of functional groups.

# Unit IV <sup>1</sup>H-NMR

The spinning nucleus – The effect of an external magnetic field, precessional motion, precessional frequency, energy transitions.

Theory of NMR – Measurement of chemical shifts – Internal standards – Units used in NMR. Factors influencing chemical shift – electronegativity, shielding and deshielding, Van der Walls deshielding, Anisotropic effects – Correlation data, use of correlation tables. Influence of restricted rotation. Chemically equivalent and magnetically equivalent protons. Solvents used in NMR – Choice of solvent – solvent shifts – concentration and temperature effects.

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Integrals – Spin spin splitting – The splitting of NMR signals – Theory of spin-spin splitting. Magnitude of coupling, coupling constants.Proton exchange reactions. Factors influencing geminal coupling – vicinal coupling – Hetero annular coupling, Deuterium exchange. Improving the NMR spectrum – shift reagents. Effect of changing the magnetic field. Nuclear overhauser effect, spin tickling. Problems (Problems involving UV, IR and NMR to be solved)

## Unit V <sup>13</sup>C-NMR

Carbon – 13 NMR: Principle, spin decoupled spectra, single frequency off resonance decoupled (SFORD) spectra, chemical shift values, problems.

#### Total: 60 h

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#### **Course Outcomes:**

- To learn about the energy of excitation. The absorption laws, measurement of the spectrum
- To learn about the selection rules and intensity, chromospheres, solvent effects, conjugated dienes, polyenes, ketones and aldehydes
- To understand the π − π\* transitions, n π\* transition, ∞,β- unsaturated ketones, acids, esters, nitriles, amides.
- To learn about the high resolution and low resolution mass spectra
- To understand the fragmentation process, mcLafferty rearrangement.

#### **Text Book**

1. H.H.Willard, L.L.Meritt, J.A.Dean and F.A.Settle, Instrumental Methods of Analysis, Wadsworth, New York, 7<sup>th</sup> edition, 1986.

#### **Reference Books**

- John R.Dyer, Applications of absorption spectroscopy of Organic Compounds, Prentice Hall, London, 1987.
- Robert M.Silverstein, Clayton Bassler and Terence C.Morril, Spectrophotometer Identification of Organic Compounds, 6<sup>th</sup> Edition, John Wiley & Sons, New York, 2002.

# INORGANIC CHEMISTRY 4004

#### **Course Objective**

To learn about the basic concepts of bonding in metal carbonyls and nitrosyls and other inorganic compounds. To learn about the reactions of organometallic compounds and their magnetic properties.

#### Unit I Bonding in inorganic compounds

Alkyls and arene complexes; metalation, bonding in metal carbonyls and nitrosyls, chain and cyclic donors, olefin, acetylene and allyl systems, synthesis, structure and bonding metallocenes.

#### Unit II Organometallic reactions

**Catalysis:**Hydrogenation of olefins (Wilkinson's catalyst), hydroformylation of olefins using cobalt or rhodium catalysts (oxoprocess), oxidation of olefins to aldehydes and ketones (Wacker process) polymersiation (Zeigler-Natta catalyst); cyclooligomerisation of acetylene using nickel catalyst (Reppes' catalyst)-Synthetic Gasoline-mobile Reaction.

#### Unit III Magnetic properties

Spectral and magnetic properties of transition metal complexes-Guoy method, Faraday method.Applications of IR, Raman, NMR, ESR, Massbauer to the study of coordination compounds.

#### Unit IV The chemistry of solid state

Structure of solids: Comparison of X-ray, Neutron and Electron diffraction,

structure of ZnS, Rutile, Per voskite, Cadmium iodide and Nickel arsenide: Spinels and inverse spinels: defects in solids, non-stochiometric compounds.

#### Unit V Semiconductors

Band theory, semiconductors, superconductors, solid state electrolytes, types of magnetic behaviour, Dia, Para, Ferro, Antiferro and ferri magnetism: Hysterisis, Solid state lasers, inorganic phosphors.

## Total: 60 h

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#### **Course Outcomes:**

- To learn about the alkyls and arene complexes
- To learn about the synthesis, structure and bonding metallocenes.
- To understand Hydrogenation of olefins, hydroformylation of olefins

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- To learn about the oxidation of olefins to aldehydes and ketones (Wacker process) polymersiation, cyclo oligomerisation of acetylene using nickel catalyst and synthetic Gasoline-mobile Reaction
- To understand the Guoy method, Faraday method.

#### **Text Books**

- J.E. Huheey, Inorganic Chemistry Principles, Structure and Reactivity: Harper Collins, New York, IV Edition, 1993.
- 2. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry- A Comprehensive

Text, John Wiley and Sons 5<sup>th</sup>Edition, 1998.

#### **Reference Books**

- 1. K. F. Purcell and J.C. Kot, Inorganic Chemistry-WB Saunders Co., USA 1977
- 2. M.C. Day and J. Selbin, Theoretical Inorganic Chemistry, Van Nostrand Co., New York,1974
- 3. D.F. Shrivers, P.W. Atkins and C.H. Langfor, Inorganic Chemistry, CH Langford, 1990
- 4. N.N. Greenwood and Earnshaw, Chemistry of the Elements Pergamon, Press New York, 1984.

# Syllabus Generic Elective Courses

#### SOFT SKILL I

**Course Objective:** The ability to create an open environment for communication. An understanding of other people communication styles and needs. To create an environment for open discussion and ongoing dialogue is crucial for communication success.

#### Unit I Reading Comprehension and Vocabulary

Definitions of reading – types of reading – oral reading – silent reading – reading process – classification of reading – nature of reading – Filling in the blanks – Cloze Exercises – Vocabulary building – Reading and answering question.

#### Unit II Listening and Answering Question

Listening process – speaker – hearer – types of listening – transitional listening – critical listening – recreational listening – listening for appreciation – selective listening – intensive listening – listening and sequencing sentences – filling in the blanks – listening and answering questions.

#### Unit III Group Discussion

Introduction – Why GD Part of a selection process – Structure of a GD-Strategies in GD – Team work – body language – Debating various points of views – interaction with peers.

#### Unit IV Conversations

Introducing oneself and others, narrating events – making telephonic conversation – Giving instruction – Giving instruction- Expressing purposes and functions- obligation and preferences, Accepting offers and Counseling Face to face Conversations

#### Unit V Self – Introduction and Role Play

Introduction self and greetings- asking for information- offerings- requisitions- inviting – vocabulary building- asking for description.

#### TOTAL: 45 h

#### **Course outcomes:**

- Cloze exercises provide support to build vocabulary.
- Sense of logic develops from sequencing sentences.
- Group discussion infuses team spirit and sense of competition.
- Face to face and telephone conversation builds up self confidence.

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• Self introduction and role play facilitate cultivation firmness of mind and empathy.

## **TEXT BOOKS:**

- 1. Barun K. Mitra, "Personality Development and Soft Skills". Oxford University Press. New Delhi. 2011.
- 2. S.P. Sharma, "Personalilty Development", Pustaq Mahal. New Delhi. 2010.

- 1. Meenakshi Raman and Sangeetha Sharma, "Technical Communication", Oxford University Press. New Delhi, 2009.
- 2. A.S. Hornby: "Oxford Advanced Learner's Dictionary of Current English", Oxford University Press, 2007

#### SOFT SKILL II 1022

**Course Objective:** To provide basic information about presentation skill and train the students for letter writing, creation of resume and develop the interview skills. To provide information about the Process, types and patterns of communication.

#### Unit I Presentation Skills

General presentation methods and developing presentation skill

#### Unit II Soft skills (Time Management, Stress Management and Body Language) 09

Time management: Importance, Plan and Execution, Default reason and rectification methods. Stress Management: Stress Impacts over Efficiency and how to manage. Body Language: Its importance and need

# Unit IIIResume / Report / Letter Writing09

Resume: Basic components of a resume, Preparation of a resume, Types of resume Report: How to prepare reports, reports components and structure Letter writing: types of letters, framing letters, basic structure, how to draft a letter

Unit IV	Frequently asked Questions	09
Unit V	Interview Skills	09

Aims of Interview expectations and how to fulfill, developing skills

## TOTAL: 45 h

## **TEXT BOOKS:**

- 1. Barun K. Mitra, "Personality Development and Soft Skills". Oxford University Press. New Delhi. 2011.
- 2. S.P. Sharma, "Personalilty Development", Pustaq Mahal. New Delhi. 2010.

#### **Course Outcome:**

- Self introduction and role play facilitate cultivation firmness of mind and empathy
- Group discussion infuses team spirit and sense of competition
- Listening regenerates transformation empathetically
- Cloze exercises provide support to build vocabulary
- Implementation of assertive thoughts can be acquired through writing skills

- 1. Meenakshi Raman and Sangeetha Sharma, "Technical Communication", Oxford University Press. New Delhi, 2009.
- A.S. Hornby: "Oxford Advanced Learner's Dictionary of Current English" Oxford University Press, 2007

#### GREEN CHEMISTRY 2002

**Course Objective:** To train the students to use eco-friendly approaches in synthesizing agrobased chemicals viz. insecticides, fungicides, herbicides, bactericides acaricides, weedicides. To emphasize green chemistry approach in crop protection which help to reduce global warming.

#### Unit I Introduction

Current status of chemistry and the Environment-Evolution of the Environmental movement: Public awareness - Dilution is the solution to pollution-Pollution prevention

#### Unit II Green Chemistry

Definition – Principles of Green Chemistry - Why is this new area of Chemistry getting to much attention - Why should chemist pursue the Goals of Green Chemistry - The roots of innovation – Limitations

#### Unit IIIGreen Chemistry using Bio Catalytic Reactions06

Introduction - Fermentation and Bio transformations - Production of Bulk and fine chemicals by microbial fermentation- Antibiotics – Vitamins - Bio catalyses synthesis of industrial chemicals by bacterial constructs - Future Tends.

#### Unit IV Green House Effect and Global Warming

Introduction - How the green house effect is produced - Major sources of green house gases - Emissions of  $CO_2$  - Impact of green house effect on global climate - Control and remedial measures of green house effect - Global warming a serious threat - Important points

#### Unit V Future Trends in Green Chemistry

Green analytical methods, Redox reagents, Green catalysts; Green nano-synthesis, Green polymer chemistry, Exploring nature, Biomimetic, Proliferation of solvent-less reactions; Non-covalent derivatization, Biomass conversion, emission control.

#### TOTAL: 30h

#### **Course Outcomes:**

- To learn about the environment
- To learn about pollution and prevention methods
- To understand the principle, instrumentation, structure determination of nuclear magnetic resonance

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- To learn about the goals of green Chemistry
- To understand the principle, instrumentation, structure determination of Mass Spectrometry

#### **TEXT BOOKS:**

- 1. M. Lancaster, "Green Chemistry: an Introductory Text", RSC, 2002
- 2. Sheldon, Arends, Hanefeld, "Green Chemistry and Catalysis", Wiley, New York, 2007

- 1. Anastas & Warner, Green Chemistry : Theory & Practice ,Oxford Univ. Press,New York, 1998
- 2. S. E. Park, J. S. Chang, S. H. Jhung, "The Role of Catalyst for Green Chemistry", Chemworld, Vol. 44 (8), 38, 2004

# CHEMINFORMATICS 2002

#### **Course Objective:**

Students completing this paper should be able to understand concepts of molecular chemistry that are basic to cheminformatics. This course will train the students to use QSAR, docking etc.

#### **Unit I Mathematics Process**

Graph theory and molecular numerology; Logic, sets and functions; Algorithms, integers and matrices; Mathematical reasoning, induction and recursion; Counting; graphs, trees and sets, basic probability and statistics; Markov processes

## Unit II Basics of Stereochemistry

Basic Stereochemistry, Amino acids and Proteins and Properties; pKa, pH and ionization of acids and bases; Protein structure - Primary structure, Secondary structure - helix & sheet; Tertiary structure; Quaternary structure; covalent and non-covalent forces that maintain structures.

#### Unit III Chem Information

History of scientific information communication-chemical literature-chemical informationchemical information search-chemical information sources-chemical name and formula searching-analytical chemistry-chemical history-biography-directories and industry sources

#### Unit IV Biological Databases

Introduction; Experimental sources of biological data; Publicly available databases; Gene expression monitoring; Genomics and Proteomics; Metabolomics; Visualisation of sequence data; Visualization of structures using Rasmol or SPDB Viewer or CHIME; Genetic basis of disease; Personalised medicine and gene-based diagnostics.

## Unit V Drug Design

Introduction to drugs, structure-based drug design. QSAR and 3D-QSAR Methods. Pharmacophore Design, Ligand-Based Design and De Novo Drug Design Virtual screening/docking of ligands. Protein structure, Drug action & enzymes. Drug action & receptors. Prediction of Binding Modes, Protein–Ligand binding free energies, Fragment-Based Drug Design, ADMET prediction.

TOTAL: 30h

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#### **Course Outcomes:**

- To learn about the Graph theory and molecular numerology
- To learn about the Markov processes
- To understand the Basic Stereochemistry and properties of Amino acids and Proteins
- To learn about the pKa and pH and ionization of acids and bases
- To understand the History of scientific information communication and chemical literature

## **TEXT BOOKS**

- 1. P. Shanmughavel, "Principles of Bioinformatics", Pointer publishers, 2005.
- 2. Arfken, "Mathematical Methods for Physicists" Academic Press, 1985

- 1. P. Shanmughavel, "Trends in Bioinformatics", Pointer publishers, 2006.
- 2. Francis A. Carey and Richard J. Sundberg, "Advanced Organic Chemistry-Part A & B" Third Edition, 1990.

#### FOOD CHEMISTRY AND ADULTERATION 2002

#### **Course Objective:**

To understand the basic information of food chemistry and adulteration. To appreciate the importance of food additives and pesticide control. To provide an information about food preservatives.

#### Unit I Introduction

Food: source, functions of food – food groups – food guide – basic five food groups, usage of the food guide – food in relation to health – objectives of cooking.

Water: Purification processes - Ion exchangers, reverse osmosis, activated charcoal treatment - Use of chlorination, ozone, and UV light disinfection. Specification of drinking water.

#### Unit II **Constituents of Foods**

Carbohydrates: Classification, Principles involved in the analysis of carbohydrates estimation of carbohydrates.

**Proteins:** amino acids – peptides - Analysis of proteins – Separation of amino acids by paper chromatography.

Minerals and vitamins: Sources, functions, deficiency of the following minerals (calcium, iron, iodine, fluorine, sodium and potassium (elementary treatment). Vitamins classification, sources, Vitamins – A, D, E and K, C, B Complex, - B6 & B12.

#### **Unit III Food Additives**

Artificial sweeteners – saccharin, cyclomate, asparatame – food flavours – esters, aldehydes and heterocyclic compounds. Antioxidants. Food colours - changes in cooking..Restricted use. Spurious colours. Emulsifying agents, preservatives - leavening agents. Baking powder -Yeast. Taste enhancers - MSG-vinegar

#### Unit IV **Pesticides Control**

Spoilage of foods by insects and pests, loss in food quantity and quality Various pesticides used in agriculture and post-harvest storage, uses of pesticides for food grain application.

#### Unit V **Food Adulteration**

Common adulterants in different foods - milk and milk products, vegetable oils, and fats, spices and condiments, cereals, pulses, sweetening agents and beverages. Contamination with toxic chemicals - pesticides and insecticides. .

## TOTAL: 30h

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#### **Course Outcomes:**

- To learn about the source, functions of food
- To learn about the Purification processes of water
- To understand the classification, principles involved in the analysis of carbohydrates and estimation of carbohydrates.
- To learn about the amino acids peptides Analysis of proteins and separation of amino acids by paper chromatography
- To understand the Sources, functions, deficiency of the minerals and vitamins

# **TEXT BOOKS**

- 1. Owen R Fennema, "Food Chemistry", Marcel Decker Inc., New York. 1996.
- 2. M. Swaminathan "Text Book on Food chemistry", Printing and Publishing CO., Ltd. 1993.

- 1. B. Siva Sankar, "Food Processing and Preservatio", Prentice Hall of India Pvt. Ltd., New Delhi. 2002.
- 2. S. Ramakrishnan, K. G. Prasannam, R. Rajan, "Principles Text book of medical biochemistry", Orient Longman Ltd. Third Edition, 2001.