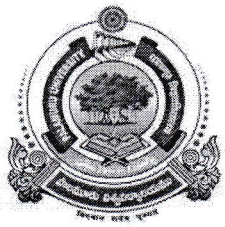

DEPARTMENT OF CHEMISTRY,
PALAMURU UNIVERSTY, MAHABUBNAGAR, TELANGANA

M. Sc., CHEMISTRY

ORGANIC CHEMISTRY SPECIALIZATION

SYLLABUS For III & IV SEMESTERS

WITH EFFECT FROM THE ACADEMIC YEAR (2021– 22)

REVISED AS PER NEW (CBCS) SYLLABUS

DEPARTMENT OF CHEMISTRY,
PALAMURU UNIVERSTY, MAHABUBNAGAR, TELANGANA

Minutes of Meeting

The meeting of board of studies in Chemistry is held on 08-09-22 at 10.30 am in the Department of Chemistry, Palamuru University, Mahabubnagar for the operational syllabi from the academic year 2022-23.

The following members were present:

1.	Prof. K.Girija Managatayaru, Dept.of Chemistry, Palamuru University	Chairperson
2.	Prof. P. Leelavathi, Dept. of Chemistry, Osmania University	Member
3.	Dr. M. Noorjahan, HoD, Dept. of Chemistry, Palamuru University	Member
4.	Dr. N. Chandrakiran, Asst. Prof, Dept. of Chemistry, Palamuru University	Member
5.	Dr. S. Vijaya Laxmi, Asst.Prof, Dept. of Chemistry, Palamuru University	Member
6.	Dr. K. Rajender Reddy, Sr. Principal Scientist, IICT, Hyd	Member
7.	Dr. K. Padmavathi, Principal, NTRGDC for Women, M BNR	Member
8.	Dr. G. Suresh Kumar, Group Leader, Hetero Drugs Ltd, Hyderabad	Member
9.	Dr. A. Hari Padmashri, Asst.Prof, Dept. of Chemistry, Osmania University	Member
10.	Mr. G. Satyanarayana Goud, Asst. Prof, Dr. BRR GDC, Jadcherla	Member

After the discussion the following resolutions were taken.

Resolutions:

1. The Members of the BOS have thoroughly discussed about the existing syllabus and suggested some changes as per the need of current research and Industrial requirements.
2. It is resolved to introduce revised syllabi in accordance with the requirements of CBCS (A copy of the revised syllabus in CBCS pattern is enclosed)
3. Based on the suggestions given by the BOS members, modifications in the syllabus were enclosed in Annexure - II
4. The proposed syllabus for the subject of chemistry is approved unanimously.

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ANNEXURE- II

Following modifications in the III & IV Semester syllabus were approved by BOS members

Semester - III

Paper 1– CH (OC) 301T: Title of this paper has been changed
Asymmetric Synthesis, New techniques and concepts inorganic synthesis and Bio molecules (New chapter)
Conformational Analysis, Asymmetric Synthesis and Bio molecules (old chapter)

OC09: Principles of Asymmetric synthesis

OC09 from old syllabus shifted to semester-II, previous OC-10 is replaced as OC-9

OC10: Methodologies in asymmetric synthesis

Previous OC-11 is replaced as OC10

OC11: New techniques and concepts in organic synthesis

OC -16 is replaced in the place of OC 11

OC12: Biomolecules

No change

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

OC13- Synthetic Reagents I

Protecting groups topic is completely modified as a new chapter and typographical mistake f) Hydrogenolysis g) use of tri-n-butyl tin hydride; Radical reductions is rectified as f) Hydrogenolysis use of tri-n-butyl tin hydride; Radical reductions.

The syllabus of previous synthetic reagents – I requires more no.of classes and protecting groups which itself requires equal no. of classeshas been separated as separate Chapter.

OC 14- Synthetic Reagents II

Below given two topics included

i) **Carbene insertions:** Rh based carbene complexes, cyclopropanations.
ii) **C-H Activation:** Introduction, Rh catalysed C-H activation.

OC 15- Protecting groups

Old syllabus OC 15 is now shifted to OC-16 in place of it protecting groups topic from OC 13 of previous syllabus with following inclusions made in to new chapter as OC- 15

Previous syllabus

Protection of alcohols by ether, silyl ether and ester formation b).Protection of 1,2-diols by acetal, ketal and carbonate formation c) Protection of amines by acetylation, benzoylation, benzyloxycarbonyl, t-butyloxycarbonyl, fmoc and triphenyl methyl groups. d) Protection of carbonyls by acetal, ketal and thiol acetal (Umpolung) groups. e) Protection of carboxylic acids by ester and ortho ester (OBO) formation.

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Modifications in the new syllabus

a) Protection and deprotection of alcohols as ether (methyl, MOM, MEM, THP, benzyl, PMB, trityl), silyl ether (TMS, TES, TBDMS, TBDPS) and ester formation (acetate, benzoate, pivolate).

b) Protection and deprotection of 1, 2-diols and 1, 3-diols as acetonides, cycloalkylidene and benzylidene (comparative study) and carbonate formation.

c) Protection and deprotection of amines as carbamates (Fmoc, BOC, Cbz), amides and sulfonamides formation(Ts).

d) Protection and deprotection of carbonyls as acetals (dioxolanes, dioxanes) and thio acetals (Umpolung) formation.

e) Protection and deprotection of carboxylic acids as ester (alkyl,benzyl), ortho ester and oxazoline formation.

OC 16- New Synthetic reactions

As previous OC-16 is shifted to OC-11 of new syllabus in place of which OC-15 of old syllabus is now made into OC-16.

Paper 3: CH (OC) 303T: Title of this paper has been changed

Organic Spectroscopy and synthetic strategies (New chapter)

Organic Spectroscopy and Pericyclic reactions (old chapter)

OC-17: ^{13}C NMR spectroscopy

No change

OC-18: Title of this chapter has been changed

2D NMR techniques (New chapter)

2D NMR techniques and ORD (old chapter)

Optical Rotatory Dispersion (ORD) and CD Spectroscopy topic is removed as it is shifted to semester –II

OC-19: Title of this chapter has been changed

Synthetic strategies – I (New chapter)

Pericyclic reactions I (old chapter)

Previous syllabus OC-22 is now modified as OC -19

OC-20: Title of this chapter has been changed

Synthetic strategies – II (New chapter)

Pericyclic reactions II (old chapter)

Previous syllabus OC-23 is now modified as OC -20

Paper-4 CH (OC) 304T: Title of this paper has been changed

Pericyclic reactions, Photochemistry and Green Chemistry (New chapter)

Photochemistry, Synthetic strategies and Green Chemistry (old chapter)

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Paper-3 CH (OC) 403T: Advanced Heterocyclic Chemistry
No change

OC-33: Title of this chapter has been changed
Nonaromatic (Three and four membered) heterocyclics (New chapter)
Nonaromatic heterocyclics (old chapter)

OC-34: Five and six membered heterocyclics with two hetero atomsOC-35: Heterocyclics with more than two hetero atoms

OC-36: Larger ring and other heterocycles

Paper-4 – CH (OC) 404(CB_1)T: Advanced Natural Products
No change

OC(CB_1)-1: Biosynthesis of natural products
OC(CB_1)-2-: Structure determination and stereochemistry of natural products by chemicalmethods.
OC(CB_1)--3: Structure determination and stereochemistry of natural products by spectralmethods.
OC(CB_1)--4: Total stereo selective synthesis of natural products.

Paper-4 CH (OC) 404T (CB_2): Bioorganic Chemistry
OC (CB_2) -1: Enzymes and their action
OC (CB_2) -2: Enzyme models and enzymatic transformations
OC (CB_2) -3: Recombinant DNA and Fermentation technologyOC
OC (CB_2) -4: Coenzymes

Paper-4 CH (OC) 404 T (CB_3): Physical- Organic Chemistry
OC (CB_3) -1: MO and VB theory of reactivity
OC (CB_3) -2: Kinetic, isotopic, structural, solvent, steric and conformational effects
OC (CB_3) -3: Nucleophilic, electrophilic and free radical reactivity
OC (CB_3) -4: Supra molecular chemistry

Laboratory courses

PAPER-V CH (OC) 451P: Spectroscopic identification of organic compounds and Chromatography.
Separation by column chromatography is modified as Separation by column chromatography (Demonstration).

PAPER-VI CH (OC) 452P: Synthesis and analysis of drugs
Ascorbic acid (titrimetry, Iodometry and Cerimetry, Colorimetry) is modified as ascorbic acid (Iodometry)

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OC-21: Title of this chapter has been changed
Aromaticity and Pericyclic reactions I (New chapter)
Photochemistry (old chapter)
Previous OC 19 is now made as OC -21 with internal shuffling of topics where aromaticity is shifted before pericyclic topic

OC-22 Title of this chapter has been changed
Pericyclic reactions II (New chapter)
Synthetic strategies – I (old chapter)
Previous syllabus OC-20 is now modified as OC -22

OC-23 Title of this chapter has been changed
Photochemistry (New chapter)
Synthetic strategies – II (old chapter)
Previous syllabus OC-21 is now modified as OC -23

OC-24 Green Chemistry
No change

Laboratory courses

PAPER-V CH (O) 351P: Separation and identification of organic compounds

No Change

PAPER VICH (O) 352P: Synthesis of organic molecules & isolation of natural products

Not much Change

SEMESTER IV

Paper-1 CH (OC) 401T: Drug Design and Drug Discovery
No change

OC-25: Principles of Drug design and drug discovery
OC-26: Lead modification and SAR Studies
OC 27: QSAR studies
OC 28: Combinatorial Synthesis

Paper CH (OC) 402T: Drug synthesis and mechanism of action
No change

OC-29: Drugs acting on metabolic process, cell wall and specific enzymes OC-
OC-30: Drugs acting on genetic material and immune system
OC-31: Drugs acting on receptors and ion channels
OC-32: Chiral drugs

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M. Sc. CHEMISTRY (ORGANIC CHEMISTRY)

Syllabus for III and IV Semesters

(With effect from the academic year 2021-2022 under the CBCS pattern)

[Under Restructured CBCS Scheme]

(Approved in the P.G. BOS meeting held on 08-09-2022)

Semester - III

	Instruction Hrs/week	Internal assessment marks	Semester exam marks	Total marks	Credits
CH(OC) 301T	4	20	80	100	4
CH(OC) 302T	4	20	80	100	4
CH(OC) 303T	4	20	80	100	4
CH(OC) 304T	4	20	80	100	4
SEMINAR	2	--	--	50	2
*CH(OC) 351P	9	--	100	100	4
*CH(OC) 352P	9	--	100	100	4
Total				**650**	**26**

*Theory: 3 hours; Practical's: 6 hours

Semester - IV

	Instruction Hrs/week	Internal assessment marks	Semester exam marks	Total marks	Credits
CH(OC) 401T	4	20	80	100	4
CH(OC) 402T	4	20	80	100	4
CH(OC) 403T	4	20	80	100	4
CH(OC)404T (CB)	4	20	80	100	4
SEMINAR	2	--	--	50	2
*CH(OC) 451P	9	--	100	100	4
*CH(OC) 452P	9	--	100	100	4
Total				**650**	**26**

(**Choice based paper (CB)** = Paper offered by the same Department or other Department in the Science faculty)

*Theory: 3 hours; Practical's: 6 hours

Grand total (all 4 semesters) 2400 marks and 96 credits

PAPER TITLES

M.Sc., ORGANIC CHEMISTRY
SPECIALISATION III SEMESTER SYLLABUS
(With effect from the academic year 2021-2022 under the CBCS pattern)
[Under Restructured CBCS Scheme]

Paper 1– CH (OC) 301T: Asymmetric Synthesis, New techniques and concepts in organic synthesis and Biomolecules

OC09: Principles of Asymmetric synthesis
OC10: Methodologies in asymmetric synthesis
OC11: New techniques and concepts in organic synthesis
OC12: Biomolecules

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

OC13- Synthetic Reagents- I
OC 14- Synthetic Reagents- II
OC 15- Protecting groups
OC 16- New Synthetic reactions

Paper 3: CH (OC) 303T: Organic Spectroscopy and synthetic strategies

OC-17: ^{13}C NMR spectroscopy
OC-18: 2D NMR techniques
OC-19: Synthetic strategies - I
OC-20: Synthetic strategies - II

Paper-4 CH (OC) 304T: Pericyclic reactions, Photochemistry and Green Chemistry

OC-21 Aromaticity and Pericyclic reactions- I
OC-22 Pericyclic reactions- II
OC-23 Photochemistry
OC-24 Green Chemistry

Laboratory courses

PAPER-V CH (O) 351P: Separation and identification of organic compounds
PAPER VI CH (O) 352P: Synthesis of organic molecules & isolation of natural products

PAPER TITLES

M.Sc. ORGANIC CHEMISTRY SPECIALISATION

IV SEMESTER SYLLABUS

(With effect from the academic year 2021-2022 under the CBCS pattern)

[Under Restructured CBCS Scheme]

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

OC-25: Principles of Drug design and drug discovery

OC-26: Lead modification and SAR Studies

OC 27: QSAR studies

OC 28: Combinatorial Synthesis

Paper CH (OC) 402T: Drug synthesis and mechanism of action

OC-29: Drugs acting on metabolic process, cell wall and specific enzymes

OC-30: Drugs acting on genetic material and immune system

OC-31: Drugs acting on receptors and ion channels

OC-32: Chiral drugs

Paper-3 CH (OC) 403T: Advanced Heterocyclic Chemistry

OC-33: Non aromatic (Three and four membered) heterocyclics

OC-34: Five and six membered heterocyclics with two hetero atoms

OC-35: Heterocyclics with more than two hetero atoms

OC-36: Larger ring and other heterocyclics

Paper-4 – CH (OC) 404(CB_1)T: Advanced Natural Products

OC(CB_1)-1: Biosynthesis of natural products

OC(CB_1)-2-: Structure determination and stereochemistry of natural products by chemical methods.

OC(CB_1)-3: Structure determination and stereochemistry of natural products by spectral methods.

OC(CB_1)-4: Total stereo selective synthesis of natural products.

Paper-4 CH (OC) 404T (CB_2): Bioorganic Chemistry

OC (CB_2) -1: Enzymes and their action

OC (CB_2) -2: Enzyme models and enzymatic transformations

OC (CB_2) -3: Recombinant DNA and Fermentation technology

OC (CB_2) -4: Coenzymes

Paper-4 CH (OC) T404 (CB_3): Physical- Organic Chemistry

OC (CB_3) -1: MO and VB theory of reactivity

OC (CB_3) -2: Kinetic, isotopic, structural, solvent, steric and conformational effects

OC (CB_3) -3: Nucleophilic, electrophilic and free radical reactivity

OC (CB_3) -4: Supra molecular Chemistry

Laboratory courses

PAPER-V CH (OC) 451P: Spectroscopic identification of organic compounds and Chromatography.

PAPER-VI CH (OC) 452P: Synthesis and analysis of drugs

M.Sc. ORGANIC CHEMISTRY

SPECIALISATIONIII SEMESTER SYLLABUS

(With effect from the academic year 2021-2022 under the CBCS pattern)

[Under Restructured CBCS Scheme]

Paper 1–CH(OC) 301T: Asymmetric Synthesis, New techniques and concepts in organic synthesis and Biomolecules.

OC09: Principles of Asymmetric synthesis

OC10: Methodologies in asymmetric synthesis

OC11: New techniques and concepts in organic synthesis

OC12: Biomolecules

Teaching Hours = 4/week **Marks= 80**

OC 09- Principles of asymmetric synthesis **15 Hrs**

Introduction and terminology: Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry, substitution and addition criteria. Prochirality nomenclature: Pro-R, Pro-S, Re and Si. Stereoselective reactions: Substrate stereoselectivity, product stereoselectivity, enantioselectivity and diastereoselectivity. Conditions for stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control.

Methods for inducing enantio and diastereoselectivity. Analytical methods: % Enantiomeric excess, enantiomeric ratio, optical purity, % diastereomeric excess and diastereomeric ratio. Techniques for determination of enantiomeric excess, specific rotation, Chiral NMR; Chiral derivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.

OC 10- Methodologies in asymmetric synthesis **15 Hrs**

Strategies in Asymmetric Synthesis: 1. Chiral substrate controlled, 2. Chiral auxiliary controlled, 3. Chiral reagent controlled, 4. Chiral catalyst controlled and 5. Asymmetric aldol reaction

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

2. Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral enolates, azaenolates, imines and hydrazones. 1, 4-Asymmetric induction and Prelog's rule. Use of chiral auxiliaries in Diels-Alder reaction.

3. Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC_2 BH and $IPCBH_2$.

4. Chiral catalyst controlled asymmetric synthesis: Sharpless and Jacobsen asymmetric epoxidations. Sharpless asymmetric dihydroxylation. Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalyst. Enzyme mediated enantioselective synthesis

5. Asymmetric aldol reaction: Diastereoselective aldol reaction (chiral enolate & achiral aldehydes and achiral enolate & chiral aldehydes) its explanation by Zimmerman-Traxel model.

OC-11: New techniques and concepts in organic synthesis **15 Hrs**

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.

Solid phase oligodeoxynucleotide synthesis: Triester pathway and phosphoramidite pathway

I. **Oligosaccharide synthesis:** Protection of hydroxyl groups, cylic oxocarbenium ion, glycosyl donors and glycosyl acceptors, Kahne glycosidation, convergent and linear oligosaccharide synthesis.
II. **Phase Transfer catalysis:** Onium and crwon ethers as PTC.
III. **Tandem synthesis:** Tandem reactions; conjugate addition-aldol reaction, polymerization-cyclisation, elctrocylic-Diels Alder reaction.

IV. **Baldwin Rules:** Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavoured cyclisations.

V. **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, furanonycin from D-glucose, S-(-)-ipsenol from S-leucine. 8) Determination of absolute configuration: Mosher's methods.

OC-12 Biomolecules **15 Hrs**

1. Enzymes: Definition. Classification based on mode of action. Mechanism of enzyme catalysis. Lock and Key model and Induced- Fit model. Enantiomer discrimination by Three- point Contact model. Factors affecting enzyme catalysis.Enzyme inhibition- reversible and irreversible inhibition. Enzymes in organic synthesis. Immobilised enzymes.

2. Nucleic acids: Primary, secondary and tertiary structure of DNA. Types of m-RNA, t-RNA and r-RNA. Replication, transcription and translation. Genetic code. Protein biosynthesis. Chemical Synthesis of nucleosides and nucleotides.

3. Lipids: Lipid structure- acylglycerols, phosphoglycerides and sphingolipids. Biosynthesis of Lipids and chemical Synthesis of lipids.

Recommended Books:

1. Stereo selectivity in organic synthesis by R S Ward.
2. Asymmetric synthesis by Nogradi
3. Asymmetric organic reactions by J D Morrison and H S Moschcr
4. Principles in Asymmetric synthesis by Robert E. Gawley & JEFFREY AUBE
5. Stereo differentiating reactions by Izumi
6. Some modern methods of organic synthesis by W Carruthers
7. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
8. Organic synthesis by Michael B Smith
9. Enzyme structure and mechanism by Fersht and Freeman
10. Bio-Organic chemistry by Hennan Dugas
11. Nucleic acids in Chemistry and Biology by G M Blackbum MI Gait
12. Lehninger Principles of Biochemistry by D L Nelson and M M Cox
13. Outlines of Biochemistry by Conn and Stumpf
14. Biotransformations in Organic Chemistry by K Faber.
15. Principles of biochemistry by Horton & others.
16. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.
17. Fudamentals of asymmetrc synthesis by G.L.David Krupadanam

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

OC13- Synthetic Reagents -I
OC 14- Synthetic Reagents -II
OC 15- Protecting groups
OC 16- New Synthetic reactions

Teaching Hours = 4/week **Marks= 80**

OC-13 Synthetic Reagents - I **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, Swern oxidation d). Oxidative cleavage of 1,2-diols: Periodic acid and Lead tetra acetate

ii) **Reductions:** a). Catalytic hydrogenation: Homogenous (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-14: Synthetic Reagents -II

15 Hrs

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

ii) Carbonyl methylenation:
a) Phosphorous ylide mediated olefination: 1) Wittig reaction 2) Horner-Wordsworth-Emmons reaction
b) Titanium- Carbene mediated olefination: 1) Tebbe reagent 2) Petasis reagent 3) Nysted reagent.

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

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

OC 15- Protecting groups **15 Hrs**

a) Protection and deprotection of alcohols as ether (methyl, MOM, MEM, THP, benzyl, PMB, trityl), silyl ether (TMS, TES, TBDMS, TBDPS) and ester formation (acetate, benzoate, pivolate).
b) Protection and deprotection of 1, 2-diols and 1, 3-diols as acetonides, cycloalkylidene and benzylidene (comparative study) and carbonate formation.
c) Protection and deprotection of amines as carbamates (Fmoc, BOC, Cbz), amides and sulfonamides formation (Ts).
d) Protection and deprotection of carbonyls as acetals (dioxolanes, dioxanes) and thio acetals (Umpolung) formation.
e) Protection and deprotection of carboxylic acids as ester (alkyl, benzyl), ortho ester and oxazoline formation.

Utility of protecting groups in the synthesis of R-Serine from S-Serine. Epoxidation of chiral cyclohexenols and oxidation of 1, 5-dioles (with and without silyl protecting groups). Importance of protecting groups in the synthesis of both natural and synthetic steroids from Weiland – Miescher ketone.

OC-16: New Synthetic reactions **15 Hrs**

1. **Metal mediated C-C and C-X coupling reactions:** Suzuki, Heck, Stille, Sonogishira 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, Hantzsch and Mannich reactions.
4. **Ring Formation Reactions:** Pausan-Khand reaction, Bergman cyclisation, Nazerov cyclisation.
5. **Click Chemistry:** Criteria for Click reaction, Sharpless azides cycloadditions.
6. **Metathesis:** Grubb's 1st and 2nd generation catalyst, Olefin cross coupling metathesis(OCM), ring closing metathesis(RCM), ring opening metathesis(ROM), applications.
7. **Other important synthetic reactions:** Baylis-Hilman reaction, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction, Stork-enamine reaction and Michael reactions.

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. Total synthesis of natural products: the Chiron approach by S. Hanesian
9. Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren

Paper 3: CH (OC) 303T: Organic Spectroscopy and Synthetic strategies.

OC-17: ^{13}C NMR spectroscopy
OC-18: 2D NMR techniques
OC-19: Synthetic strategies -I
OC-20: Synthetic strategies –II

Teaching Hours = 4/week **Marks= 80**

OC-17: ^{13}C NMR spectroscopy **15 Hrs**

CW and PFT techniques. 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.

OC-18 2D NMR techniques **15 Hrs**

1). 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.

OC-22: Synthetic Strategies I **15 Hrs**

Synthetic Strategies: Introduction, Terminology: target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition, functional group elimination. Criteria for selection of target. Linear and convergent synthesis. Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations. Order of events in synthesis by retrosynthetic approach, explanation with examples: S-salbutamol, Propoxycaine and Dinocap. Introduction to one group C-C and C-X disconnections. One group C-C disconnections, Alcohols and carbonyl compounds. One group C-X disconnections, Carbonyl compounds, alcohols, ethers and sulphides.

OC-23: Synthetic Strategies II **15 Hrs**

Introduction to two group C-C and C-X disconnections, Two group C-X disconnections; 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- difunctionalised compounds, Michael addition and Robinson annulation. Control in carbonyl condensations, explanation with examples oxanamide and mevalonic acid. Strategic bond: definition, choosing disconnection/ 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. Other approaches to retro synthesis – biomimetic approach (Johnsons polyene cyclisation), and retro mass spectral fragmentation. Application of the strategies to the synthesis of (+) Disparlure, Retronecene, longifoline.

Recommended Books:

1. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
2. Organic Spectroscopy by William Kemp
3. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
4. Modern NMR techniques for chemistry research by Andrew B Derome
5. NMR in chemistry - A multinuclear introduction by William Kemp
6. Spectroscopic identification of organic compounds by P S Kalsi
7. Introduction to organic spectroscopy by Pavia
8. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
9. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
10. Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and RichardJ.Sundberg
11. Mechanism and Structure in Organic chemistry by S Mukherjee
12. Advanced Organic Chemistry: Reactions, Mechanisms & Structure by Michael B Smith & Jerry March
13. Pericyclic Reactions by Mukherjee S M
14. Conservation of Orbital Symmetry by Woodward and Hoffmann
15. Organic Reactions and Orbital Symmetry, Gilchrist and Storr
16. Pericyclic Reactions — a problem solving approach, Lehr and Merchand
17. The Nature of Chemistry — Units 17-19 - Aromaticity — Open University, U K. Publications
18. The aromaticity III level, units 17-19 British open university volumes
19. Aromatic character and aromaticity by G.M.Badger
20. Non-benzenoid aromatic compounds by D.Ginsberg
21. Nonbenzenoid compounds by Lloyds

Paper-4 CH (OC) 304T: Pericyclic reactions, Photochemistry and Green Chemistry

OC-21 Aromaticity and Pericyclic reactions I
OC-22 Pericyclic reactions II
OC-23 Photochemistry
OC-24 Green Chemistry

Teaching Hours =4/week **Marks= 80**

OC-19 Aromaticity and Pericyclic reactions I — 15 Hrs

Aromaticity: Aromatic and anti-aromatic compounds. Criteria for aromaticity. Huckel's 4n+2 electron rule for benzene and non benzenoid aromatic compounds. Eg. Cyclopropenium ion, cyclopentadienyl ion, cycloheptatrienium ion, azulene and annulenes.

Introduction - Characteristics and classification of pericyclic reactions— Electrocyclic, cycloaddition & cycloreversions and sigmatropic reactions—4ne and 4n+2e type examples.
Approaches for the interpretation of mechanism of pericyclic reactions-Aromatic Transition States (ATS)/Perturbation Molecular Orbitals (PMO) approach-Concept of Huckel –Mobius aromatic and antiaromatic transition states. Framing Woodward-Hofmann selection rules for all the pericyclic reactions by ATS approach. Solving problems based on ATS approach.

OC-20 Pericyclic reactions II — 15 Hrs

Molecular orbitals-definition and their origin-Non-mathematical writing up of molecular orbitals and their symmetry properties for acyclic conjugated systems. Frontier Molecular Orbital (HOMO-LUMO) approach-concept-Framing Woodward-Hofmann selection rules for all the pericyclic reactions by Frontier Molecular Orbital (FMO) approach. Solving problems based on FMO approach. Conservation of orbital symmetry (Correlation Diagrams) approach-concept- Framing Woodward-Hofmann selection rules for electrocylic and cycloadditions & cycloreversions by Conservation of orbital symmetry approach.

OC-21: Photochemistry — 15Hrs

Photochemistry of (π, π^*) transitions: Excited states of alkenes, cis-trans isomerisation, photostationary state, electrocyclisation and sigmatropic rearrangements, di-π methane rearrangement. Intermolecular reactions, photocycloadditions, photodimerisation of simple and conjugated olefins, addition of olefins to α, β-unsaturated carbonyl compounds. Excited states of aromatic compounds, Photoisimerisation of benzene
Photochemistry of (n-π^*) transitions: Excited states of carbonyl compounds, homolytic cleavage of α-bond, Norrish type I reactions in acyclic and cyclic ketones and strained cycloalkanediones. Intermolecular abstraction of hydrogen: photoreduction - influence of temperature, solvent, nature of hydrogen donor and structure of the substrate
Intramolecular abstraction of hydrogen: Norrish type II reactions in ketones, Esters and 1, 2- diketones, Addition to carbon-carbon multiple bonds, Paterno-Buchi reaction, Photochemistry of nitrites-Barton reaction.

OC-24: Green Chemistry **15Hrs**

Introduction. Principles, atom economy and scope. Introduction to alternative approaches.

1. Solvent free reactions-principle, scope, utility of solvent free condition reactions. Organic Synthesis in solid state (without using any solvent): Michael addition, Beckmann rearrangement, Synthesis of aziridines; solid supported organic synthesis: Synthesis of aziridines, pyridines, chromenes and flavones.
2. Aqueous Phase Reactions: Diels-Alder Reaction, Heck reaction, epoxidation, Dihydroxylation (Syn- & Anti-)
3. Microwave Technology: Microwave equipment, activation-benefits, limitations, microwave effects.

a) Microwave Solvent free reactions (Solid state Reactions) - Deacetylation, deprotection, saponification of esters, alkylation of reactive methylene compounds, synthesis of nitriles from aldehydes, reductions.

b) Microwave assisted reactions in water — Hoffmann elimination, hydrolysis, oxidation, saponification reactions.

c) Microwave assisted reactions in organic solvents — Esterification reactions, Fries rearrangement, Ortho ester Claisen rearrangement, Diels- Alder reaction, decarboxylation.

d) Microwave assisted reactions under PTC conditions:

4. Ultrasound assisted reactions: introduction, substitution reactions, addition, oxidation, reduction reactions.
5. Organocatalysis: Aldol reactions, Acyl transfer reactions, nucleophilic N-heterocyclic carbenes in asymmetric organocatalysis, setter reaction and Baker's Yeast.
6. Ionic liquids: Introduction and applications in organic synthesis (illustrate with two examples).

Recommended Books

1. Green chemistry, Theory and Practical, Paul T.Anastas and John C.Warner.
2. New trends in green chemistry By V.K.Ahulwalia and M.Kidwai.
3. Organic Synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal.
4. Enantioselective organocatalysis, Peter I Dallco, Willey-VCH.
5. Molecular Reactions and Photo chemistry by Depuy and Chapman
6. Photochemistry by C W J Wells
7. Organic Photochemistry by Turro
8. Molecular Photochemistry by Gilbert & Baggo
9. Organic Photochemistry by D Coyle
10. Organic Synthesis-The disconnection approach by S Warren
11. Organic Synthesis by C Willis and M Willis
12. Problems on organic synthesis by Stuart Warren

Semester III

Laboratory courses

Paper CH (O) 351P: Separation and identification of organic compounds

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 10 mixtures should be separated and analyzed by these procedures.

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

Paper CH (O) 352P: Synthesis of organic molecules & isolation of natural products

(A) Laboratory synthesis of the following compounds:

2-Phenyl indole (Fischer indole synthesis), 7-hydroxy-3-methyl flavone (Baker - Venkatramanreaction), 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 ofmaleic 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.

(B) Demonstration for the 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 (solvent extraction).

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

M.Sc. CHEMISTRY (ORGANIC CHEMISTRY)IV SEMESTER SYLLABUS
(With effect from the academic year 2021-2022 under the CBCS pattern)
[Under Restructured CBCS Scheme]

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

OC-25: Principles of Drug design and drug discovery
OC-26: Lead modification and SAR Studies
OC 27: QSAR studies
OC 28: Combinatorial Synthesis

Teaching Hours = 4/week **Marks= 80**

OC- 25: 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. cimitidine) 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-26: 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-27: Quantitative Structure- Activity Relationship (QSAR) studies **15 Hrs**

Introduction, physicochemical properties - pKa, electronic effects and Hammett constants(σ), lipophilicity constant(π), steric effects and Taft's constant, linear and nonlinear relationship between biological activity and Hammett/ Lipophilicity Substituent constants. Lipenski rule of five. Hansch analysis, Craig's plot, Topliss scheme, Free Wilson approach, cluster significantanalysis. Three case studies. Principles of molecular modeling in drug design.

OC-28: Combinatorial Synthesis **15Hrs**

Introduction. Combinatorial approach. Combinatorial libraries, technologies. Solid phase synthesis, types of resins. Linkers. Reactants for solid phased synthesis. Methods of Parallel synthesis: Haughton's tea bag procedure. Automated parallel synthesis. Methods in Mixed combinatorial synthesis: general principles. Furkas mix and split combinatorial synthesis, Structure determination of active compounds-Deconvolution, Methods in deconvolution- recursive deconvolution, tagging and use of decoded sheets. Examples of Combinatorial Chemistry. Planning and designing of combinatorial synthesis, Spider like scaffolds, drug molecules. Automation in Combinatorial chemistry. High throughput screening.

Recommended 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.
20. Medicinal Chemistry by G. Patricks.
21. Text book of Drug Design and Discovery, Edited by Povl Krogsgaard – Larsen Tommy Liljefors.
22. 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 CH (OC) 402T: Drug synthesis and mechanism of action

OC-29: Drugs acting on metabolic process, cell wall and specific enzymes
OC-30: Drugs acting on genetic material and immune system
OC-31: Drugs acting on receptors and ion channels
OC-32: Chiral drugs

Teaching Hours = 4/week **Marks= 80**

OC-29: Drugs acting on metabolic process, cell wall and specific enzymes

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-30: Drugs acting on genetic material and immune system

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 of loxacin and Lomefloxacin.

f) Inhibitors of transcribing enzymes: Anti-TB and anti-leprosy 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

Drugs acting on immune system: Introduction to immune system. Immuno-suppressing agent-structural formula of Cyclosporin. Immuno-enhancers-use of vaccines and structural formula of levamisol.

OC-31: Drugs acting on receptors and ion channels

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, Chloropheneramine, 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.

OC-32: Chiral drugs

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.

Synthesis and pharmacological activity of S-Ibuprofen, S- Metaprolol, Ininavir sulfate, Levocetrazine, 2S-Verapamil, S,S-Ethambutol, (+)Lomefloxacin, Fluvastatin,Dextropropoxyphen, (+)Ephedrine, (+)Griseofulvin, Dexormaplatin, R-Indacrinone, Nateglinide, Oxybutynin hydrochloride, S,S- Captopril and S,S,S- Enalaprilate.

Recommended 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: Advanced Heterocyclic Chemistry

OC-33: Nonaromatic (Three and four membered) heterocyclics
OC-34: Five and six membered heterocyclics with two hetero atoms
OC-35: Heterocyclics with more than two hetero atoms
OC-36: Larger ring and other heterocyclics

Teaching Hours = 4/week **Marks= 80**

OC-33: Nonaromatic (Three and four membered) heterocyclics **15 Hrs**

Different types of strains, interactions and conformational aspects of nonaromatic heterocycles. Synthesis, reactivity and importance of the following ring systems. Azirines, Aziridines, Oxiranes, Thiiranes, Diazirenes, Diaziridines, Oxaziridines, Azetidines, Oxetanes and Thietanes

OC-34: Five and six membered heterocyclics with two hetero atoms **15 Hrs**

Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine.Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole.

OC-35: Heterocyclics with more than two hetero atoms **15 Hrs**

Synthesis, reactivity, aromatic character and importance of the following Heterocycles: 1,2,3-triazoies,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, 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.

OC-36: Larger ring and other Heterocyclics **15 Hrs**

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. Synthesis of selenophenes, Tellerophenes, Phospholes and Boroles.

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

Paper-4 – CH (OC) 404T(CB_1): Advanced Natural Products

OC(CB_1)-1: Biosynthesis of natural products

OC(CB_1)-2-: Structure determination and stereochemistry of natural products by chemical methods.

OC(CB_1)-3: Structure determination and stereochemistry of natural products by spectral methods.

OC(CB_1)-4: Total stereo selective synthesis of natural products.

Teaching Hours = 4/week **Marks= 80**

OC(CB_1)-1: 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(CB_1)-2: Structure determination and stereochemistry of natural products by chemical methods **15 Hrs**

Determination of structure and stereochemistry of morphine, reserpine, abietic acid, cholesterol and rotenone.

OC(CB_1)-3: Structure determination and stereochemistry of natural products by spectral methods **15 Hrs**

Spectroscopic techniques IR, UV, ^{1}Hnmr, ^{13}Cnmr, COSY, HETEROCOSY, NOESY, 2D-INADEQUATE and MS in the structure elucidations of natural products, Examples, flavones, biflavones, flavanones, isoflavones, coumarins, quinolines, isoquinolines.

Study of the following solved problems: Mass, IR, ^{1}H, ^{13}C NMR, HOMOCOSY, HECTOR, DEPT, 2D-INADEQUATE and NOE of **Geraniol**, INEPT of **menthol**, NOESY of **buxaquamarine**, HETEROCOSY of **strictanol**, 2D-INADEQUATE of **α-picoline** and **β- methyl tetrahydran furan**.

OC(CB_1)-4: Total stereoselective synthesis of natural products. **15 Hrs**

Woodward's synthesis of reserpine and cholesterol, Corey's synthesis of prostaglandins (E2, F2α), Nicolaous synthesis of taxol, Takasago synthesis of menthol, Hoffmann-LaRoche synthesis of Biotin.

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) 404 T(CB_2): Bioorganic Chemistry

OC (CB_2) -1: Enzymes and their action
OC (CB_2) -2: Enzyme models and Enzymatic transformations OC
(CB_2) -3: Recombinant DNA and Fermentation technology OC
(CB_2) -4: Coenzymes

Teaching Hours = 4/week **Marks= 80**

OC (CB_2)-1: 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 (CB_2)-2: 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 (CB_2) -3: 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.

OC (CB_2) -4: Coenzymes — 15 Hrs

Introduction. Co factors — cosubstrates — 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 I)nicotinamide adenosine dinucleotide / their phosphates (NAD), NADH, $NADP^+$ NADPH) ii) Flavin adenine nucleotide FAD, $FADH_2$ and iii) Flavin mononucleotide (FMN, $FMNH_2$) lipoic acid, biotin, tetrahydrofolate and ubiquinone. Adenosine triphosphate (ATP) and adenosine diphosphate (ADP), S-adenosyl methionine (SAM) and uridine diphospho sugars (UDP-sugars) Mechanism of reactions catalyzed by the above coenzymes.

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) 404 T(CB_3): Physical- Organic Chemistry

OC (CB_3) -1: MO and VB theory of reactivity

OC (CB_3) -2: Kinetic, isotopic, structural, solvent, steric and conformational effects

OC (CB_3) -3: Nucleophilic, electrophilic and free radical reactivity

OC (CB_3) -4: Supramolecular chemistry

OC (CB_3) -1- Molecular Orbital (MO) and Valence Bond (VB) theory of reactivity

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 (CB_3) -2: Kinetic,isotopic, structural,solvent, steric and conformational effects

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 (CB_3) -3: Nucleophilic,electrophilic and free radical reactivity

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. Bronstéd 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.

OC (CB_3) -4: Supramolecular chemistry

Properties of covalent bonds- bond length, inter-bond angles, force constant, bond and molecular dipole moments. Molecular and bond polarisability, bond dissociation enthalpy, entropy. Intermolecular forces, hydrophobic effects. Electrostatic, induction, dispersion and resonance energy, magnetic interactions, magnitude of interaction energy, forces between macroscopic bodies, medium effects, Hydrogen bond. Principles of molecular association and organization as exemplified in biological macromolecules like enzymes, nucleic acids, membranes and model systems like micelles and vesicles. Molecular receptors and design principles. Cryptands, cyclophanes, calixeranes, cyclodextxins. Supramolecular reactivity and catalysis. Molecular channels and transport processes. Molecular devices and nanotechnology.

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

Semester-IV

Laboratory courses

Paper CH (OC) 451P: Spectroscopic identification of organic compounds andChromatography:

1. Identification of unknown organic compounds by interpretation of IR, UV, ^{1}H -NMR, ^{13}C NMR and mass spectral data. A minimum of 30 representative examples should be studied.
2. Thin layer chromatography: Determination of purity of a given sample, monitoring the progress of chemical reactions, identification of unknown organic compounds by comparing the R_f values of known standards.
3. Separation by column chromatography(**Demonstration**): Separation of a mixture of *ortho* and *para*- nitroanilines using silicagel as adsorbant and chloroform as the eluent. The column chromatography should be monitored by TLC.

Paper CH (OC) 452P: Synthesis and analysis of drugs

(A) Laboratory Synthesis of the following drugs:
Paracetamol, Phenytoin, Benzocaine, 6-Methyluracil, Chloritone,4-Aminobenzene sulfonamide, FIuorescien and antipyrine.

(B) Estimation of the following drugs:
Aspirin (titrimetry), Ibuprofen (titrimetry), Analgin (titrimetry),Chloride in Ringer's lactate (argentometry), ascorbic acid (Iodometry), Isoniazid (Iodometry), Riboflavin (colorimetry), Zn ions in Bactracin Zinc, Ca^{+2} ions in Calcium gluconate injection (complexometry), Diazepam (UV-Visible Spectrophotometer).

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.