

॥ सा विद्या या विमुक्तये ॥



स्वामी रामानंद तीर्थ मराठवाडा विद्यापीठ, नांदेड

“ज्ञानतीर्थ” परिसर, विष्णुपुरी, नांदेड - ४३१६०६ (महाराष्ट्र)

SWAMI RAMANAND TEERTH MARATHWADA UNIVERSITY NANDED

“Dnyanteerth”, Vishnupuri, Nanded - 431606 Maharashtra State (INDIA)

Established on 17th September 1994 – Recognized by the UGC U/s 2(f) and 12(B), NAAC Re-accredited with 'A' Grade

ACADEMIC (1-BOARD OF STUDIES) SECTION

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संलग्नित महाविद्यालयांतील विज्ञान व तंत्रज्ञान विद्याशाखेतील पदव्युत्तर स्तरावरील द्वितीय वर्षाचे CBCS Pattern नुसारचे अभ्यासक्रम शैक्षणिक वर्ष २०२०-२१ पासून लागू करण्याबाबत.

प रि प त्र क

या परिपत्रकान्वये सर्व संबंधितांना कळविण्यात येते की, दिनांक २० जून २०२० रोजी संपन्न झालेल्या ४७व्या मा. विद्या परिषद बैठकीतील विषय क्र.११/४७-२०२०च्या ठरावानुसार प्रस्तुत विद्यापीठाच्या संलग्नित महाविद्यालयांतील विज्ञान व तंत्रज्ञान विद्याशाखेतील पदव्युत्तर स्तरावरील द्वितीय वर्षाचे खालील विषयांचे C.B.C.S. (Choice Based Credit System) Pattern नुसारचे अभ्यासक्रम शैक्षणिक वर्ष २०२०-२१ पासून लागू करण्यात येत आहेत.

1. M.Sc.-II Year-Botany
2. M.Sc.-II Year-Herbal Medicine
3. M.Sc.-II Year-Analytical Chemistry
4. M.Sc.-II Year-Biochemistry
5. M.Sc.-II Year-Organic Chemistry
6. M.Sc.-II Year-Physical Chemistry
7. M.Sc.-II Year-Computer Management
8. M.Sc.-II Year-Computer Science
9. M.Sc.-II Year-Information Technology
10. M.C.A. (Master of Computer Applications)-II Year
11. M.Sc.-II Year-Software Engineering
12. M.Sc.-II Year-System Administration & Networking
13. M.Sc.-II Year-Dairy Science
14. M.Sc.-II Year-Environmental Science
15. M.Sc.-II Year-Applied Mathematics
16. M.Sc.-II Year-Mathematics
17. M.Sc.-II Year-Microbiology
18. M.Sc.-II Year-Physics
19. M.Sc.-II Year-Zoology
20. M.Sc.-II Year-Biotechnology
21. M.Sc.-II Year-Bioinformatics

सदरील परिपत्रक व अभ्यासक्रम प्रस्तुत विद्यापीठाच्या www.srtmun.ac.in या संकेतस्थळावर उपलब्ध आहेत. तरी सदरील बाब ही सर्व संबंधितांच्या निदर्शनास आणून द्यावी.

‘ज्ञानतीर्थ’ परिसर,

विष्णुपुरी, नांदेड - ४३१ ६०६.

जा.क्र.: शैक्षणिक-१/परिपत्रक/पदव्युत्तर-सीबीसीएस अभ्यासक्रम/
२०२०-२१/३३५

दिनांक : १६.०७.२०२०.

प्रत माहिती व पुढील कार्यवाहीस्तव :

- १) मा. कुलसचिव यांचे कार्यालय, प्रस्तुत विद्यापीठ.
- २) मा. संचालक, परीक्षा व मूल्यमापन मंडळ यांचे कार्यालय, प्रस्तुत विद्यापीठ.
- ३) प्राचार्य, सर्व संबंधित संलग्नित महाविद्यालये, प्रस्तुत विद्यापीठ.
- ४) साहाय्यक कुलसचिव, पदव्युत्तर विभाग, प्रस्तुत विद्यापीठ.
- ५) उपकुलसचिव, पात्रता विभाग, प्रस्तुत विद्यापीठ.
- ६) सिस्टम एक्सपर्ट, शैक्षणिक विभाग, प्रस्तुत विद्यापीठ.

स्वाक्षरित / -

उपकुलसचिव

शैक्षणिक (१-अभ्यासमंडळ) विभाग

**Swami Ramanand Teerth Marathwada University,
Nanded-431 606**



**CHOICE BASED CREDIT SYSTEM (CBCS)
SEMESTER PATTERN
Post Graduate (PG) Programme in Chemistry
(Affiliated Colleges)**

**SYLLABUS FOR
M. Sc. PART – II
ORGANIC CHEMISTRY
w. e. f. Academic year 2020-21**

Program Specific Outcomes

1. Global level research opportunities to pursue Ph. D. program targeted approach of CSIR–NET examination.
2. Enormous job opportunities at all level of chemical, pharmaceutical, food products, life oriented material industries.
3. Specific placements in R & D and synthetic division of polymer industries as well as in allied division.
4. To impart the chemistry knowledge of global standard.
5. Discipline specific competitive examinations conducted by different organization.

Choice Based Credit System (CBCS)
Draft Syllabus Prescribed for
M. Sc. Second Year, ORGANIC CHEMISTRY
Semester-III & IV

Semester	Paper	Course No.	Course	Periods / week	Total Periods	Credit
Theory III	XV	OCH-511	Advanced Spectroscopic Methods	04	60	04
	XVI	OCH-512	Natural Product	04	60	04
	XVII	OCH-513	Organic Synthesis	04	60	04
	XVIII	OCH-514	Elective Paper (Any One)			
			A] Medicinal Chemistry	04	60	04
			B] Green Chemistry	04	60	04
			C] MOOCS NPTEL Course	04	60	04
	XIX		Seminar		15	01
					Total	17
Theory IV	XX	OCH-521	Advanced Heterocyclic Chemistry	04	60	04
	XXI	OCH-522	Advanced Organic Chemistry	04	60	04
	XXII	OCH-523	Organic Synthesis: Retro synthetic Approach	04	60	04
	XXIII	OCH-524	Elective Paper (Any One)			
			A] Medicinal Chemistry	04	60	04
			B] Environmental Chemistry	04	60	04
			C] MOOCS NPTEL Course	04	60	04
	XXIV		Seminar		15	01
					Total	17
Practical III & IV	XXV	OCH-525	Mixture Analysis (Laboratory Course-V)	06	120	04
	XXVI	OCH-526	Synthesis of Organic Molecules (Laboratory Course-VI)	06	120	04
	XXVII	CH-527	Physico-organic estimation (Laboratory Course-VII)	06	120	04
	XXVIII	CH-528	Project (Laboratory Course-VIII)	06	120	04
					Total	16
					Grant Total	50 Credits

Instructions

- I] Each Laboratory Course of 6 Hrs duration should be completed in 6 Hrs per day.
- II] Assessment shall consist of continuous assessment (CA) and end of Semester examination (ESE).
- III] 75% for ESE and 25% for CA.
- IV] Paper-(Elective): Transfer of credit as per student choice.

Draft Syllabus Prescribed for
M. Sc. Second Year, ORGANIC CHEMISTRY
Semester-III & IV

Semester	Paper	Course No	External (ESE)	Internal (CA)	Total Credits (Marks)
Theory III	XV	OCH-511	75 Marks	2 Tests: 15 marks + Assignment: 10 Marks = 25 marks	04 (100)
	XVI	OCH-512	75 Marks	2 Tests: 15 marks + Assignment: 10 Marks = 25 marks	04 (100)
	XVII	OCH-513	75 Marks	2 Tests: 15 marks + Assignment: 10 Marks = 25 marks	04 (100)
	XVIII	OCH-514	75 Marks	2 Tests: 15 marks + Assignment: 10 Marks = 25 marks	04 (100)
	XIX		25 Marks		01
Theory IV	XX	OCH-521	75 Marks	2 Tests: 15 marks + Assignment: 10 Marks = 25 marks	04 (100)
	XXI	OCH-522	75 Marks	2 Tests: 15 marks + Assignment: 10 Marks = 25 marks	04 (100)
	XXII	OCH-523	75 Marks	2 Tests: 15 marks + Assignment: 10 Marks = 25 marks	04 (100)
	XXIII	OCH-524	75 Marks	2 Tests: 15 marks + Assignment: 10 Marks = 25 marks	04 (100)
	XXIV		25 Marks		01
Practical III & IV	XXV	OCH-525	75 Marks	2 Tests: 25 marks	04 (100)
	XXVI	OCH-526	75 Marks	2 Tests: 25 marks	04 (100)
	XXVII	OCH-527	75 Marks	2 Tests: 25 marks	04 (100)
	XXVIII	OCH-528	75 Marks	2 Tests: 25 marks	04 (100)
Total Credits Semester III & IV + Lab Course = 17 + 17 + 16 = 50					

M. Sc. Second Year, Semester-III
Paper–XV, [OCH-511]
Advanced Spectroscopic Methods

Credits: 04

Periods: 60

Objectives:

- ❖ Students are acquainted with various spectroscopic techniques to elucidate the known and unknown organic molecules.
- ❖ Students are familiar with the ultra-violet and visible spectroscopy by determining the absorption maximum of various dienes, enones and aromatic organic compounds.
- ❖ Student develops the detail knowledge to get the different peaks of functional groups in organic molecules by infra-red spectroscopy.
- ❖ Students understand the importance and applications of proton magnetic resonance spectroscopy for determination of structure of unknown organic compounds.
- ❖ Students are recognizable with CMR to authenticate the position of carbon atom in organic molecules.
- ❖ Students identified the structure of compounds by fragmentation of various classes of organic molecules.

SM-1: UV-Vis Spectroscopy:

09P

Fieser-Woodward rules for conjugated dienes and carbonyl compounds, Fieser-Kuhn rules for polyenes. UV spectra of aromatic compounds and heteroaromatic compounds. Calculation of λ_{\max} for the benzene derivatives (R-C₆H₄-Co-G) by A. I. Scott empirical rules.

SM-2: IR spectroscopy:

09P

Recapitulation, Characteristic vibration frequencies of Alkanes, Alkenes, Alkynes, Aromatic compounds, Alcohols, Ethers, Phenols and Amines. Detailed study of vibrational frequencies of carbonyl compounds Ketones, Aldehydes, Esters, Amides, Acids, Anhydride, Lactose, Lactams and Conjugated Carbonyl compounds. Factors affecting group frequencies: overtones, combination bands and Fermi-resonance. FITR and sampling techniques.

SM-3: ¹H NMR Spectroscopy:

12P

General introduction and definitions, Chemical shift, Spin-spin interaction, Shielding mechanism of measurement of chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehyde and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides and mercapto). Factors affecting chemical shift. Deuterium exchange. Spin-spin coupling, factors affecting coupling constant. Complex spin-spin interaction between two and three nuclei. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique. Nuclear Over-Hauser effect (NOE). Resonance of other nuclei; ¹⁹F and ³¹P.

SM-4: ¹³C NMR:

06P

Resolution and multiplicity of ¹³C NMR, ¹H-decoupling, noise decoupling, broad band decoupling; Deuterium, fluorine and phosphorus coupling; NOE signal enhancement, off-resonance, proton decoupling, Structural applications of CMR.

SM-5: Mass Spectroscopy:**09P**

Theory, instrumentation and modifications; Unit mass and molecular ions; Important terms- singly and doubly charged ions, metastable peak, base peak, isotopic mass peaks, relative intensity, FTMS, etc.; Recognition of M^+ ion peak; General fragmentation rules: Fragmentation of various classes of organic molecules, including compounds containing oxygen, sulfur, nitrogen and halogens; α , β -, allylic and benzylic cleavage; McLafferty rearrangement.

SM-6: Structural Problems:**15P**

- a) Combined problems on UV, IR, NMR and Mass spectral data for structure determination.
- b) Elucidation of structure of organic molecules using spectra (IR, PMR & CMR).

Outcomes:

- Learn the structure determination of organic molecules by spectroscopic methods.
- Know the use of electronic spectroscopy to determine absorption maximum in dienes, enones and aromatic compounds.
- Know the applications of IR spectroscopy for functional group determination.
- Learn the structure elucidation of organic compounds by PMR spectroscopy.
- Gather basic knowledge to know the position of carbon in carbon compounds.
- Recognize the molecular mass of the organic molecule by fragmentation pattern.
- Know the complete structure of compounds using UV, IR, PMR, CMR and Mass spectroscopic methods.

Reference Books:

01. Spectroscopic Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill.
02. Introduction to NMR spectroscopy, R. J. Abraham, J. Fisher and P. Loftus.
03. Application of spectroscopy of organic compounds, J. R. Dyer.
04. Spectroscopy of organic compounds, P. S. Kalsi.
05. Organic Spectroscopy, William Kemp.
06. Organic Chemistry, R. T. Morrison and R. N. Boyd.
07. Practical NMR spectroscopy, M. L. Martin, J. J. Delpench and G. J. Martin.
08. Spectroscopic methods in organic Chemistry, D. H. Williams, I. Fleming.
09. Fundamentals of Molecular spectroscopy, C. N. Banwell.
10. A Handbook of Spectroscopic Data of Chemistry, B. D. Mistry.
11. Elementary Organic Spectroscopy, Y. R. Sharma.

M. Sc. Second Year, Semester-III
Paper–XVI, [OCH-512]
Natural Products

Credits: 04

Periods: 60

Objectives:

- ❖ To study the different natural products, and their Nomenclature, occurrence, deficiency syndromes.
- ❖ To study the Biogenesis of Natural Products.
- ❖ To study the Structure elucidation and synthesis of Vitamins, Terpenoids and Steroids.
- ❖ To study the physiological effects of prostoglandins, pyretheroids.

NP-1: Vitamins:

10P

Classification, Occurrence Chemistry of Vitamins A, Vitamin C and Vitamin E Structure elucidation and synthesis. Deficiency syndromes etc.

NP-2: Terpenoids and Carotenoids:

10P

Classification, nomenclature, Occurrence, isolation, isoprene rule, structure determination, stereochemistry and biogenesis of the following molecules Citral, Camphor, Menthol, Farnesol, Zingiberene, Abietic acid. Biosynthesis of terpenoids

NP-3: Alkaloids:

08P

Structure, stereochemistry and synthesis of quinine and morphine

NP-4: Steroids:

12P

Occurrence, Nomenclature, Basic Skeleton, Diel's hydrocarbon and Stereochemistry. Structure determination and synthesis of Cholesterol, Bile acid, Androsterone, Testosterone, Oestrone, Aldosterone and Progesterone.

NP-5: Plant pigments:

10P

Occurrence, nomenclature and general methods of structure determination of Anthocyanidins. Synthesis of Cyanidin Chloride, Chalcones, Flavones, Quercetin.

NP-6: Prostaglandins, pyrethroids, Rotenones and pheromones.

10P

Occurrence, classification. Biogenesis, physiological effects and synthesis of PGE and PGF_{2z}. Natural and synthetic of pyrethroids, Rotenones and pheromones. Synthesis of Bombykol.

Outcomes:

1. Structure elucidation, degradation, applications, stereochemistry of Vitamins, Terpenoids, Steroids.
2. Synthetic methods for total synthesis of natural products
3. Medicinal Application of different natural products
4. Rotenones, pyretheroids, prostoglandins and their applications

Books Suggested:

1. Natural products : Chemistry and Biological significance, J. Mann, R. S. Davidson, J. B. Hobbs, D. V., Banthropde& J. B. Harborne.
2. Organic Chemistry, vol-2, I. L. Finar,ELBS.
3. Stereoselective synthesis: a practical Approach, M. Nogrudi.
4. Rodd's Chemistry of carbon compounds, Ed. S. Coffey.
5. Chemistry, Biological and Pharmacological properties of Medicinal plants from the Americans, Ed. Kurt. Hostettmann, M. P. Gupta and A. Marston.
6. Introduction to Flavonoids, B. A. Bohm.
7. Neco trends in natural products Chemistry, Ata-ur-Rahaman and M. I. Choudhary.
8. Natural Products : Chemistry and Biological Significance, J. Mann, R.S. Davidson, J. B. Hobbs, D. V. Banthrope and J. B Harborne, Longman, Essex.

M. Sc. Second Year, Semester-III
Paper–XVII, [OCH-513]
Organic Synthesis

Credits: 04

Periods: 60

Objectives:

- ❖ To learn the mechanism of condensation, oxidation and reduction.
- ❖ Synthetic application of reagent

OS-1: Oxidation:

12P

- a) Oxidation of alcohol to aldehyde, ketone or acid: Jones reagent, Swern oxidation, Collins reagent, Fetizon's reagent, PCC, PDC, PFC, IBX, Activated MnO₂, Chromyl chloride (Etard reaction), TEMPO, CAN, NMO, Moffatt oxidation, Baeyer-Villiger, Woodward and Prevost dihydroxylation,
b) Oxidative cleavage of Carbon-Carbon double bonds: KMnO₄, Ozonolysis.
c) Oxidations using SeO₂, PhSeBr.
d) Selective cleavages at functional groups: Cleavage of glycols, IO⁻, Pb(OAc).

OS-2: Reductions:

12P

- a) Catalytic Hydrogenation; (b) Reduction of nitriles, oximes and nitro compounds; (c) Reduction of acids and Esters; (d) Reduction with metal hydride- Sodium cyanoborohydride, Diborane, L- & K- Selectrides, LiBH₄, DIBAL-H; (e) Birch reduction and related reactions, (h) Luche reagent, Wolf-Kishner reduction, Clemmensen reduction, Wilkinson catalyst, TBTH.

OS-3: Organic Reagents:

12P

DCC, EDC, DDQ, 1,3 Dithiane, LDA, DMDO, OsO₄, RuO₄, SmI₂, Dess-Martin Periodinane, Diazomethane, Lawesson's reagent.

OS-4:

12P

(A) Ylides and Enamines

- (i) Ylides: Preparation and their synthetic applications along with their stereochemical aspects of Phosphorous, Sulphur and Nitrogen ylides.
(ii) Enamines: Generation & application in organic synthesis with mechanistic pathways, stork enamine reaction.

(B) Rearrangements

Pummerer, Payne, Eschenmoser fragmentation, Brook, Wagner-Meerwein, Wolf, Semipinacol, Epoxide rearrangement with Lewis acid, Dienone-Phenol rearrangement, Tiffeneau-Demjanov, Favorskii, von Richter, Wittig, Neber, Smiles, Fries, Curtius, Lossen, Schmidt, Stevens, Hofmann, Iodolactonisation.

OS-5: Name Reactions:

12P

Hunsdiecker reaction, Dakin, Gabriel synthesis, Michael, Darzens, Prins, Henry, Reimer-Tiemann, Hoffmann-Löffler-Freytag, Dieckmann cyclization, Chichibabin, Vilsmeier, Ene, Ullmann reaction, Mannich, Strecker amino acid synthesis. Bamford-Stevens, Baylis-Hillmann, Corey-Fuchs Reaction, Julia olefination, Mukaiyama aldol, Mitsunobu, Peterson olefination, Corey-Winter olefination, Shapiro, Ritter, Stille, Heck, Sonogashira, Suzuki, Duff, Chugaev, Petasis, McMurry reaction and Coupling. Ring closing metathesis (Grubbs' metathesis), Aldol- Tishchenko (Evans-Tishchenko reaction), Ugi, Passerini, Biginelli, Hantzsch condensation.

Outcomes:-

- 1) To understand the Dakin reaction, Etard reaction, HVZ reaction, Umpolung synthesis and Stephen reaction .
- 2) To know about the Barton reaction, Jones oxidation, Oppenauer oxidation and Michel addition .
- 3) To familiarize the different types of reduction reaction .
- 4) To learn about the synthesis and applications of the organic reagents like 9-Borabicyclo(3.3.1)nonane (9-BBN) and n-butyl lithium .
- 5) To learn the synthesis and applications of the organic reagents like ceric ammonium nitrate (CAN), DCC, Grignard reagent, LDA, Gilman reagent, NBS and PCC.
- 6) To know about the complex metal hydrides, Hilman's reagent, lithium dimethyl cuprate and dicyclohexyl carbodimide, 1,3-dithiane.
- 7) To know the detail study of Woodward, Woodward hydroxylation, selenium dioxide, crown ethers and Peterson's synthesis, Wilkinson's catalyst and Baker yeast.

Reference Books:

1. Organic Chemistry: Clayden, Greeves, Warren and Wothers
2. Stereochemistry of Organic Compounds (Principle and application): D. Nasipuri
3. Stereochemistry of Organic compounds: Ernest L. Eliel / Samuel H. Wilen
4. Organic Synthesis: W. Carruthers
5. Organic Reagents: Fieser & Fieser
6. Organic Synthesis: M. B. Smith
7. Advanced Organic Chemistry; Part A and B: F. A. Carey & R. J. Sundberg
8. Modern Organic Synthesis: An Introduction: G. S. Zweifel & M. H. Nantz
9. A Guidebook To Mechanism In Organic Chemistry: Peter Sykes
10. Organic Synthesis Concepts, Methods, Starting Materials: J. Fuhrhop, G. Penzlin
11. Organic Chemistry: An Intermediate Text: Robert V. Hoffmann
12. Advanced Organic Chemistry: Jerry March
13. Organic Synthesis: R. O. C. Norman and Coxan
14. Name Reactions: Jie Jack Li

M. Sc. Second Year, Semester-III
Paper–XVIII, [OCH-514]
Medicinal Chemistry

Credits: 04

Periods: 60

Objectives:

- Learn basic principles involved in drug discovery and designing process
- To know the role of medicinal chemist in development of medicinal agents
- Learn insight knowledge to analyze and perform SAR and QSAR
- Learn how to analyze and perform SAR of Antimicrobial drugs, Antibiotics, Coagulants and Anticoagulants

MC-1: Concepts of Medicinal Chemistry, Classification of Drugs: 04P

A) Concepts of Medicinal Chemistry: Important terminologies in Medicinal Chemistry:

Drugs, Pharmacy, Pharmaceutics, Toxicology; Pharmacodynamic agents, Pharmacophore, Pharmacodynamics, metabolites and antimetabolites, Chemotherapy.

Mechanism of chemotherapeutic actions: 1) Biological defences 2) Chemical defences. a) Surface active agent, b) Metabolic antagonism. Assay of Drugs: Chemical assay, Biological assay, Immunological assay

B) Classification of Drugs:

i) Classification of drugs on the basis of therapeutic action.

a) Chemotherapeutic agents, b) Pharmacodynamic agents.

iii) Differentiate medicine and drugs.

MC-2: Drug Design: 24P

A) Drug Discovery.

i) Introduction

ii) Procedure followed in drug design.

a) Drug discovery without a lead, b) Lead discovery, rational approaches to lead discovery

iii) Lead modification: Drug design and development, a) Identification of the active part: The pharmacophore, b) Functional group modification, c) Structure-activity relationship, Qualitative versus quantitative approaches- advantages and disadvantages d) Structure modification to increase potency and the therapeutic index; 1) Homologation, 2) Chain branching, 3) Ring-chain transformation., 4) Bioisosterism,

5) Combinatorial chemistry.

iv) Structural modification to increase oral bioactivity.

1) Electronic effect, 2) The Hammett equation, 3) Lipophilicity effect.

B) Concept of prodrugs and soft drugs

a) Prodrugs: i) Prodrugs designing, types of prodrugs, ii) Prodrug formation of compounds containing various chemical groups, Prodrugs and drug delivery system

b) Soft drugs: i) Soft drug concept ii) Properties of soft drugs.

C) Theories of drug activity

Drug-receptor interactions, receptor theories and drug action,

i) Occupancy theory, ii) Rate theory, iii) Induced theory; LD-50 and ED-50, Therapeutic index

D] QSAR method:

Introduction, Methods used in QSAR studies, Hansch method, Free-Wilson method (Mathematical derivations of equations excluded), Advantages and disadvantages of free approach, Computer based methods of QSAR related to receptor binding, Physico-Chemical properties, Lipophilicity, Electronic parameters, Steric substituent constants, Experimental determination of partition coefficients.

E] Molecular docking:

Rigid docking, flexible docking, manual docking; Advantages and disadvantages of flex-X, flex-S, Autodock and Dock softwares, with successful examples.

F] Structure based drug design.

i) Process of structure based drug design, ii) Deactivation of certain drug, iii) Determination of the structure of the protein, iv) Design of inhibitors.

G] Molecular modelling using computers

i) Introduction

ii) Uses of molecular modelling: a) Manual use, b) Further-computer programming

iii) Artificial Intelligence Methods in molecular modelling

c) X-ray crystallography.

H] Design of Enzyme inhibitors

i) Introduction, ii) Competitive inhibitors, iii) Active-site directed irreversible inhibition of enzymes, iv) Suicide enzyme inactivation. Drug action through enzyme inhibition. Theories of enzyme inhibition and inactivation, Enzyme activation of drugs and prodrugs.

I] Nucleic acids: Nucleic acids (NA) as targets for drug action, NA-interactive agents, Classes of drugs that interact with nucleic acids, Intercalation, NA-alkylation, NA-strand breaking and their importance in drug action.

J] New developments Gene therapy and drug resistance

K] Informatics methods in drug design: Brief introduction to bioinformatics, cheminformatics, their relation to drug design as per the topics discussed above.

MC-3: Pharmacokinetics and Pharmacodynamics**06P****A] Pharmacokinetics:**

a) Drug absorption, b) Distribution, c) Elimination d) Disposition; Chemistry of ADME and toxicity properties of drugs. Uses of pharmacokinetics in drug development process.

B] Pharmacodynamics

a) Introduction, Elementary treatment of enzyme inhibition, b) Membrane active drug, c) Sulphonamides

MC-4: Drug metabolism**04P**

I] Introduction, II] Oxidation, III] Reduction, IV] Hydrolysis, V] Conjugation, Significance of drug metabolism in Medicinal Chemistry

MC-5: Antimicrobial drugs**08P****A] Antitubercular drugs:** Introduction.

Mechanism of action of anti-tuberculosis drugs, Targets for anti-tuberculosis drug development, Mechanism of drug-resistance in tuberculosis

a) First-line agents (Primary tubercular drugs): Structure and activity of streptomycin and dihydro-streptomycin, Synthesis and SAR of 4-amino salicylic acid and isoniazid.

b) Second line agents (Secondary antitubercular agents): Structure and activity of Rifampicin, Cycloserine, Viomycin, Ethionamide, Ethambutol, Thioacetazone.

(Synthesis of Cycloserine and Ethambutol expected)

B) Antileprotic drugs

Chaulmoogra and hydnocarpus oil, Multidrug therapy, SAR of sulphones, Dapsone (DDS), Acedapstone, Solapstone, Diaminodipheylthiourea, Rifampicin. (Synthesis of Acedapstone expected)

MC-6: Antibiotics

08P

1. Introduction, classification of antibiotics, 2. Cell wall synthesis, 3. Mechanism of action of antibiotics, a) Inhibition of cell-wall synthesis, b) Inhibition of bacterial protein synthesis, c) Disorganization of the cytoplasmic membrane, d) Interference in the bacterial nucleic acid synthesis, e) Inhibition of the tetrahydro-folate biosynthesis

I) Cell wall synthesis inhibitors (β -Lactam antibiotics): Synthesis of Penicillin-V, Penicillin-G, amoxicillin, ampicillin from 6-APA, cephalixin, Structure and activity of benzyl penicillin, semi-synthetic penicillin, cephalosporin, Mode of action of penicillin and cephalosporin.

II) Protein synthesis inhibitors: Structure activity of tetracycline and synthesis of chlortetracycline, Synthesis and SAR of chloramphenicol, Mode of action of chloroamphenicol.

MC-7: Coagulants and Anticoagulants

06P

Mechanism of blood clotting, Coagulant, Vitamin-K, Vitamin-K analogues, anticoagulant, Action of anticoagulant, Heparin, Coumarin derivatives, Synthesis of 4-hydroxy coumarin, Dicoumarol, Structure and activity coumarin derivatives.

Home assignment:

Modern approaches in drug discovery of antimycobacterial agents and antibiotics and related research papers

Outcomes:

- Understand key component of drug discovery process and drug designing
- Understanding the role of medicinal chemist in development of medicinal agents
- Have understanding about functional group modification and their utility in SAR and QSAR.
- Analyze the recent research articles related with drug design of antimycobacterial agents and antibiotics.

Recommended study materials:

1. Medicinal chemistry-William O. Foye
2. T. B. of Organic medicinal and pharmaceutical chemistry-Wilson and Gisvold's (Ed. Robert F. Dorge)
3. An introduction to medicinal chemistry- Fourth Edition Graham L. Patrick Oxford Press
4. Principles of medicinal chemistry (Vol. I and II)-S. S. Kadam, K. R. Mahadik and K. G. Bothara (Niraliprakashan)
5. Burger's Medicinal Chemistry, Drug Discovery and Development, 8 Volume Set (Burger's Medicinal Chemistry and Drug Discovery) Donald J. Abraham and David P. Rotella
6. An introduction to drug design-S. S. Pandeya and J. R. Dimmock (New age international)
7. The organic chemistry of drug design and drug action-R. B. Silverman (Academic Press)
8. Strategies for organic drug synthesis and design-D. Lednicer Wiley
9. Pharmacological basis of therapeutics-Goodman and Gilman's (McGraw Hill)

M. Sc. Second Year, Semester-III
Paper–XVIII, [EOCH-514]
Elective: Green Chemistry

Credits: 04

Periods: 60

Objectives:

To learn about basic concepts of structure and functionality, membranes, structure, function transport properties, aspects of electrochemical phenomena of biological system, enzyme, co enzyme, nitrogen fixation and photosynthesis

GC-1: Introduction to Green Chemistry

Green chemistry, relevance and goals, Anastas' twelve principles of green chemistry-Tools of green chemistry: alternative starting materials, reagents, catalysts, solvents and processes with suitable examples.

GC-2: Microwave mediated organic synthesis (MAOS):

Microwave activation, advantage of microwave exposure, specific effects of microwave, Neat reactions, solid supports reactions, Functional group transformations, condensations reactions, oxidations, reductions reactions, multi-component reactions.

GC-3: Ionic liquids and PTC

Introduction, synthesis of ionic liquids, physical properties, applications in alkylation, hydroformylations, epoxidations, synthesis of ethers, Friedel-craft reactions, Diels-Alder reactions, Knoevenagel condensations, Wittig reactions, Phase transfer catalyst, Synthesis, applications.

GC-4: Supported catalysts and bio-catalysts for Green chemistry

Introduction, the concept of atom economy, supported metal catalysts, mesoporous silicas, the use of Biocatalysts for green chemistry, modified bio catalysts, fermentations and biotransformations, fine chemicals by microbial fermentations, vitamins and amino acid, Baker's yeast mediated biotransformations, Biocatalyst mediated Baeyer-Villiger reactions.

GC-5: Supramolecular Chemistry and Biomimetic Chemistry

Host-Guest approach, Chiral recognition, Ionophores, Crown ethers, cryptands, Micelles, Cyclodextrins, calixarenes.

Outcomes:-

- 1) To learn about the different enzymes participating in the chemical reactions inside the body and their functions
- 2) To study about the different oxygen carriers present in the body with their structure and stereochemistry
- 3) To study in detail about nitrogen fixation reactions and microorganisms involved in nitrogen fixation reactions
- 4) To know about the biological redox systems and their classifications
- 5) To create awareness about metal toxicities, their detection and permissible levels in

Reference Books

1. Green Chemistry-Environmentally benign reactions. V. K. Ahluwalia. Ane Books India.
2. Green Chemistry-Designing Chemistry for the Environment. Paul T. Anastas & Tracy C. Williamson.
3. Green Chemistry-Frontiers in benign chemical synthesis and processes. Paul T. Anastas & Tracy C. Williamson.
4. Green Chemistry- Environment friendly alternatives. Rashmi Sanghi & M. M. Srivastava

M. Sc. Second Year, Semester-IV
Paper-XX, [OCH-521]
Advanced Heterocyclic Chemistry

Credits: 04

Periods: 60

Objectives:-

The course gives a broad introduction to heterocyclic chemistry. Emphasis is given on the most important heterocyclic systems, such as pyridines, quinolines, isoquinolines, pyrroles, furanes, tiophenes, indoles, pyrimidines, purines, imidazoles, aziridines and oxiranes. For each group, ring synthesis, chemical properties and characteristic reactions will be discussed. Aromaticity applied to heterocyclic compounds, general methods for ring synthesis (by a number of cyclisation and cycloaddition reactions) as well as different systems for nomenclature will be presented.

HC-1: Nomenclature of heterocycles: 10P

Systematic nomenclature system (Hantzsch-Widman system). Trivial nomenclature system. Fusion nomenclature system and Replacement nomenclature system.

HC-2: Nonaromatic heterocycles: 12P

Synthesis, reactivity, and importance of the following ring systems. Azirines, Oxaranes, Thiiranes, Diazirenes, Diaziridines and Azetidines.

HC-3: Five and six-membered heterocycles with two hetero atoms: 12P

Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Pyrimidine and Pyrazine.

HC-4: Heterocycles with more than two hetero atoms: 10P

Synthesis, reactivity, aromatic character and importance of the following heterocycles: Triazoles, Oxadiazoles, Thiadiazoles and Triazines.

HC-5: Larger ring and other heterocycles: 10P

Synthesis and reactivity of Azepines, Oxepines and Thiopines. Synthesis of Benzoazepines, Benzooxepines, Benzothiepinines, Azocines and Azonines.

HC-6: Banzanellated azoles and heterocycles with ring-junction nitrogen: 06P

Banzanellated azoles: Synthesis and chemical properties of Benzimidazoles, Benzoxazoles and Benzothiazoles. Heterocycles with Ring-Junction nitrogen: Synthesis and reactivity of Quinolizines and Indolizines.

Outcomes:-

- 1) This course aims at giving a fundamental theoretical understanding of heterocyclic chemistry, including alternative general methods for ring synthesis and application of such methods for the preparation of specific groups of heterocyclic systems.
- 2) The student will get familiar with particular properties and reactions for the most important heterocycles as well as different systems of nomenclature.

Recommended books:

1. Heterocyclic Chemistry, T. L. Gilchrist.
2. An Introduction to the Chemistry of Heterocyclic compounds, R. M. Acheson.
3. Heterocyclic chemistry, J. A. Joule & K. Mills.
4. Principals of Modern Heterocyclic Chemistry, A. Paquette.
5. Heterocyclic Chemistry, J. A. Joule & Smith.
6. Handbook of Heterocyclic Chemistry, A. R. Katritzky
7. Heterocyclic Chemistry by R. R. Gupta, M. Kumar, V. Gupta
8. Heterocyclic Chemistry-IIIrd Edt. by Raj K Bansal

M. Sc. Second Year, Semester-IV
Paper-XXI, [OCH-522]
Advanced Organic Chemistry

Credits: 04

Periods: 60

Objectives:

1. To study the applications and Mechanism of Enzymes
2. To study the supramolecular chemistry with mechanism
3. To study Free radical reaction
4. To study Asymmetric synthesis

UNIT-I: Enzyme Chemistry

12P

Introduction, Nomenclature, Classification and Extraction of enzymes, Introduction to catalysis and enzymes; Multifunctional catalysis, Intramolecular Catalysis, Mechanism of enzyme action, Factors responsible for enzyme specificity, Enzyme activity and kinetics (Michaelis Menten and Lineweaver-Burk plots), Enzyme Inhibitions (Reversible and irreversible), Structure, Mechanism of action and applications of α -Chymotrypsin, Ribonuclease, lysozyme and Carbopeptidase-A. Enzymes in synthetic organic chemistry [Additions, eliminations, substitutions, condensations, cyclocondensations, oxidations, reductions and rearrangement one example each to be covered] .

UNIT-II: Mechanism of enzyme action and co-enzyme chemistry

12P

Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Example of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

Chemical structures of co-enzymes and cofactors, Oxidoreduction (NAD^+ , NADP^+), Pyridoxal phosphate (PLP), Thiamine pyrophosphate (TPP), Biotin (CO_2 carrier).

UNIT-III: Asymmetric Synthesis

16P

Chiral pool, Chiral auxiliary, Enantio- & Diastereoselective synthesis, Chiral reagent and chiral catalyst including CBS reagent, NADH, Asymmetric hydrogenation including BINAP, Hydroboration- Ipc_2BH , IpcBH_2 , Asymmetric epoxidation- (+) DET & (-) DET, Sharpless, Jacobson, Asymmetric dihydroxylation- $(\text{DHQD})_2\text{PHAL}$ & $(\text{DHQ})_2\text{PHAL}$, Felkin-Anh model, Zimmermann-Traxler transition state model, Proline catalyzed asymmetric reactions.

UNIT-IV: Formation of Carbon-Carbon bonds via organometallic reagents

20P

Synthesis and applications of organo, Magnesium, Titanium, Cerium, Boron, Silicon, Cadmium. Introduction, generation, stability, reactivity, characteristics, structural and stereo chemical properties of free radicals.

Reaction of free radicals: Addition, substitutions, fragmentations, Oxidations and reductions, Detection of free radicals, Homolysis and free radical displacement. Radical chain reactions, Addition and rearrangements, radical cyclization, reactivity of aliphatic and aromatic substrates at bridgehead, Coupling of alkynes and arylation of aromatic compound by diazonium salt, Sandmeyer reaction, Hunsdieker reaction, , McMurry reaction, Acyloin condensation, , Bouveault-Blank reduction.

Outcomes:

1. The basic Principles of Green Chemistry,
2. Applications and uses of Green catalysts and Reagents.
3. Use of Ionic Liquids and PTC in Green Synthesis.

Reference Books:

1. Bioorganic chemistry (A chemical approach to enzyme action): Hermann Dugas.
2. Biotransformation in Organic chemistry: K. Faber
3. Enzyme structure and Mechanism: Alan Fersht.
4. Enzyme catalysis in organic synthesis vol.1: KarlheinzDrauz and Herbert Waldmann.
5. Bioorganic, Bioinorganic and supramolecular chemistry: P. S. Kalsi and J. P. Kalsi.
6. Organic chemistry IVthEdn.: G. Marc Loudon.
7. Stereochemistry of Organic Compounds (Principle and application): D. Nasipuri
8. Stereochemistry of Organic compounds: Ernest L. Eliel / Samuel H. Wilen
9. Advanced Organic Chemistry; Part A and B: F. A. Carey & R. J. Sundberg
10. Organic Chemistry: Clayden, Greeves, Warren and Wothers
11. Organic Synthesis: W. Carruthers
12. Organic Synthesis: M. B. Smith
13. Name Reactions: Jie Jack Li
14. Name Reactions and Reagents in Organic Synthesis: B. P. Mundy, M. G. Ellerd, F. G. Favaloro

M. Sc. Second Year, Semester-IV
Paper-XXII, [OCH-523]
Organic synthesis: Retro synthetic Approach

Credits: 04

Periods: 60

Objectives:

- ❖ Gathering the information of disconnection of functional group in organic transformations.
- ❖ To study the protection and deprotection group approach.
- ❖ To learn the C-C bond disconnections in various organic molecules.
- ❖ To know the ring synthesis for cyclic molecules.
- ❖ To develop synthetic routes based on retrosynthetic analysis for molecules.

OS-1: Disconnection Approach

18P

Introduction to: (i) Grounding of organic chemistry for understanding retrosynthesis; Retrosynthetic analysis and designing of the synthesis; Disconnection approach: An introduction to synthons, synthetic equivalents, disconnection approach, functional group interconversions, importance of order of events in organic synthesis, one and two group C-X disconnections, selective organic transformations: chemoselectivity, regioselectivity, stereoselectivity, enantioselectivity, Reversal of polarity, cyclization reactions, amine synthesis.

OS-2: Protecting Groups:

06P

Protection and deprotection of hydroxyl, carbonyls in aldehydes and ketones, amines, carboxylic acids, alkenes and alkynes.

OS-3: C-C Disconnections

12P

(i) One group C-C Disconnections:

Alcohols (including stereoselectivity), carbonyls (including regioselectivity), Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

(ii) Two group C-C Disconnections:

Diels-Alder reactions, 1,3 difunctionalized compounds and α , β -unsaturated compounds, control in carbonyl condensations, 1,5 difunctionalized compounds, Michael addition and Robinson annelation.

OS-4: Ring Synthesis:

12P

Introduction to ring synthesis, saturated heterocycles, synthesis of 3, 4, 5 and 6 membered rings, rearrangements and photochemistry in synthesis, aromatic heterocycles.

OS-5: Complex molecules:

12P

Synthetic routes based on retrosynthetic analysis for following molecules: Longifoline, Reserpine, Juvabione, Aphidicoline, Taxol.

Outcomes:

- 1) To persuade the subject specific knowledge as well as relevant understanding of the Retrosynthesis
- 2) The academic and professional skills required for Chemistry-based professions.
- 3) Learning experiences gained from this Disconnection approach is important for industrial purpose.

Reference Books:

1. Organic Synthesis: The Disconnection Approach: Stuart Warren
2. Designing Organic Synthesis: Stuart Warren
3. Organic Synthesis: Strategy and Control: Paul Wyatt and Stuart Warren
4. The Logic of Chemical Synthesis: E. J. Corey and Xue-Min Chelg
5. Classics in Total Synthesis I, II and III: K. C. Nicolaou and others

6. Organic Synthesis Concepts, Methods, Starting Materials: J. Fuhrhop, G.Penzlin
7. Some Modern Methods of Organic Synthesis: W.Carruthers
8. Organic Synthesis: M. B.Smith
9. Principles of Organic Synthesis: R. Norman and J. M.Coxan.
10. Advanced Organic Chemistry: JerryMarch
11. Organic Chemistry: Clayden, Greeves, Warren and Wothers

M. Sc. Second Year, Semester-IV
Paper-XXIII, [OCH-524]
Medicinal Chemistry

Credits: 04

Periods: 60

Objectives:

- Learn basic principles involved in Anti-cancer and Anti-AIDS agents, Hypoglycemic agents, Cardiac drugs, antiviral antimalarials.
- To know the role of medicinal chemist in development of medicinal agents for analgesic agents, Anti-inflammatory drugs, Anaesthetics, depressants, Anticonvulsant agents, Drug acting on Gastrointestinal tract infections
- Learn how to analyze and perform SAR of Anti-cancer Agents, Hypoglycemic agents, Cardiac drugs, Antimalarials, Analgesic and Anti-inflammatory drugs, Anaesthetics, Psychoactive Drugs
- Learn how to file the patents

MC-1: Anti-cancer and Anti-AIDS agents

8P

A] Anti-cancer Agents (Anti-neoplastic agents): Introduction, Cancer or tumor, Types of tumor, Terminology: Neoplasma, Sarcoma, Carcinoma, Blastoma, Cancers of blood, Metastases. Mechanism of tumor formation, Treatment of cancer: a) Surgery, b) Photo radiation, c) Radiation therapy, d) Immunology, e) Cancer Chemotherapy. Role of alkylating agents and antimetabolites in the treatment of cancer, i) Alkylating agents, Mustard gas, nitrogen mustards (General methods of preparations), Mechloethamine, melphalan (synthesis) and chlorambucil (synthesis), ii) Antimetabolites, Synthesis and structure activity of 6-mercaptopurine, 5-fluorouracil. Brief discussion regarding use of hormones, natural products, carcinolytic antibiotics and mitotic inhibitors.

B] Anti-AIDS agents:

Introduction, structure and life cycle of the AIDS virus, Mechanism of action of anti-HIV drugs, Targets for anti-HIV drug development, Taxol and Azedothymidine (AZT) derivatives.

MC-2: A: Insulin and Hypoglycemic agents.

10P

Introduction, Types of diabetics, Insulin and its preparation, Storage, secretion, and function of insulin, SAR and mechanism action of Sulphonyl urea and Biguanides, Sweetening agents: Saccharin and p-Phenyl urea (Dulcin), (Synthesis of sodium saccharin expected).

B] Cardiac drugs:

Introduction, Myocardial cell, Molecular basis of myocardial contraction, cardiovascular diseases, pathophysiology heart failure. i) Cardiotonic (Cardiac glycosides): Structure and activity of glycosides, ii) Antianginal drugs. Types of angina pectoris, Mechanism of action of antianginal drugs. Classification of antianginal drugs, a) Nitrates and nitrites, b) Non-nitrate. SAR of Dipyridamol, Khellin, Xanthines and Papavarine, iii) Antiarrhythmic drugs: Synthesis and SAR of guanidine, procainamide, iv) β -Adrenergic blocking agents: Synthesis and SAR of propranolol and isoproterenol, v) Calcium channel blockers: Structure activity of 1,4-dihydropyridines, synthesis of Verapamil and Diltiazem, vi) Antihypertensive drug: Primary and secondary hypertension agents like Rauwolfia alkaloids, Synthesis and structure activity of methyl dopa, Clonidine, Hydralazine

MC-3: Antiviral agents, Antimalarials

08P

Antiviral Agents: : Introduction, Classification of antiviral agents, viral diseases, viral replication and transformation of cells, SAR of amantadine hydrochloride and interferons.

Coronavirus: Introduction, genome structure and life cycle, COVID-19 drug development.

Antimalarials: Introduction, life cycle of plasmodia, chemotherapy of malaria, Mechanism of action of anti-malarial drugs, Targets for anti-malarial drug development, Mechanism of drug-resistance in malaria types of antimalarial drugs. SAR of 8-aminoquinoline derivatives, 4-aminoquinoline derivatives, pyrimidine and biguanide derivatives. Synthesis of pamaquine, primaquine, santoquine, camaquine, and pyrimethamine and choroquine phosphate (expected).

MC-4: A) Analgesic and Anti-inflammatory drugs:

10P

I) Analgesics:

- i) SAR of piperidine, meperidin, methadone, and 6, 7-benzomorphans
- ii) Synthesis of mepiridine, methadone and 6, 7-benzomorphans (expected)

II) Anti-inflammatory drugs:

-Introduction, classification on non-steroidal anti-inflammatory drugs, SAR of methyl salicylate, aspirin, iodomethazone, mefenamic acid, phenyl butazone, oxyphenbutazone, naproxen, rofecoxib, celecoxib, Synthesis of ibuprofen and phenylbutazone.

III) Treatment of Gout:

-Introduction, synthesis and uses of Allopurinol.

B) Antifungal agents.

-Introduction, SAR and synthesis of Fluconazole.

MC-5: Drugs acting on CNS:

10P

A) Anaesthetics:

- i) General anaesthetics: Synthesis of methohexital, structure activity of divinyl ether, nitrous oxide, Pentothal.
- ii) Local anaesthetics: Introduction, development of local anaesthetics, classification (according to chemical structure), a) Procaine and related amino benzoic acid, b) Stovain and its analogues, c) Lidocaine and its analogues, d) Synthesis and SAR of procaine, lidocaine and stovaine

B) Depressants:

-Introduction

- i) Sedative and hypnotics, SAR of aldehydes, ketones and sulphones
- ii) Anticonvulsant: Introduction, Structure and activity of substituent barbiturates. Synthesis of Phenobarbital sodium (expected), Hydantoin: General synthesis and SAR of hydantoin.

C) Antipsychotic agents (Neuroleptic agents): Selective modifier of CNS (Tranquillizers)

Introduction, Classification,

- i) Phenothiazine derivatives: SAR and synthesis of chlorpromazine and related compounds.
- ii) Butyrophenones derivatives: Synthesis of haloperidol, spiroperidol. SAR of butyrophenones derivatives
- iii) Central nervous system stimulants (Antidepressants): Introduction Tricyclic system with central seven membered ring: Dibenzepine and related compounds, SAR of dibenzepine derivatives Synthesis of imipramine, amitriptyline, Chlorpromazine and Diazepam.

MC-6: A) Intellectual property right (IPR):

10P

Manual of patent practices and procedure, Introduction, Patentable subject matter, Application for patents, Patent application under PCT, Publication and examination of application.

B) Agents for organ image OR Diagnostic agents.

Introduction, Classification, Radiopague agents (contrast media), Water soluble and Water insoluble contrast media. Synthesis of Metrizamide, Iopanoic acid and Propylidone. Diagnostic chemicals: i)

Drugs used to test kidney functions, ii) Drugs used to test liver functions, iii) Agents used to test gastric function, iv) Agents used to test cardiac function

C) Drug acting on Gastrointestinal tract (Drug acting on GIT).

Introduction, a) Gastric antacid: i) Treatment of gastric hyperacidity, ii) H₂-receptor antagonists- Synthesis of Ranitidine (Zantac) and Famotidine. b) Ulcerative colitis. c) Antispasmodics agents (Spasmolytic agents), d) Anthelmintic agents: Introduction, anthelmintic agents, synthesis of mebendazole.

Outcomes:

• Understand key components of drug discovery of Anti-cancer and Anti-AIDS agents, Hypoglycemic agents, Cardiac drugs, antiviral antimalarial agents

Recommended study materials:

1. Medicinal chemistry-William O. Foye
2. T. B. of Organic medicinal and pharmaceutical chemistry-Wilson and Gisvold's (Ed. Robert F. Dorge)
3. An introduction to medicinal chemistry-Graham L. Patrick
4. Principles of medicinal chemistry (Vol. I and II)-S. S. Kadam, K. R. Mahadik and K. G. Bothara.
5. Medicinal chemistry (Vol. I and II)-Burger
6. An introduction to drug design-S. S. Pandeya and J. R. Dimmock (New age international)
7. The organic chemistry of drug design and drug action-R. B. Silverman (Academic Press)
8. Strategies for organic drug synthesis and design-D. Lednicer Wiley
9. Pharmacological basis of therapeutics-Goodman and Gilman's (McGraw Hill)
10. Manual of patent practice and procedure-Patent office, India (2005)

M. Sc. Second Year, Semester-IV
Paper–XXIII [EOCH-521]
Elective: Environmental Chemistry

Credits: 04

Periods: 60

Objectives:

Environmental chemistry focuses on the presence and impact of chemicals in soil, surface water, and groundwater. Environmental chemists study how chemicals - usually contaminants - move through the environment. This is referred to as chemical “fate and transport”.

EC-1: Introduction to Environmental Chemistry

12P

Concept and scope of environmental chemistry, Environmental terminology and nomenclatures, Environmental segments, The natural cycles of environment (Hydrological, Oxygen, Nitrogen)

EC-2: Atmosphere, Hydrosphere and Lithosphere

12P

Atmosphere: Regions of the atmosphere, Reactions in atmospheric chemistry, Earth’s radiation balance, Particles, ion and radicals in atmosphere; Chemistry of ozone layer.

Hydrosphere: Complexation in natural water and waste-water, Micro-organisms in aquatic chemical reactions, Eutrophication, Microbiology mediated redox reactions.

Lithosphere: Inorganic and organic components in soil, acid-base and ion-exchange reactions in soil, micro and macro nutrients, nitrogen pathways and NPK in soil.

EC-3: Chemical Toxicology

12P

Toxic chemicals in the environments, Impact of toxic chemicals on enzymes, Biochemical effects of arsenic, cadmium, lead, mercury, carbon monoxide, nitrogen oxides, sulphur oxides.

EC-4: Air Pollution

12P

Particulates, Aerosols, SO_x, NO_x, CO_x and hydrocarbon, Photochemical smog, Air-quality standards

EC-5: Water Pollution

12P

Water-quality parameters and standards: physical and chemical parameters, Dissolved oxygen, BOD, COD, Total organic carbon, Total nitrogen, Total sulfur, Total phosphorus and Chlorine, Chemical speciation (Pb, As, Hg)

Outcomes:

- Familiar with environmental chemistry and its effects on living organisms.

Reference Books:

1. G.W. Vanloon, S.J. Duffer, Environmental Chemistry - A Global Perspective, Oxford University Press (2000).
2. F.W. Fifield and W.P.J. Hairens, Environmental Analytical Chemistry, 2nd Edition (2000), Black Well Science Ltd.
3. Colin Baird, Environmental Chemistry, W.H. Freeman and Company, New York (1995).
4. A.K. De, Environmental Chemistry, 4th Edition (2000), New Age International Private Ltd., New Delhi.
5. Peter O. Warner, Analysis of Air Pollutants, 1st Edition (1996), John Wiley, New York.
6. S.M. Khopkar, Environmental Pollution Analysis, 1st Edition (1993), Wiley Eastern Ltd., New Delhi.
7. S.K. Banerji, Environmental Chemistry, 1st Edition (1993), Prentice-Hall of India, New Delhi.

M. Sc. Second Year, Semester-IV
Paper–XXV [LOCH-525]
Mixture Analysis

Credits: 04

Periods: 120

Objectives:

- ❖ To study the qualitative analysis of ternary mixture in organic chemistry.
- ❖ To understand the analysis of organic compounds by spectral techniques.

Qualitative Analysis (At least 10 Organic Mixtures): Semi-micro Qualitative Analysis of Ternary Mixtures (Solids; Two Solids and One Liquid, One Solid and Two Liquids) containing single/poly functional compounds by Chemical and Physical Method with Chromatographic Separation (TLC) for purity of all three components and its Expected Theoretical Spectral Data (IR, ^1H NMR & ^{13}C NMR).

Outcomes:

- Learn basics practical knowledge of qualitative analysis.
- Become skilled at organic compounds determination.

M. Sc. Second Year, Semester-IV
Paper–XXVI [LOCH-526]
Synthesis of Organic Molecules

Credits: 04

Periods: 120

Objectives:

- ❖ To trained the multistage synthesis of organic molecules.
- ❖ Become skilled for the synthesis of drug molecules in the laboratory.
- ❖ Gain the practical knowledge of organic synthesis by microwave irradiations.

1. Multistage Synthesis (At least three)

- a) Benzophenone → benzopinacol → benzopinacolone
- b) Benzoin → benzil → benzilic acid
- c) Benzaldehyde → chalcone → chalcone epoxide,
- d) Acetanalide → 4-bromoacetanalide → 4-bromoaniline.
- e) Cyclohexanone → cyclohexanoneoxime → caprolactone
- f) Anthranilic acid → o-chlorobenzoic acid → N-phenyl anthranilic acid.

2. Synthesis of Drug Molecules (At least three)

- a) Synthesis of anaesthetic drug Benzocaine.
- b) Synthesis of anticancer drug 6-methyl uracil.
- c) Synthesis of antibacterial drug sulfanilamide.
- d) Synthesis of anti-epileptic drug antypyrine.
- e) Synthesis of anti-convulsant drug Phenytoin.

3. Use of microwaves in organic synthesis (At least one)

- a) The Hantzsch dihydropyridine synthesis from aldehydes, ethyl acetoacetate and urea in microwave irradiation (*Synthetic Letters*, 8, 1296-1298, 2001; *Synthetic Communications*, 31, 425-430, 2001).
- b) Synthesis of coumarin by Knoevenagel synthesis using salicylaldehyde, ethylacetate in presence of base in microwave irradiation (*J. Chem. Res. (S)*, 468-469, 1998).

c) Synthesis of dihydropyrimidones from Biginelli Reaction by acid-catalyzed, three-component reaction between an aldehyde, β -ketoester and urea (*Tetrahedron*, **2005**, 61, 4275-4280).

Outcomes:

- Learn basics practical knowledge of multistage synthesis of organic molecules.
- Learn fundamentals of organic synthesis in drug discovery.
- Learn about the one-pot organic synthesis by microwave techniques.

Note:

1. Synthesis is carried out in molar quantities (Less than 5 gm).
2. Reaction with possible mechanism.
3. Calculate Theoretical and practical % yield.
4. Product conformation by Physical constant and TLC.
5. Give expected spectral data (IR and NMR) of starting material, intermediate and final product.
6. All the prepared organic compounds should be stored as a sample and present at the time of University examination.

M. Sc. Second Year, Semester-IV
Paper–XXVIII [LOCH-527]
Physico-Organic Estimations

Credits: 04

Periods: 120

Objectives:

- ❖ To trained the estimation of different organic molecules in day to day's life chemistry.
- ❖ Gain the practical knowledge to estimate the drug molecules by instrumentation methods.

A) Estimation of Drugs by Titrimetric: (At least three)

a) Assay of Aspirin. b) Assay of Ibuprofen. c) Assay of Analgin. d) Determination of Chloride in Ringer Lactate solution for Injection. e) Determination of Calcium ions in Calcium Gluconate Injection.

B) Isolation of natural products. (At least three)

a) Isolation of caffeine from tea leaves. b) Isolation of piperine from black pepper c) Isolation of β -carotene from carrots d) Isolation of lycopene from tomatoes e) Isolation of limonene from lemon peel f) Isolation of eugenol from cloves

C) Estimation of Drugs by Instrumental Methods: (At least Four)

a) Assay of sulfanilamide by Potentiometry. b) Assay of Riboflavin by Colorimetry. c) Assay of ascorbic acid by Colorimetry. d) Assay of Diazepam by UV-Vis Spectrophotometer. e) Assay of Riboflavin by UV-Vis Spectrophotometer. f) Estimation of carbohydrates, amino acids, proteins by UV-Vis spectrophotometer. g) Determination of Hammett constants and determine its substitution effect. i) Benzoic acid, ii) P-Nitro Benzoic acid, iii) P-Methoxy Benzoic acid, iv) PMethyl benzoic acid, v) P-Chloro benzoic acid. (Out of two compounds one compound must be benzoic acid and another should be substituted benzoic acid is given to the students)

Note:

1. All required solutions must be prepared by the students.
2. In examination one experiment is on Instrumental and one should be on non-instrumental.

Outcomes:

- Gain the knowledge of estimation of drugs by Titrimetric.
- Learn about the Isolation of natural products.
- Develops the techniques for the estimation of drugs by Instrumental Methods.

Books Referred:

1. Modern Experimental organic chemistry by Royston M. Robert, John C. Gilbert, Lyuu B. Rodewald & alan S. Wingrove, Saunder International Edition
2. Advanced practical organic chemistry by N.K.Vishnoi
3. Experimental organic chemistry by L. M. Harwood & C. I. Moody,
4. The systematic identification os organic compounds by R.L.Shriner&D.Y.Curtin
5. Semi-microqualitative organic analysis by N.D.Cheronis, J.B.Entrikin&E.M.Wodnett
6. small scale organic preparation by P.J.Hill
7. Vogel's textbook of practical organic chemistry by ELBS, Longmann.

M. Sc. Second Year, Semester-IV
Paper–XXVIII [LOCH-528]
Project

Credits: 04

Periods: 120

Literature Survey, Studies of Reactions, Synthesis, Mechanism, Isolation of Natural Products, Standardization of Reaction Conditions, New Synthetic Methods etc.

Note:

1. External and Internal Examiners will examine this project jointly at the time of Practical examination.
2. The students will have to give at least one seminar in each semester in their subject of specialization is compulsory.
3. Project work must be carried out only in specialized branch.
4. All synthesized organic compounds should be submitted at the time of University Examination.
5. The project work carried out during the year should be presented in power point presentation in presence of University Examiners.