DEPARTMENT OF CHEMISTRY,
PALAMURU UNIVERSTY, MAHABUBNAGAR, TELANGANA

M. Sc., CHEMISTRY

ORGANIC CHEMISTRY SPECIALIZATION

SYLLABUS for III & IV SEMESTERS

WITH EFFECT FROM THE ACADEMIC YEAR (2023– 24)

REVISED AS PER NEW (CBCS) SYLLABUS

M. Sc. CHEMISTRY (ORGANIC CHEMISTRY)

Syllabus for III and IV Semesters

(With effect from the academic year 2023-2024 under the CBCS pattern)

[Under Restructured CBCS Scheme]

(Approved in the P.G. BOS meeting held on)

Semester - III

	Instruction Hrs. /week	Internal assessment marks	Semester exam marks	Total marks	Credits
CH(OC) 301T(Core)	3+1 (T)	40	60	100	3
CH(OC) 302T(Core)	3+1 (T)	40	60	100	3
CH(OC)303T(Elective)	3+1 (T)	40	60	100	3
CH(OC)304T(Elective)	3+1 (T)	40	60	100	3
SEMINAR	2	--	50	50	2
*CH(OC) 351P (LAB 1)	6	--	50	50	2
*CH(OC) 352P (LAB 2)	6	--	50	50	2
**CH(OC) 353P (LAB 3)	3	--	25	25	1
**CH(OC) 354P (LAB 4)	3	--	25	25	1
Total				**600**	**20**

Theory: 3 hours, *Practical's: 6 hours/ week, **Practical's: 3 hours/ week. T=Tutorial hour.

Semester – IV

	Instruction Hrs. /week	Internal assessment marks	Semester exam marks	Total marks	Credits
CH(OC) 401T(Core)	3+1 (T)	40	60	100	3
CH(OC) 402T(Core)	3+1 (T)	40	60	100	3
CH(OC)403T(Elective)	3+1 (T)	40	60	100	3
CH(OC)403T(Elective)	3+1 (T)	40	60	100	3
SEMINAR	2	--	50	50	2
*CH(OC) 451P (LAB 1)	6	--	50	50	2
*CH(OC) 452P (LAB 2)	6	--	50	50	2
**CH(OC) 453P (LAB 3)	3	--	25	25	1
**CH(OC) 454P (LAB 4)	3	--	25	25	1
Total				**600**	**20**

Theory: 3 hours; *Practical's: 6 hours/ week, **Practical's: 3 hours/ week. T=Tutorial hour.

Lab (Practical's) are conducted in two batches (Batch-I & II) with a minimum of 12-15 students/ Batch

Grand total (all 4 semesters) 2400 marks and 80 credits

Kiranmai (Dr N. Chandra Kiran) HOD

Board of Studies (BoS) Meeting

Dept of Chemistry, Palamuru University

Agenda:

To reorganise the credit frame work and examination pattern for the **II-year** students which is effective from the ACY 2023-24 as per the instructions of TSCHE.

Minutes of the meeting:

From the academic year 2023-24, it is decided to follow the guidelines suggested by TSCHE (Telangana State Council for Higher Education) for that the committee decided to follow same curriculum of dept. of Chemistry, Osmania University is to be followed i.e.

1. The total number of credits for II-year is 40 (20 credits each for Semester-III and Semester-IV).

2. In each paper the evaluation weightages will be as follows

   - Internal examination - 40 marks
   - External examination - 60 marks

The internal examination in each paper consists of 04 internal examinations which are to be conducted at equal intervals.

Each internal examination is for 50 marks which are mentioned below

1. Class test - 20 marks
2. Assignment - 10 marks
3. Seminar - 10 marks
4. Attendance - 10 marks (65 to 74%- 04 marks; 75-84% - 06 marks; 85-95% - 08 marks and above 95%-10 marks)

After conduction of each examination, each paper is scaled down from 50 marks to 10 marks.

Kiranmai (HOD)

External Theory Examination pattern

Total Marks- 60 M

Section-A (Short answer questions) 3 x 8 = 24 M

1. a) Cahpter-1
   b) Cahpter-1
2. a) Cahpter-2
   b) Cahpter-2
3. a) Cahpter-3
   b) Cahpter-3

Section-B (Essay answer questions) 3 x 12 = 36 M

4. a) Cahpter-1
   b) Cahpter-1
   (OR)
   c) Cahpter-1
   d) Cahpter-1
5. a) Cahpter-2
   b) Cahpter-2
   (OR)
   c) Cahpter-2
   d) Cahpter-2
6. a) Cahpter-3
   b) Cahpter-3
   (OR)
   c) Cahpter-3
   d) Cahpter-3

Kinnera (HoD)

Internal Class test Examination pattern

Total Marks- 20 M

1. **Section-A** (Multiple Choice questions) 10 x 1/2 = 5 M
2. Section-B (Fill in the blanks) 10 x 1/2= 5 M
3. Section-C (Short answer questions) 5 x 2 = 10 M

Kirubagaran (HoD)

PAPER TITLES

M.Sc., ORGANIC CHEMISTRY SPECIALISATION
III - SEMESTER SYLLABUS
(With effect from the academic year 2023-2024 under the CBCS pattern)
[Under Restructured CBCS Scheme]

Paper 1– CH (OC) 301T (Core): Synthetic reagents, ^{13}C & 2D NMR

OC-07: Synthetic Reagents- I
OC-08: Synthetic Reagents- II
OC-09: ^{13}C NMR & 2D NMR spectroscopy

Paper 2– CH (OC) 302T (Core): Modern Organic Synthesis

OC-10: Asymmetric synthesis
OC -11: Synthetic strategies
OC-12: New Synthetic reactions

Paper 3: CH (OC) 303T (Elective IIIA): Bioorganic Chemistry - I & Conformational Analysis and ORD

OC(CB1)-13: Carbohydrates, Nucleic acids & Coenzymes
OC(CB1)-14: Proteins, Enzymes and Lipids
OC(CB1)-15: Conformational analysis – II (Cyclic systems) & ORD

Paper-3 CH (OC) 303T (Elective IIIB): Process Chemistry and Development

OC(CB1)-13: Process Chemistry and Principles
OC(CB1)-14: Process Development /Optimization - I
OC(CB1)-15: Process Development /Optimization – II

Paper 4: CH (OC) 304T (Elective IVA): Green chemistry and New techniques

OC(CB2)-16: Principles of Green chemistry and Green synthesis
OC(CB2)-17: Organic nano materials and Supramolecular chemistry
OC(CB2)-18: New techniques and concepts in organic synthesis

Paper-4 CH (OC) 304T (Elective IVB): Pesticides

OC(CB2)-16: Introduction to pesticides
OC(CB2)-17: Synthetic insecticides
OC(CB2)-18: Natural insecticides & herbicides

Laboratory courses

PAPER-V CH (O) 351P: Synthesis of organic molecules
PAPER VI CH (O) 352P: Separation and identification of organic compounds
PAPER-VII CH (O) 353P: Isolation of natural products & Thin layer Chromatography
PAPER-VIIICH (O) 354P: Separation of three component mixtures by Chemical methods and column Chromatography

Seminar

PAPER TITLES

M.Sc. ORGANIC CHEMISTRY SPECIALISATION
IV SEMESTER SYLLABUS
(With effect from the academic year 2023-2024 under the CBCS pattern)
[Under Restructured CBCS Scheme]

Paper 1– CH (OC) 401T(core): Drug Design and Drug Discovery

OC-19: Principles of Drug design and drug discovery
OC-20: Lead modification and SAR studies
OC-21: QSAR studies and computer aided drug design

Paper 2– CH (OC) 402T (core): Advanced Heterocyclic Chemistry

OC-22: Heterocyclic compounds, Nonaromatic heterocyclics and Five membered heterocyclics with two heteroatoms
OC-23: Six membered heterocyclics with two hetero and Five membered heterocyclics with more than two heteroatoms
OC-24: Six membered heterocyclics with more than two heteroatoms and Larger ring heterocyclics

Paper 3: CH (OC) 403T (Elective IIIA): Drug synthesis and mechanism of action

OC(CB1)-25: Drugs acting on metabolic process, cell wall and specific enzymes
OC(CB1)-26: Drugs acting on genetic material and immune system
OC(CB1)-27: Drugs acting on receptors and ion channels

Paper-3 CH (OC) 403T (Elective IIIB): Bioorganic chemistry – II

OC(CB1)-25: Enzymes and their action
OC(CB1)-26: Enzyme models and Enzymatic Transformations
OC(CB1)-27: Recombinant DNA and Fermentation technology

Paper 4: CH (OC) 404T (Elective IVA): Advanced Natural Products

OC(CB2)-28: Biosynthesis of natural products
OC(CB2)-29: Structure determination of natural products
OC(CB2)-30: Total stereoselective synthesis of natural products

Paper-4 CH (OC) 404T (Elective IVB): Physical- Organic Chemistry

OC(CB2)-28: MO and VB theory of reactivity
OC(CB2)-29: Kinetic, isotopic, structural, solvent, steric and conformational effects
OC(CB2)-30: Nucleophilic, electrophilic and free radical reactivity

Laboratory courses

PAPER-V CH (O) 451P: Spectroscopic identification of organic compounds
PAPER VI CH (O) 452P: Synthesis of drugs
PAPER-VII CH (O) 453P: Assay of Drugs
PAPER-VIII CH (O) 454P: Practice of Chemistry Software Programs

Seminar

M.Sc. ORGANIC CHEMISTRY SPECIALISATION
IV SEMESTER SYLLABUS
(With effect from the academic year 2023-2024 under the CBCS pattern)
[Under Restructured CBCS Scheme]

Paper 1– CH (OC) 301T(core): Synthetic reagents, ^{13}C & 2D NMR

OC-07: Synthetic Reagents- I

OC-08: Synthetic Reagents- II

OC-09: ^{13}C NMR & 2D NMR spectroscopy

(Teaching Hours = 3/week) **(Marks= 60)**

OC-07: Synthetic Reagents- I

15 Hrs.

I) Protecting groups:

a) Protection of alcohols by silyl ether (TBDMS, TBDPS) and ester formation.
b) Protection of 1, 2-diols (acetals, ketals and carbonate formation.)
c) Protection of amines by carbamates (Fmoc, BOC).
d) Protection of carbonyls by thio acetals (Umpolung) groups.
e) Protection of carboxylic acids by ortho ester (OBO) formation.

II) Organometallic Reagents: Preparation and application of the following in organic synthesis:
a) Organo lithium b) Organo copper reagents c) Organo boranes in C-C bond formation
d) Organo silicon reagents: reactions involving β-carbocations and α- carbanions, utility of trimethyl silyl halides, cyanides and triflates

III) Carbonyl methylenation:

a) Phosphorous ylide mediated olefinations:
1) Wittig reaction 2) Horner-Wordsworth-Emmons reaction.

IV) Carbene insertions: Rh based carbene complexes, cyclopropanations.

V) C-H Activation: Introduction, Rh catalysed C-H activation.

OC-08: Synthetic Reagents- II

15 Hrs.

I) Oxidations:

a) Oxidation of active C-H functions: DDQ and SeO_2.
b) Alkenes to diols: Prevost and Woodward oxidation
c) Alcohol to carbonyls; Cr(VI) oxidants (Jones reagent, PCC, PDC) IBX, DMP, CAN, TEMPO, TPAP, and Swern oxidation

II) Reductions:

a) Catalytic hydrogenation: Homogeneous (Wilkinsons's catalytic hydrogenation) and heterogeneous catalytic reduction.
b) Non-metallic reductions: Diimide reduction
c) Dissolving metal reductions: Birch reduction.
d) Nucleophilic metal hydrides: $LiAlH_4$, $NaBH_4$, and their modifications.
e) Electrophilic metal hydrides: BH_3, AlH_3 and DIBAL.
f) Use of tri-n-butyl tin hydride: Radical reductions.

OC-09: ^{13}C NMR & 2D NMR spectroscopy

15 Hrs.

I) **^{13}C NMR Spectroscopy:** Introduction, Types of ^{13}C NMR spectra: undecoupled, proton-decoupled and off- resonance decoupled spectra. ^{13}C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear (^{13}C-^{13}C J) and heteronuclear (^{13}C-^{1}H J and ^{13}C-^{2}H J) coupling. Applications of ^{13}C-NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. ^{13}C-NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.

II) 2D-NMR techniques: Principles of 2D-NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMO COSY (^{1}H-^{1}H COSY), TOCSY (Total Correlation Spectroscopy), Hetero COSY (^{1}H, ^{13}C COSY, HMQC), long range ^{1}H, ^{13}C COSY (HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

Recommended Books:

1. Some modern methods of organic synthesis by W. Carruthers
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
3. Organic Synthesis by O House
4. Organic synthesis by Micheal B Smith
5. Reagents for organic synthesis, by Fieser & Fieser, Vol 1-11 (1984)
6. Organic synthesis by Robert E Ireland
7. Handbooks of reagents for organic synthesis by Reich and Rigby, Vol-I-IV
8. Organic chemistry by Jonathan Clayden, Nick Greeves and Stuart Warren
9. Organic Reactions and their mechanisms by P.S. Kalsi
10. Organic reaction mechanisms by V. K. Ahulwalia and Rakesh Kumar Parashar
    Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
11. Organic Spectroscopy by William Kemp
12. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
13. Modern NMR techniques for chemistry research by Andrew B Derome
14. NMR in chemistry - A multinuclear introduction by William Kemp
15. Spectroscopic identification of organic compounds by P S Kalsi
16. Introduction to organic spectroscopy by Pavia
17. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
18. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
19. Basic one and two-dimensional NMR spectroscopy by Horst Friebolin
    NMR spectroscopy by H. Gunther
20. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri
21. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. wilen
22. Stereochemistry: Conformation & Mechanism by P S Kalsi
23. The third dimension in organic chemistry, by Alan Bassendale
24. Stereo selectivity in organic synthesis by R S Ward.
25. Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg
26. Optical rotatory dispersion by C Djerassi
27. Optical rotatory dispersion and circular dichroism by P Crabbe
28. Mechanism and Structure in Organic chemistry by S Mukherjee

Paper 2– CH (OC) 302T(core): Modern Organic Synthesis

OC-10- Asymmetric synthesis
OC-11- Synthetic strategies
OC-12- New Synthetic reactions

(Teaching Hours = 3/week) **(Marks= 60)**

OC- l0- Asymmetric synthesis **15 Hrs.**

Introduction: Brief revision of classification of stereoselective reactions

Pro-stereoisomerism: Topicity in molecules Homotopic, stereo heterotopic (Enantiotopic and Diastereotopic) groups and faces- symmetry criteria.

Pro-chiral nomenclature: Pro chirality and Pro-R, Pro-S, Re and Si faces.

Conditions for stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods of inducing enantioselectivity.

Analytical methods: % Enantiomeric excess and diastereomeric ratio. Determination of enantiomeric excess: specific rotation, Chiral NMR; Chiral derivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.

Chiral Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1,2-asymmetric induction, Cram's rule and Felkin-Anh model.

Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral enolates, Evan's oxazolidinone, 1,4-Asymmetric induction and Prelog's rule.

Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC_2BH and $IPCBH_2$.

Chiral catalyst controlled asymmetric synthesis: Sharpless epoxidation. Asymmetric hydrogenations using Chiral Wilkinson biphosphine catalyst.

Asymmetric aldol reaction: Diastereoselective aldol reaction (achiral enolate & achiral aldehydes) its explanation by Zimmerman-Traxler model.

OC-11- Synthetic Strategies **15 Hrs.**

Introduction: Terminology, Target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition. Criteria for selection of target. Linear and convergent synthesis. Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations.

Order of events: S-Salbutamol, Propoxycaine.

One group C-C and C-X disconnections: Introduction. One group C-C disconnections in alcohols and carbonyl compounds. One group C-X disconnections in Carbonyl compounds, alcohols, ethers and sulphides.

Two group C-C and C-X disconnections: Introduction. Two group C-X disconnections in 1,1-difunctionalised, 1,2-difunctionalised and 1,3-difunctionalised compounds. Two group C-C disconnections: Diels-Alder reaction, 1,3-difunctionalised compounds, 1,5- difunctionalized compounds, Michael addition and Robinson annulation.

Control in carbonyl condensations: oxanamide and mevalonic acid.

Strategic bond: definition, guidelines for disconnection; disconnection of C-X bonds, disconnect to greatest simplification, using symmetry in disconnection, disconnection corresponding to known reliable reaction, high yielding steps and recognizable starting materials. Retrosynthesis of Retronecine, longifolene.

OC-12- New Synthetic reactions **15 Hrs.**

1. **Metal mediated C-C and C-X coupling reactions:** Suzuki, Heck, Stille, Sonogashira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions.
2. **C=C Formation Reactions:** Shapiro, Bamford-Stevens, McMurrey reactions, Julia-Lythgoe olefination and Peterson's stereoselective olefination.
3. **Multicomponent Reactions:** Ugi, Passerini, Biginelli, Bergman and Mannich reactions.
4. **Ring Formation Reactions:** Pausan-Khand reaction, Nazerov cyclisation.
5. **Click Chemistry:** Click reaction, 1,3-dipolar cycloadditions.
6. **Metathesis:** Grubb's 1st and 2nd generation catalyst, Olefin cross coupling metathesis (OCM), ring closing metathesis (RCM), ring opening metathesis (ROM), applications.

Reference Books:

1. Asymmetric synthesis by Nogradi
2. Asymmetric organic reactions by J D Morrison and H S Moscher
3. Principles in Asymmetric synthesis by Robert E. Gawley & Jeffrey aube
4. Stereo differentiating reactions by Izumi
5. Some modern methods of organic synthesis by W Carruthers
6. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
7. Organic synthesis by Michael B Smith
8. Organic Synthesis-The disconnection approach by S Warren
9. Organic Synthesis by C Willis and M Willis
10. Problems on organic synthesis by Stuart Warren
11. Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren
12. The logic of chemical synthesis by Elias James Corey and Xue-Min Cheng
13. Name reactions by Jie Jacj Li
14. Fundamentals of asymmetric synthesis by G.L.

Paper 3: CH (OC) 303T (Elective IIIA): Bioorganic Chemistry - I & Conformational Analysis-II and ORD

OC(CB1)-13: Carbohydrates, Nucleic acids & Coenzymes
OC(CB1)-14: Proteins, Enzymes and Lipids
OC(CB1)-15: Conformational analysis-II (Cyclic systems) & ORD

(Teaching Hours = 3/week) **(Marks= 60)**

OC(CB1)-13: Carbohydrates, Nucleic acids & Coenzymes — 15 Hrs.

Carbohydrates: Introduction to the importance of Carbohydrates. Types of naturally occurring sugars. Deoxy sugars, amino sugars, branched chain sugars. Determination of configuration and determination of ring size of D-glucose and D-Fructose. Conformational analysis of monosaccharides. Synthesis of amino, halo and thio sugars. Conformational structures of sucrose. Structure and biological functions of starch, cellulose, glycogen and chitin.

Nucleic acids: Retrosynthetic analysis of Nucleic Acids-Nucleotides, Nucleosides, Nucleotide bases and Sugars. Structure and synthesis of nucleosides and nucleotides. Primary, secondary and tertiary structure of DNA.

Coenzymes: Introduction. Co-factors, Co substrates - prosthetic groups. Classification-Vitamin derived coenzymes and metabolite coenzymes. Structure and biological functions of coenzyme A, Thiamine pyrophosphate (TPP), Pyridoxal phosphate (PLP), oxidized and reduced forms of Nicotinamide adenosine dinucleotide their phosphates (NAD, NADH, $NADP^+$, NADPH).

OC(CB1)-14: Proteins and Enzymes and Lipids — 15 Hrs.

Proteins: Introduction. Peptide bond, classification and nomenclature of peptides. Amino acid sequence of polypeptides and proteins: terminal residue analysis and partial hydrolysis. Peptide synthesis by solution phase and solid phase synthesis methods.

Enzymes: Definition. Classification based on mode of action. Mechanism of enzyme catalysis - Lock and Key, Induced- Fit and three-point contact models. Enzyme selectivity – chemo, regio, diastereo and enantio selectivity – illustration with suitable examples. Factors affecting enzyme catalysis.

Lipids: Introduction and classification of lipids. Stereochemical notation in lipids. Chemical synthesis and biosynthesis of phospholipids and glycolipids

OC(CB1)-15: Conformational analysis-II (Cyclic systems) & ORD — 15 Hrs.

Conformational analysis (Cyclic systems)

Study of conformations of cyclohexane, mono, di and tri substituted cyclohexanes, (1,3,5-trimethyl cyclohexanes and Menthols), cyclohexanone (2-alkyl and 3-alkyl ketone effect), 2-halocyclohexanones, cycloheptane. Stereo chemistry of bicyclo [3,3,0] octanes, hydrindanes, decalins and perhydroanthracenes. Conformational structures of piperidine, N-Methylpiperidine, tropane, tropine, pseudotropine, decahydroquinoline and quinolizidine. Factors governing the reactivity of axial and equatorial substituents in cyclohexanes. (oxidation, S_N2 reaction, rearrangements, Ester hydrolysis) Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.

Optical Rotatory Dispersion (ORD) and CD Spectroscopy: Optical rotation, circular birefringence, circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempirical rules-The axial haloketone rule, the octant rule, Helicity rule, Exciton chirality method. Application of the rules to the study of absolute configuration and conformations of organic molecules.

Reference Books:

1. Organic Chemistry Vol. I and Vol. II by I. L. Finar
2. Carbohydrate Chemistry by Barton Volumes
3. Carbohydrate chemistry by G. J. Boons
4. The chemistry of natural Products: vol.V - carbohydrates by S. F. Dyke
5. Organic Chemistry by McMurry
6. Nucleic acids in Chemistry and Biology by G M Blackbum MI Gait
7. Lehninger Principles of Biochemistry by D L Nelson and M M Coxon
8. Outlines of Biochemistry by Conn and Stumpf

9. Enzyme structure and mechanism by Fersht and Freeman 10. Enzymes for green organic synthesis by V. K. Ahluwalia
10. Biotransformations in Organic Chemistry by K Faber.
11. Principles of biochemistry by Horton & others.
12. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.
13. Concepts in Biotechnology by D. Balasubramanian & others
14. Chemistry and physiology of the vitamins by H. R. Rosenberg.
15. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri
16. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. wilen
17. Stereochemistry: Conformation & Mechanism by P S Kalsi
18. The third dimension in organic chemistry, by Alan Bassendale
19. Stereo selectivity in organic synthesis by R S Ward.
20. Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg.
21. Optical rotatory dispersion by C Djerassi
22. Optical rotatory dispersion and circular dichroism by P Crabbe
23. Mechanism and Structure in Organic chemistry by S Mukherjee

Paper-3 CH (OC) 303T (Elective IIIB): Process Chemistry and Development

OC(CB1)-13: Process Chemistry and Principles
OC(CB1)-14: Process Development /Optimization - I
OC(CB1)-15: Process Development /Optimization – II

(Teaching Hours = 3/week) **(Marks= 60)**

OC(CB1)-13: Process Chemistry and Principles **15 Hrs.**

Introduction to pharmaceutical industry, Product life cycle and its different functions in product life cycle Management, Research and development, production /manufacturing, Quality control, Quality Assurance, Intellectual property, Regulatory affairs.

Root selection: SELECT (Safety, Environment, Legal, Economics, Control, Throughput) Safe route, Environment friendly route, Legal (more insights into intellectual property on patent infringement related topic), Economic and commercially viable route, control and scalable route, Feasibility of selected route/s for optimum throughput (Depends on number of routes proposed for development), Structure confirmation of product at each stage by IR, NMR, Mass conclusion of feasibility study.

OC(CB1)-14: Process Development /Optimization – I **15 Hrs.**

Process chemistry: Introduction and importance of process Optimization in product development, Starting material/s: Definition, Reagent/s: Definition, different types of reagents, catalysts, Stoichiometric calculations, Solvent/s: Definition, different types of solvents and their compatibility. **Process Safety Engineering:** Reaction condition/s: Definition, different reaction conditions, exothermic and endothermic conditions, (DSC/TSU, Reaction calorimetry and gas evolution study) endothermic conditions. **Analytical:** Reaction monitoring technique/s or In-process controls: Definition, different types of monitoring techniques: TLC, HPLC and GC, Impurity identification and their structure elucidation: UV, IR, Mass, NMR. Fixing Specifications, Different detectors (UV, RI, ELSD, CAD).

OC(CB1)-15: Process Development /Optimization – II **15 Hrs.**

Reaction parameters: Reaction kinetics (Homogeneous, Heterogeneous reactions, Mixing, Temperature, Time and Critical process parameter identification). **Work up and product isolation:** Definition, different type of work ups: Quenching, extraction and distillation/ concentration and isolation. **Purification**: Definition, different types of purifications: Washing, Precipitation, Crystallization. **Filtration study. Drying**: Different types of drying methods ATD (Air tray dryer) VTD (vacuum tray dryer), RCVD (rotatory cone vacuum dryer), FBD (Fluid bed dryer), Lyophilization, Spray Drying. **What -if and stability study:** Definitions and its requirement in scale up, Finalizing the critical process parameters based on the Optimisation and what if study. Risk mitigations by considering critical Material Attributes and Critical process parameter. **Report writing.**

Reference Books:

1. Practical process Research & Development- neal Anderson(Chapter-2)
2. Process Chemistry in pharmaceutical Industry by kumar Gadasetti, Voll & II.CRC Press

Paper 4: CH (OC) 304T (Elective IVA): Green chemistry and New techniques

OC(CB2)-16: Principles of Green chemistry and Green synthesis
OC(CB2)-17: Organic Nanomaterials and Supramolecular chemistry
OC(CB2)-18: New techniques and concepts in Organic synthesis

(Teaching Hours = 3/week) **(Marks= 60)**

OC(CB2)-16: Principles of Green chemistry and Green synthesis **15 Hrs.**

Introduction of Green Chemistry. Principles of Green Chemistry. Introduction to alternative approaches.

i) Microwave Assisted Organic Synthesis (MAOS): introduction, benefits and limitations

a) Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Claisen rearrangement and Diels- Alder reaction.

b) Microwave assisted Solvent-free reactions: Deacetylation, saponification of esters, alkylation of reactive methylene compounds and synthesis of nitriles from aldehydes.

ii) Ultrasound Assisted Organic Synthesis: introduction, applications of ultrasound Cannizaro reaction, Reformatsky reaction and Strecker synthesis.

iii) Organic Synthesis in Green Solvents: introduction

a) Aqueous Phase Reactions: Diels-Alder Reaction, Heck reaction, Hoffmann elimination, Claisen-Schmidt condensation, hydrolysis and dihydroxylation reactions.

b) Organic Synthesis using Ionic liquids: Introduction, applications-Beckmann rearrangement, Suzuki Cross-Coupling Reaction and Diels- Alder reaction.

iv) Green Catalysts in organic synthesis: introduction

a) Phase Transfer Catalysts in Organic Synthesis: Introduction, Williamson ether synthesis and Wittig reaction

b) Biocatalysts in Organic Synthesis: Biochemical (microbial) oxidations and reductions.

OC(CB2)-17: Organic Nanomaterials and Supramolecular chemistry **15 Hrs.**

Organic Nanomaterials :

Introduction. The 'top-down' approach, the 'bottom-up' approach and Nanomanipulation.

Molecular Devices: Photochemical devices, Liquid crystals.

New Carbon family: Types of Fullerenes, Types of Carbon nanotubes (Zig-Zag, Armchair and Chiral), Graphenes. Types of Fullerenes, CNTs (Zig Zag, Armchair and Chiral), single walled CNTs (SWCNTs) and multi walled MWCNTs) and Graphenes.

Supramolecular Chemistry

Introduction: Supramolecular interactions (ion-ion, ion-dipole, H-bonding, cation-π, anion-π, π-π and Van der Walls interactions), Ionophore and molecular receptors.

Host-Guest Chemistry: Lock and key analogy, Structures and applications of Cryptands, Spherands, Calixerenes, Cyclodextrins, Cyclophanes, Carcerands and hemicarcirands.

Self-assembly: Ladder, polygons, helices, rotaxanes, catanenes, Molecular necklace, dendrimers, self-assembly capsules their synthesis, properties and applications.

OC(CB2)-18: New techniques and concepts in organic synthesis **15Hrs.**

1. Techniques in peptide synthesis: Solid phase peptide synthesis, commonly used resins (Rink resin, Wang resin and Ellman resin, synthesis of cross linked Merrifield resin and drawbacks of solid phase synthesis.

2. Solid phase oligodeoxynucleotide synthesis: Phospho triester, Phosphite triester and phosphoramidite pathway

3. Oligosaccharide synthesis: glycosidation: cylic oxocarbenium ion, glycosyl donors and glycosyl acceptors, Kahne glycosidation, convergent and linear oligosaccharide synthesis.

4. Phase Transfer catalysis: Onium and crown ethers as PTC.

5. Tandem synthesis: Tandem reactions: conjugate addition-aldol reaction, polymerization- cyclisation, electrocyclic-Diels Alder reaction.

6. Baldwin Rules: Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems,favoured and disfavoured cyclisations.
7. Chiron approach in organic synthesis: Nature's chiral pool, carbohydrates, amino acids, hydroxy acids, terpenes as chiral precursors. Synthesis of shikimic acid from D-arabinose, furanomycin from D-glucose, S-(-)-ipsenol from S-leucine.
8. Determination of absolute configuration: Mosher's methods.

Recommended books:

1. P.T. Anastes & J.K. Warmer: Oxford Green Chemistry- Theory and Practical, University Press (1998).
2. A.S. Matlack: Introduction to Green Chemistry, Marcel Deckkar, (2001).
3. M.C. Cann & M.E. Connely: Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
4. M.A. Ryan & M. Tinnesand, Introduction to Green Chemistry, American Chemical Society, Washington (2002).
5. V.K. Ahluwalia & M.R. Kidwai: New Trends in Green Chemistry, Anamalaya Publishers
6. Enantioselective organocatalysis, Peter I Dallco, Willey-VCH
7. Core Concepts in Supramolecular Chemistry and Nanochemistry by Jonathan W. Steed, David R. Turner and Karl J. Wallace; John-Wiley and Sons Publications
8. Supramolecular Chemistry by Jonathan W. Steed and Jerry L. Atwood, John-Wiley and Sons Publications
9. Supramolecular Chemistry-Concepts and Perspectives by J M. Lehn; Wiley-VCH (1995) Publications
10. Supramolecular Chemistry by P. D. Beer, P. A. Gale and D. K. Smith; Oxford University Press (1999)
11. Stereochemistry of organic compounds - Principles & Applications by D Nasipuri
12. Nanochemistry by G.B. Sergeev; Elsevier
13. Nanochemistry: A chemical approach to nano materials , G.A. Ozin & A.C. Arsenault; RSC publishers.
14. Stereo differentiating reactions by Izumi
15. Some modern methods of organic synthesis by W Carruthers
16. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
17. Organic synthesis by Michael B Smith
18. Organic Synthesis-The disconnection approach by S Warren
19. Organic Synthesis by C Willis and M Willis
20. Problems on organic synthesis by Stuart Warren
21. Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren
22. The logic of chemical synthesis by Elias James Corey and Xue-Min Cheng
    Name reactions by Jie Jack Li

paper-4 CH (OC) 304T (Elective IVB): Pesticides

OC(CB2)-16: Introduction to pesticides
OC(CB2)-17: Synthetic insecticides
OC(CB2)-18: Natural insecticides & herbicides

(Teaching Hours = 3/week) **(Marks= 60)**

OC(CB2)-16: Introduction to pesticides **15 Hrs.**

i) Definition, Classification and importance of pesticides

ii) Pest control: Different methods- chemical-insecticides, fungicides, herbicides, rodenticides, fumigants, chitin synthesis inhibitors and insect repellents.

a) Biological-pheremones: Definition and classification, synthesis of Disparlure, Exobrevicomin, Endobrevicomin, frontalin and grandiso pheromones, synthetic sex attractants.

b) Insect juvenile hormones: JH-A, JH-B,Synthesis of juvabione. Structural formula and importance of methopren.

c) Moulting harmones: tructural formulae and mode of action of ecdysones

d) Antibiotics and secondary metabolites of microbial origin as insecticides and fungicides in agricultiure. Structural formula and importance of Blasticidin-S, Kasugamycin, Avermectin-B, Invermectin, piercidins and phytoalexins.

iii) Environmental pollution from pesticides.

iv) Integrated pest management.

v) Pesticide formulations: Dusts, Granules, Wettable powders, Emmulsions and Aerosols.

OC(CB2)-17: Synthetic insecticides **15 Hrs.**

i) Organochlorine insecticides: Synthesis and mode of action of methoxychlor, perthan, Dicofol, Heptachlor, Dieldrin and Endosulfan.

ii) Organophosphorous insecticides: Synthesis and mode action of Phosphoric acid derivatives, phosdrin, Dichlorophos, parathion, Zolone, Aninphomethyl, TEPP and Sachradan.

iii) Carbamate insecticides- Synthesis and mode of action of carbamyl, Furadan, Baygon, Aldicarb and Zectron.

iv) Formulation and residue analysis of organochlorine, organophophorous and carbamate insecticides.

OC (CB2) - 18: Natural insecticides and herbicides **15 Hrs.**

i) Insecticides of plant origin: Synthesis and importance of pyrethrins (I and II) , Rotenone and Nicotine. Main constituents Neem-structural formula of Azadirachtin. Synthesis of polygodial and warbunganol(Antifeedants).

ii) Synthesis of pyrethroids: Synthesis of Allethrin, Bioallethrin, Cypermethrin, Fenvalerate, Decemethrin and pyrithrelone.

iii) Concept of Bioinsecticides: Bacillus thiuringiensis.

iv) Concept of pro-insecticides: Structure and mode of action of pro-pheremones and pre-pro-insecticides.

V) Herbicides: Synthesis, applications and mode of action of the following

a) Aryloxyalkyl carboxylic acid derivative: 2,4-D, MCPA, 2,4,5-T and 2,4,5-TP.

b) Carbamatespropham and chloropham, c) Urea derivatives: Monouron and diuron, d) Aliphatic acids: Dalapon, TCA, e) Aromatic acids: 2,3,6-TBA, Dicomba and Amiben, f) Nitrogen heterocyclic dericvatives: Simazine, Atrazine, Amitrole, Maleic hydrazide Diquat and paraquat, g) Phenols PCP and Dinoseb, h) Benzonitrile compounds.

Reference books:

1) Naturally occurring insecticides: M.Jacobson and D.G.Crosby.
2) Insecticides for future:Jacobson

3) Insect juvenile harmone chemistry and action: J.J Mann and M.Beroza
4) Polygodial and warburganal.Terpenoid antifeedants part-II rec,Tran,chin 106
5) Insect antifeedants :S.V.ley &P.L Toogood,chemistry in Britain ,Jan 1990 P.31
6) Synthesis of Insecticides: Metcalf
7) Fungicides-Frear
8) Fungicides-Nene
9) Residue reviews vol.36: Melnikov
10) Safer insecticides: E.Hodgson
11) Crop protection agents from Nature: leonard G Copping
12) Biofertilizers and Bioinsecticides: A.M.Deshmukh
13) Insecticides and Fungicides: U Sriramulu.
14) Organo chlorine insecticides: persistent organic pollutants: F.Moriary
15) Herbicides :P.C.Kearney & D.D.Kaufnan
16) Analytical Method for pesticides: Z.Weig (Vol III)
17) Pesticide formulations: Van Valkenburg
18) Insecticides: A.S.Tahori
19) Herbicides,fungicides,formulation chemistry-A.S.Tahori
20) Environmental pollution by pesticides: C.A.Edwards
21) Pespticides managements and insecticide resistance: Watson and brown.

Laboratory courses

PAPER-V CH (O) 351P: Synthesis of organic molecules **(6 Hrs./Week)**

Synthesis of the following compounds: 2-Phenyl indole (Fischer indole synthesis), 7-hydroxy-3-methyl flavone (Baker - Venkatraman reaction), 2,5-Dihydroxy acetophenone (Fries reaction), 4-Chlorotoluene from p-toluidine (Sandmeyer reaction), Benzilic acid from benzoin (Benzillic acid rearrangement), Benzpinacol (photochemical reaction), 7-hydroxy coumarin (Pechman synthesis), Photo-dimerization of maleic anhydride, benzophenone (Friedel-Crafts reaction), Benzanilide (Beckmann rearrangement), Vanillyl alcohol from vanillin ($NaBH_4$ reduction), 2-and-4-nitrophenols (nitration and separation by steam distillation), Acridone from Phthalic anhydride.

PAPER VI CH (O) 352P: Separation and identification of organic compounds

(6 Hrs./Week)

Separation of two component mixtures by chemical methods and their identification by chemical reactions — separation by using solvent ether, 5 % aqueous sodium bicarbonate, 5% sodium hydroxide and dil hydrochloric acid, checking the purity of the two components by TLC, identification of the compounds by a systematic study of the physical characteristics (mp /bp), extra elements (nitrogen, halogens and sulfur), solubility, functional groups, preparation of crystalline derivatives and identification by referring to literature. A minimum of **09** mixtures should be separated and analyzed by these procedures

PAPER-V CH (O) 353P: Isolation of natural products & Thin layer Chromatography

(3 Hrs./Week)

A) Isolation of the following natural products:

Caffeine from tea leaves (solvent extraction), Piperine from pepper (Soxhlet extraction), Eucalyptus oil from leaves (steam distillation), Lycopene from tomatoes.

B) Identification of components in the extracts by TLC

PAPER-V CH (O) 354P: Separation of three component mixtures by Chemical methods and column Chromatography **(3 Hrs./Week)**

Separation of three component mixtures by chemical methods. A minimum of four mixtures should be separated and analyzed.

Column chromatography: Separation of four mixtures of two components each using silica gel as adsorbent and with suitable polar eluent. The column chromatography should be monitored by TLC.

Recommended Books:

1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Ralph L. Shriner, Christine K. F. Hermann, Terence C. Morrill and David Y. Curtin

PAPER TITLES

M.Sc. ORGANIC CHEMISTRY SPECIALISATION
IV-SEMESTER SYLLABUS
(With effect from the academic year 2023-2024 under the CBCS pattern)
[Under Restructured CBCS Scheme]

Paper 1– CH (OC) 401T(Core): Drug Design and Drug Discovery

OC-19: Principles of Drug design and drug discovery
OC-20: Lead modification and SAR Studies
OC-21: QSAR studies and computer aided drug design

(Teaching Hours = 3/week) **(Marks= 60)**

OC- 19: Principles of Drug design and drug discovery **15 Hrs.**

Introduction to drug discovery. Folklore drugs, stages involved in drug discovery- disease, drug targets, bioassay. Discovery of a lead- screening of natural products and synthetic compound libraries. Existing drugs as leads (me too drugs). Pharmacokinetics (ADME), pharmacodynamics. Nature of drug-receptor interactions and their theories - Occupancy theory, Induced-fit theory, Macromolecular perturbation theory and Two-state model of receptor activation. Natural products as lead structures in drug discovery – Pharmacophore - structure pruning technique e.g. morphine. Discovery of lead structure from natural hormones and neurotransmitters. Principles of design of agonists (e.g. Salbutamol), antagonists (e.g. cimetidine) and enzyme inhibitors (e.g. captopril). Drug discovery without lead – serendipity- Penicillin and Librium as examples. Principles of prodrug design. Introduction to drug patents and Clinical trials.

OC-20: Lead modification and SAR Studies **15 Hrs.**

SAR: Lead modification strategies, Bioisosterism, variation of alkyl substituents, chain homologation and branching, variation of aromatic substituents, extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead. Discovery of oxaminquine, salbutamol, cimitidine and captopril. Structure-Activity Relationship studies in sulfa drugs, benzodiazepines, and taxol analogs.

OC-21: QSAR studies and computer aided drug design **15Hrs.**

QSAR: Introduction, physicochemical properties - pKa, electronic effects and Hammett constant (σ), lipophilicity constant (π), steric effects and Taft's constant, linear and nonlinear relationship between biological activity. Lipophilicity Substituent constants. Lipinski's rule of five. Hansch analysis, Craig's plot, Topliss scheme, Free Wilson approach, cluster significant analysis. Two case studies (QSAR study on pyranenamine and design of Crizotinib). **Computer aided drug design:** Introduction, active site, allosteric binding site, use of grids in docking, rigid docking, flexible docking and induced fit docking of ligands. Basic principles and difference between structure and ligand-based drug design, denovo drug design and utility to optimize the lead structure.

Reference books

1. Burger's medicinal chemistry and drug discovery by Manfred E. Wolf.
2. Introduction to Medicinal chemistry by Patrick.
3. Introduction to drug design by R Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. by William Foye
6. Biochemical approach to medicinal chemistry. by Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis by Roth and Kleeman
8. Drug design by E.J.Arienes

9. Principles of Medicinal Chemistty Vol I & II by Kadam et al
10. Medicinal chemistry an introduction by Garreth Thomas
11. Organic and Pharmaceutical Chemistry by Delgrado
12. Organic Pharmaceutical Chemistry by Harikishan singh
13. Medicinal Chemistry by Ashtoshkar
14. Medicinal Chemistry by Chatwal
15. Organic Drug Synthesis by Ledneicer Vol 1-6
16. Strategies for organic drug synthesis and design by Daniel Ledneicer.
17. Top Drugs: Top synthetic routes by John Saunders
18. Chirotechnoiogy by Roger A. Sheldon
19. Burger's Medicinal Chemistry and Drug Discovery: Principles and Practices. Vol. 1. Medicinal Chemistry by G. Patricks.
20. Text book of Drug Design and Discovery, Edited by Povl Krogsgaard – Larsen Tommy Liljefors.
21. Structure Based Drug Design of Crizotinib (PF-02341066), a Potent and Selective Dual Inhibitor of Mesenchymal–Epithelial Transition Factor (c-MET) Kinase and Anaplastic Lymphoma Kinase (ALK) Martin P. Edwards, J. Med. Chem., 2011, 54 (18), pp 6342– 6363. http://www.pfizer.com/news/featured_stories/featured_stories_martin_edwards.jsp

Paper 2– CH (OC) 402T (Core): Advanced Heterocyclic Chemistry

OC-22- Heterocyclic compounds, Nonaromatic heterocyclics and Five membered heterocyclics with two heteroatoms

OC-23- Six membered heterocyclics with two hetero and Five membered heterocyclics with more than two heteroatoms

OC-24- Six membered heterocyclics with more than two heteroatoms and Larger ring heterocyclics

(Teaching Hours =3/ week) **(Marks= 60)**

OC-22- Heterocyclic compounds, Nonaromatic heterocyclics and Five membered heterocyclics with two Heteroatoms **15 Hrs.**

Heterocyclic compounds: Introduction, Nomenclature Synthesis and reactivity of Indole, Quionoline, Isoquinoline and Acridine.

Nonaromatic heterocyclics: Synthesis, reactivity and importance of the following ring systems. Azirines, Aziridines, Oxiranes, Thiiranes, Diazirenes, Diaziridines, Oxaziridines, Azetidines, Oxetanes and thietanes.

Five and six membered heterocyclics with two hetero atoms: Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole.

OC-23- Six membered heterocyclics with two hetero and Five membered heterocyclics with more than two Heteroatoms **15 Hrs.**

Six membered heterocyclics with two Heteroatoms: Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyridazine, Pyrimidine, Pyrazine, Oxazine, Thiazine.

Five membered heterocyclics with more than two Heteroatoms: Synthesis, reactivity, aromatic character and importance of the following heterocycles: 1,2,3- triazoles,1,2,4-triazoles, Tetrazoles, 1,2,4-oxadiazole, 1 ,3,4-oxadiazole, 1,2,5- oxadiazole, 1,2,3-thiadiazoles, 1,3,4-thiadiazoles, 1,2,5- thiadiazoles.

OC-24- Six membered heterocyclics with more than two heteroatoms and Larger ring Heterocyclics **15 Hrs.**

Six membered heterocyclics with more than two heteroatoms: 1,2,3-triazine, 1,2,4- triazine, 1,3,5- triazine, tetrazines. Synthesis and importance of purines and pteridines. Syntheis of Caffeine, theobromine and theophylline.

Larger ring heterocyclics: Synthesis, structure, stability and reactivity of Azepines, Oxepines and Thiepines. Synthesis of Diazepines rearrangements of 1,2 - diazepines. Synthesis of Benzoazepines, Benzodiazepines, Benzooxepines, Benzothiepines, Azocines and Azonines.

Recommended Books:

1. Heterocyclic Chemistry, T. Gilchrist
2. An introduction to the Chemistry of heterocyclic compounds, R. M. Acheson
3. Heterocyclic Chemistry, J. A. Joule & K. Mills
4. Principles of Modern Heterocyclie Chemistry, A. Paquette
5. Heterocyclic Chemistry, J, A. Joule & Smith
6. Handbook of Heterocyclic Chemistry, A. R. Katritzky
7. The aromaticity III level, units 17-19 British open university volumes
8. Aromatic character and aromaticity by G. M. Badger
9. Non-benzenoid aromatic compounds by D. Ginsberg
10. Nonbenzenoid compounds by Lloy

Paper 3: CH (OC) 403T (Elective IIIA): Drug synthesis and mechanism of action.

OC(CB1)-25: Drugs acting on metabolic process, cell wall and specific enzymes
OC(CB1)-26: Drugs acting on genetic material and immune system
OC(CB1)-27: Drugs acting on receptors and ion channels

(Teaching Hours = 3/week) **(Marks= 60)**

OC(CB1)-25: Drugs acting on metabolic process, cell wall and specific enzymes. **15 Hrs.**

Basic concepts of mechanism of drug action: Introduction to macromolecular targets, carbohydrates, proteins, lipids and nucleic acids as possible drug targets. Classification of drugs. Enzyme inhibition and its types.

a) Drugs acting on metabolic process: Antifolates –Discovery and mechanism of action of sulphonamides, Synthesis of sulfomethoxazole, sulfodoxine, sulfaguanidine and dapsone. Diaminopyrimidines -trimethoprim, bacterial resistance to sulfonamides and drug synergism.

b) Drugs acting on cell wall: Structure of bacterial cell wall, β-Lactam antibiotics – mechanism of action of penicillins and cephalosporins. Synthesis of pencillin-G and Cephalosporin-C, cefalexin and cycloserine. Resistance to pencillins, broad spectrum penicillins – cloxacillin, methicillin, ampicillin, amoxicillin and carbenicillin. β-Lactamase inhibitors - Structural formulae and mode of action of clavulanic acid and sulbactum

c) Drugs acting on specific enzymes: H^+/K^+ -ATPase inhibitors- synthesis of Omeprazole and Carbonic anhydrase inhibitors-synthesis of Acetazolamide.

OC(CB1)-26: Drugs acting on genetic material and immune system. **15 Hrs.**

Drugs acting on genetic material: Introduction, classification and mechanism of action.

a) **DNA-intercalating Agents**-Anticancer and antimalarial agents. Structural formulae of Daunomycin, Adriamycin and Amsacrine. Synthesis of Amscarine, Nitracrine, Quinacrine and Chloroquine.
b) **DNA- Binding and nicking agents:** Antiprotozoal drugs. Synthesis of Metronidazole, Dimetridazole and Tinidazole.
c) **DNA-Alkylators:** Synthesis of Cyclophosphamide and Bisulphan.
d) **DNA-Polymerase inhibitors:** Antiviral agents- Synthesis of Acyclovir and AZT.
e) **DNA-Topoisomerase inhibitors:** Anti-bacterial agents. Synthesis of Ciprofloxacin and Norfloxacin. Structural formulae ofloxacin and Lomefloxacin.
f) **Inhibitors of transcribing enzymes:** Anti-TB and antileprosy agents-structural formulae of Rifamycins and partial synthesis of Rifampicin.
g) **Drugs interfering with translation process:** Antibacterial drugs- Structural formulae of Erythromycin, 5-Oxytetracycline and Streptomycin. Synthesis of Chloromycetin.

Introduction to chiral drugs. Three-point contact model, Eutomer, Distomer and eudesmic ratio. Pfeiffer's rule. Role of chirality on biological activity: Distomers – a) with no side effects b) with undesirable side effects c) both isomers having independent therapeutic value d) combination products having therapeutic advantages e) metabolic chirality inversion.

OC(CB1)-27: Drugs acting on receptors and ion channels. **15 Hrs.**

Introduction to nervous system: structure of neuron, nerve transmission. Definition and examples of agonist, antagonist, neurotransmitters and receptors. Drugs acting on receptors:

a. **Adrenergic receptors:** Introduction and classification. α-Adrenergic-receptor agonists and antagonists- Synthesis and biological activity of Nor-adrenaline, Methyl L-dopa and Tetrazosin. β-Adrenergic-receptor - agonists and antagonists – Synthesis and pharmacological activity of Salbutamol, Tetrabutalin, Propranolol and Atenolol.
b. **Cholinergic-receptors:** Introduction and classification. Cholinergic-receptor agonists and antagonists- Structural formulae of Nicotine, Atropine and Tubocurarine. Synthesis of Acetyl choline and Succinyl choline

c. **Dopamine receptors:** Introduction and classification. Dopamine- receptor agonists and antagonists- Biosynthesis of Dopamine. Synthesis of L-Dopa and Chlorpromazine.
d. **Serotonin receptors:** Introduction and classification. Serotonin receptor agonists and antagonists-synthesis and pharmacological activity of Serotonin and Metoclopramide.
e. **Histamine receptors:** Introduction and classification. Histamine receptor agonists and antagonists-synthesis and biological action of Histamine, Chloropheniramine, and Ranitidine.
f. **Hormones and their receptors:** Introduction to estrogen receptors, Structural formulae of Tamoxifen.
g. **Drugs acting on ion channels:** Introduction to ion channels, drugs acting on Ca^{2+}, Na^{+} and Cl^{-} channels and their mode of action. Structural formulae of Tetracaine and synthesis and of Nifedipine, Diltiazem, Tetracine and 4-Aminopyridine.

Reference Books:

1. Burger's medicinal chemistry and drug discovery. By Manfred B. Wolf.
2. Introduction to Medicinal chemistry. By Graham Patrick.
3. Introduction to drug design. By R. B. Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. By William O. Foye etal.
6. Biochemical approach to medicinal chemistry. By Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis By Roth and Kleeman
8. Drug design By E. J. Arienes
9. Principles of Medicinal Chemistry. Vols.1 & 2 By Kadam etal
10. Medicinal chemistry An introduction By Gareth Thomas
11. Wilson and Gisvold,s text book of Organic, Medicinal and Pharmaceutical chemistry By J.N.Delgado and W.A.Remers.
12. Organic Pharmaceutical chemistry By Harikishan singh.
13. Medicinal Chemistry By Ashutoshkar
14. Medicinal Chemistry By G.Chatwal
15. Organic Drug synthesis By Ledneiser Vol 1-6
16. Strategies for organic drug synthesis and design By Daniel Ledneiser
17. Top Drugs: Top synthetic routes By John Saunders
18. Chirotecchnology By Roger A. Sheldon.

Paper-3 CH (OC) 403T (Elective IIIB): Bioorganic chemistry – II

OC(CB1)-25: Enzymes and their action
OC(CB1)-26: Enzyme models and Enzymatic Transformations
OC(CB1)-27: Recombinant DNA and Fermentation technology

(Teaching Hours = 3/week) **(Marks= 60)**

OC(CB1)-25: Enzymes and their action **15 Hrs.**

Introduction to enzymes. Transition state theory. Acid-Base catalysis. Covalent catalysis— Binding modes of catalysis (i) Proximity effect (ii) Transition state stabilization (iii) Strain and Distortion. Examples of some typical enzyme mechanisms for (1) Triose phosphate isomerase, (i) α-chymotrypsin and serine protease (iii) Lysozyme (iv) Carboxy peptidase-A (v) Ribonuclease.

OC (CB1)-26: Enzyme Models and Enzymatic transformations **15 Hrs.**

Introduction — Biomimetic chemical approach to biological Systems-Enzyme Models Advantage of enzyme models. Requirements necessary for the design of enzyme models. Host-Guest complexation chemistry. Examples of some host Molecules-Crown ether cryptanes, cyclodextrins. Cyclodextrin based enzyme models-Valixarenes, ionophores, micelles and synzymes (synthetic enzymes) — chiral recognition and catalysis. Introduction to industrial enzymes. Enzymatic synthesis of α-amino acids and peptides. Transformations of lipases and esterases. Kinetic resolutions of catboxylic acids, esters and alcohols - Transesterification. Amine resolution-use of oxido-reductase. C-C bond formation using enzymes-asymmetric cyanohydrin formation and asymmetric aldol condensations.

OC (CB1)-27: Recombinant DNA and Fermentation technology **15 Hrs.**

Introduction to genetic engineering. Recombinant DNA technology-restriction endonuclease, cloning, linkers, adaptors. Application of recombinant DNA technology in production of pharmaceuticals, diagnosis of diseases, insect control, improved biological detergents, gene therapy-examples. Principles of finger printing technology- Site directed mutagenesis.

Fermentation technology: Introduction to fermentation. Industrial fermentation. Advantages and limitations of fermentation. Production of drugs and drug intermediates from fermentation- examples. Chiral hydroxy acids, vitamins, amino acids, β-lactam antibiotics. Precursor fermentation and microbial oxidation and reductions.

Recommended Books

1. Concepts in biotechnology by D. Balasubramananian & others
2. Principals of biochemistry by Horton & others.
3. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.
4. Chirotechnology by R.Sheldon.

Paper 4: CH (OC) 404T (Elective IVA): Advanced Natural Products

OC(CB2)-28: Biosynthesis of natural products
OC(CB2)-29: Structure determination of natural products
OC(CB2)-30: Total stereoselective synthesis of natural products

(Teaching Hours = 3/week) **(Marks= 60)**

OC(CB2)-28: Biosynthesis of natural products — 15 Hrs.

Biosynthesis of secondary metabolites: Introduction, Difference between Laboratory synthesis and biosynthesis. Methods for determination of biosynthetic mechanism. Isolation and identification of Biosynthetic precursors, Feeding experiments – use of radioisotopes. Measurement of incorporation – absolute incorporation, specific incorporation. Identification of the position of labels in labeled natural products by chemical degradation and spectral methods. Major biosynthetic pathways: 1) Acetate-Malonate pathway: Biosynthesis of aromatic compounds, 2) Shikimic acid pathway; Biosynthesis of essential amino acids – phenylalanine, tyrosine and tryptophan, carboxylic acid derivatives, flavonoids and morphine alkaloids. 3) Mevalonic acid pathway: Biosynthesis of terpenes – mono, sesqui, di, tri (β-amyrin) and carotenoids, steroids – cholesterol.

OC(CB2)-29: Structure determination of natural products — 15 Hrs.

a) By Chemical Methods: Determination of structure and stereochemistry of morphine, reserpine, abietic acid, cholesterol and rotenone.
b) By Spectral Methods:
   i) IR, UV, ^{1}H NMR, ^{13}C NMR, COSY, HETEROCOSY, NOESY, 2D-INADEQUATE and Mass spectra in the structure elucidations of natural products, Examples: flavones, flavanones, coumarins, quinolines.
   ii) DEPT and NOE of **Geraniol**, INEPT of **menthol.**
   iii) Heteronuclear 2D-J resolved spectrum of **stricticine**, HETEROCOSY of **strictanol**.

OC(CB2)-30: Total stereoselective synthesis of natural products — 15 Hrs.

Takasago synthesis of menthol, Hoffmann-LaRoche synthesis of Biotin, Corey's synthesis of prostaglandins (E2, F2α) and Paeoniflorin, Sharpless synthesis of L-hexoses, Danishefsky synthesis of Indolizomycin, Nicalou's synthesis of Taxol, Meyers synthesis of Dynemicin A.

Recommended books:

1. Textbook of organic chemistry, Vol II by I L Finar
2. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
3. An introduction to the chemistry of terpenoids and steroids, by William templeton
4. Systematic identification of flavonoid compounds by Mabry & Markham
5. Steroids by Fieser arid Fieser
6. Alkaloids by Manske
7. Alkaloids by Bentley
8. The chemistry of terpenes by A Pinder
9. The terpenes by Simenson
10. Terpenoids by Mayo
11. Alkaloids by Pelletier
12. Total synthesis of Natural Products by Apsimon Vol 1-5
13. Biosynthesis by Geismann
14. Principles of organic synthesis 3rd Ed.R O C Norman and J M Coxen
15. One and two dimensional nmr spectroscopy by Atta Ur Rahman
16. Classics in total synthesis K C Nicolaou and E J Sorenson
17. Spectrometric identification of organic compounds by Silverstein and Webster

Paper-4 CH (OC) 404T (Elective IVB): Physical-Organic Chemistry

OC(CB2)-28: MO and VB theory of reactivity
OC(CB2)-29: Kinetic, isotopic, structural, solvent, steric and conformational effects
OC(CB2)-30: Nucleophilic, electrophilic and free radical reactivity

(Teaching Hours = 3/week) **(Marks= 60)**

OC(CB2)-28: MO and VB theory of reactivity **15 Hrs.**

Introduction to Huckel molecular orbital (MO) method as a means to explain modern theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics, semiemperical methods and ab inito and density functional methods. Scope and limitations of several computational programmes. Quantitative MO theory-Huckel molecular orbital (HMO) method as applied to ethane energy levels. Orbital symmetry, orbital interaction diagrams. MO of simple organic systems such as ethane, allyl, butadiene, methane and methyl group. Conjugation and hyperconjugation. Aromaticity. Valence bond (VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Potential energy diagrams. Curve crossing model nature of activation barrier in chemical reactions. Principle of reactivity. Mechanistic significance of entropy, enthalpy and Gibbs free energy. Arrhenius equation, transition state theory. Uses of activation parameters, Hammonds postulate. Bell-Evans-Polanyi principle. Potential energy surface model. Marcus theory of electron transfer. Reactivity and Selectivity principles

OC (CB2) -29: Kinetic, isotopic, structural, solvent, steric and conformational effects **15 Hrs.**

Theory of isotope effects, Primary and secondary kinetic isotope effects. Heavy isotope effects. Tunneling effect Solvent effects. Structural effects on reactivity: Linear free energy relationship (LFER.). The Hammett equation, substituent constants, theories of substituent effects. interpretation of σ-values. Reaction constant ρ. Deviations from Hammett equation. Dual— parameter correlations, inductive substituent constant The Taft model, σ1, σR scales. Solvation and solvent effects: Qualitative understanding of solvent- solute effects on reactivity Thermodynamic measure of solvation. Effects of solvation on reaction and equilibrium. Various empirical indexes of solvation based on physical properties, solvent- sensitive reaction rates, spectroscopic properties and scales for specific solvation. Use of solvation scales in mechanistic studies. Solvent effects from the curve- crossing model. Various type of steric strain and their influence on reactivity. Steric acceleration. Molecular measurements of steric effects upon rates. Steric LFER. Conformational barrier to bond rotation-spectroscopic detection of individual conformers. Acyclic and monocyclic systems. Rotation around partial double bonds. Winstein- Holness and Curtin-Hammet principle.

OC (CB2)-30: Nucleophilic, Electrophilic and Free radical reactivity **15 Hrs.**

Bases, nucleophiles, Electrophiles and Catalysts. Acid-base dissociation. Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases. Nucleophilicity scales, Nucleofugacity. The α-effect- Ambivalent nucleophiles. Acid-base catalysis. Specific and general catalysis. Bronsted catalysis. Nucleophilic and electrophilic catalysis. Catalysis by non-covalent binding micellar catalysts. Nucleophilic and electrophilic Reactivity: Structural and electronic effects on SN1 and SN2 reactivity. Solvent effects, kinetic isotope effects. Intramolecular assistance. Electron transfer nature of SN2 reaction. Nuclcophilicity and SN2 reactivity based on curve-crossing model. Relationship between polar and electron transfer reactions. SRN1 mechanism. Electrophilic reactivity, general mechanism. Kinetics of SE2-Ar reaction, Structural effects on rates and selectivity. Curve crossing approach to electrophilic reactivity.

Radical and pericyclic reactivity. (a) Radical stability, polar influences, solvent and steric effects. A curve crossing approach to radical addition, factors affecting barrier heights in additions, regioselectivity in radical reactions. Reactivity, specificity and periselectivity in pericyclic reactions.

Recommended books:

1. Molecular mechanics. By U.Bukert and N.L.Allinger, ACS Monograph 177,1982
2. Organic Chemistry book of Orbitals. L.Salem and W.L.Jorgenson
3. Mechanism and theory in Organic Chemistry, T.M.Lowry, K.C.Richardson, Harper and Row
4. Introduction to theoretical Organic Chemistry and molecular modeling by W.B.Smith, VCH,Weinhein.
5. Physical Organic chemistry, N.S. Isaaçs
6. Suprarnolecular Chemistry - concepts and perspectives by J M. Lehn.
7. The Physical basis of Organic Chemistry by H.Maskill.
8. Physical Organic Chemistry by Jack Hine

Laboratory courses

PAPER-V CH (O) 451P: Spectroscopic identification of organic compounds
Identification of unknown organic compounds by interpretation of IR, UV, ^{1}H -NMR, ^{13}C NMR and mass spectral data (five examples with 2D-NMR). A minimum of 25 representative examples should be studied.

PAPER VI CH (O) 452P: Synthesis of following drugs
Paracetamol, Phenytoin, Benzocaine, 6-Methyluracil, Chloritone, Fluorescein, antipyrine, 4-Aminobenzene sulfonamide and phenothiazine.

PAPER-VII CH (O) 453P: Assay of Drugs
Chlorpromazine (titrimetry), Atropine (titrimetry), Analgin (titrimetry), Chloride in Ringer's lactate (argentometry), Benzylpencillin (Iodometry), Isoniazid (Iodometry), Riboflavin (colorimetry), Zn ions in Bacitracin Zinc, Ca^{+2} ions in Calcium tablet (complexometry), Diazepam (UV-Visible Spectrophotometer).

PAPER-VIII CH (O) 454P: Practice of Chemistry Software Programs
Chem Draw, analysis of NMR using MestReNova, NMR processor. EXCEL, Orgel: Drawing graphs, Molecular docking.

Recommended books:

1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Shriner et.al
4. Analytical chemistry by G N David Krupadanam et.al
5. Advanced practical medicinal chemistry by Ashutoshkar
6. Pharmaceutical drug analysis by Ashutoshkar
7. Quantitative analysis of drugs in pharmaceutical formulations by P D Sethi
8. Practical pharmaceutical chemistry part-1 and part-2 by A H Beekett and J B Stenlake
9. Spectroscopic identification of organic compounds by R M Silverstein and F X Webster.