DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY,
AURANGABAD.

DEPARTMENT OF CHEMISTRY

SYLLABUS

M. Sc. Organic Chemistry

(Semester III & IV)

Choice Based Credit and Grading System

Effective from : June 2017

The following will be the Choice Based Credit and Grading System structure of revised syllabus for M. Sc. III & IV semester Organic Chemistry effective from June 2017.

Semester	Paper Nos.	Title of Paper	Teaching (hr)/week	Marks	Credits
III- Semester	CHESC-301	Structural elucidation by spectral methods	04	100	04
	CHECO- 302	Organic synthesis	04	100	04
	CHECO- 303	Photochemistry, free radicals and pericyclic reactions	04	100	04
	CHEEO -304	Advanced organic chemistry	04	100	04
	CHEEO -305	Environmental chemistry	04	100	04
	CHEEO- 306	Green chemistry	04	100	04
	CHELO- 307	Laboratory course	06	50	03
	CHELO- 308	Laboratory course	06	50	03
	CHELO- 309	Laboratory course	06	50	03
IV semester	CHECO -401	Heterocyclic chemistry	02	50	02
	CHECO -402	Organic synthesis: Retrosynthetic approach	04	100	04
	CHECO -403	Chemistry of natural products	04	100	04
	CHEEO -404	Medicinal chemistry	04	100	04
	CHEEO -405	Organic high polymers	04	100	04
	CHEEO -406	Drug design and drug discovery	04	100	04
	CHEOR - 407	Research project (Experimental)	24	200	12
	CHEOR - 408	Research project (Dissertation, Presentation and Seminars)	06	100	06

CHESC-301: Structural elucidation by spectral methods

04 Hrs/Week **Credits: 04** **Marks 100**

UNIT-I: Nuclear Magnetic Resonance Spectroscopy (^{1}H NMR) [12 hrs]

Elementary ideas (Recapitulation); Spin-spin couplings, Different types of couplings, factors affecting on coupling constants, Karplus equation, Spin systems (AB, AX, ABX, AMX), Rate processes, spin decoupling, shift reagents, Nuclear Overhauser effect (NOE), INEPT and INADEQUATE.

UNIT-II: ^{13}C Nuclear Magnetic Resonance Spectroscopy [12 hrs]

Elementary ideas, instrumental problems, chemical shifts (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbons); Effect of substituents on chemical shifts.

UNIT-III: Mass Spectroscopy [12 hrs]

Introduction, ion production (EI, CI, FD and FAB), ion analysis, ion abundance, factors affecting on fragmentation, fragmentation of different functional groups, molecular ion peak, isotopic peaks, metastable peak, Nitrogen rule, McLafferty rearrangement, Retro-Diels-Alder reaction.

UNIT-IV [12 hrs]

Problems based on joint applications of UV, IR, ^{1}H NMR, ^{13}C NMR and Mass spectroscopy.

UNIT-V [12 hrs]

Mossbauer spectroscopy: Principle, factors affecting the line position and shape, isomer effect and Quadrupole splitting iron salt like compounds, complexes, carbonyl compounds (temperature dependence of isomer shift and Quadrupole splitting in simple compound and coordination, polynuclear complexes), Numericals.

Electron Spin Resonance Spectroscopy: Principle of ESR spectroscopy, presentation of spectrum, hyperfine splitting in various structures, hyperfine splitting diagram of representative examples, factors affecting the magnitude of 'g' values, Zero field splitting, Kramer's degeneracy, Anisotropy in the hyperfine coupling constant, electron delocalization, instrumentation and applications.

Reference Books:

1. Introduction to Spectroscopy: D. L. Pavia, G. M. Lampman, G. S. Kriz
2. Spectrometric Identification of Organic Compounds: R. M. Silverstein & F. X. Webster
3. ^{13}C NMR Spectroscopy: G. C. Levy, R. L. Lichter, G. L. Nelson

4. Spectroscopic Methods in Organic Chemistry: D. H. Williams & I. Flemming
5. Absorption Spectroscopy of Organic Compounds: V. M. Parikh
6. Mass Spectrometry: K. G. Das & James
7. Coordination Chemistry by Experimental Methods: K. Barger
8. Coordination Chemistry vol. I: E. Martell
9. Physical Methods for Chemistry: R. S. Drago
10. Structural Methods in Inorganic Chemistry: E. A. V. Ebsworth & D. W. H. Rankin
11. Organic Structure Analysis: Philips Crews

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CHECO-302: Organic synthesis

04 Hrs/Week **Credits: 04** **Marks 100**

UNIT-I Oxidation **[12 hrs]**

(a) Oxidation of alcohol to aldehyde, ketone or acid: Jones reagent, Swern oxidation, Collins reagent, Fetizones reagent, PCC, PDC, PFC, IBX, Activated MnO_2, Chromyl chloride (Etard reaction), TEMPO, CAN, NMO, Moffatt oxidation

(b) Oxidative cleavage of Carbon-Carbon double bonds: $KMnO_4$, Ozonolysis.

(c) Oxidations using SeO_2, PhSeBr.

(d) Selective cleavages at functional groups: Cleavage of glycols, IO^-_4, $Pb(OAc)_4$.

UNIT-II Reductions **[12 hrs]**

(a) Catalytic Hydrogenation; (b) Reduction of nitriles, oximes and nitro compounds; (c) Reduction of acids and Esters; (d) Reduction with metal hydride- Sodium cyanoborohydride, Diborane, L- & K-Selectrides, $LiBH_4$, DIBAL-H; (e) Birch reduction and related reactions, (h) Luche reagent, Wolf-Kishner reduction, Clemmenson reduction, Wilkinson catalyst, TBTH.

UNIT-III Organic Reagents **[12 hrs]**

DCC, EDC, DDQ, 1,3 Dithiane, LDA, DMDO, OsO_4, RuO_4, SmI_2, Dess-Martin Periodinane, Diazomethane, Lawesson's reagent.

UNIT-IV **[12 hrs]**

(A) Ylides and Enamines

(i) Ylides: Preparation and their synthetic applications along with their stereochemical aspects of Phosphorous, Sulphur and Nitrogen ylides.

(ii) Enamines: Generation & application in organic synthesis with mechanistic pathways, stork enamine reaction.

(B) Rearrangements

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

UNIT-V Formation of Carbon-Carbon bonds via organometallic reagents **[12 hrs]**

Synthesis and applications of organo Lithium, Magnesium, Titanium, Cerium, Copper, Chromium, Zinc, Boron, Silicon, Cadmium

Reference Books:

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

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CHECO-303: Photochemistry, free radicals and pericyclic reactions

04 Hrs/Week **Credits: 04** **Marks 100**

UNIT-I: Pericyclic Reactions-I **[12 hrs]**

Features and classification of pericyclic reactions, Phases, nodes and symmetry properties of molecular orbital in ethylene, 1,3-butadiene, 1,3,5-hexatriene. Allyl cation, allyl radical, pentadienyl cation and pentadienyl radical. Thermal and photochemical reactions.

Electrocyclic reactions: Woodward-Hoffmann selection rules for electrocyclic reactions. Explanation for the mechanism of electrocyclic reactions by: (i) Symmetry properties of HOMO of open chain partner; (ii) Conservation of orbital symmetry and orbital symmetry correlation diagram and (iii) Huckel-Mobius aromatic and antiaromatic transition state method.

UNIT-II: Pericyclic Reactions-II **[12 hrs]**

Cycloaddition reactions: Diels-Alder reaction. Woodward-Hoffmann selection rules for cycloaddition reactions. Explanation for the mechanism of cycloaddition reactions by 1) Conservation of orbital symmetry and orbital symmetry correlation diagrams 2) Fukui Frontier Molecular Orbital (FMO) theory and (3) Huckel-Mobius aromatic and antiaromatic transition state method. Endo-exo selectivity in Diels-Alder reaction and it's explanation by FMO theory. Examples of cycloaddition reactions.

Sigmatropic reactions: Selection rules for [i,j] shifts. Cope, degenerate Cope and Claisen rearrangements. Explanation of sigmatropic reactions by (i) symmetry properties of HOMO (ii) Huckel-Mobius aromatic and antiaromatic transition state method. Introduction to chelotropic reactions and the explanation of mechanism by FMO theory.

UNIT-III: Photochemistry-I **[12 hrs]**

Photochemistry of (π, π^*) transitions: Excited state of alkenes, cis-trans isomerisation, photochemistry state, electrocyclisation and Sigmatropic rearrangements, di π-methane rearrangement.

Intermolecular reactions: photocycloadditions, photodimerasation. Photoaddition reactions. Excited states of aromatic compounds, photodimerisation of benzene, photosubstitution reactions of aromatic compounds and Photo-Fries rearrangement.

UNIT-IV: Photochemistry-II **[12 hrs]**

Photochemistry of (n, π^*) transitions: Excited state of carbonyl compounds, Norrish-I and Norrish-II

Addition to C-C multiple bonds: Paterno-Buchi reaction, photochemistry of alkyl peroxides, hypohalites and nitriles. Barton reaction. Photochemistry of azo compounds, diazo compounds, azides and diazonium salts. Singlet oxygen-photo oxygenation reactions. Ene reaction, formation of dioxetanes and endoperoxides. Chemiluminescent reactions. Oxidative coupling.

UNIT-V: Free radical reactions **[12 hrs]**

Introduction, generation, stability, reactivity, characteristics, structural and stereo chemical properties of free radicals, Persistent free radicals.

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

Reference Books:

1. Advanced Organic Chemistry Part A & Part B: F. A. Carey & R. J. Sundberg
2. Advanced Organic Chemistry: Jerry March
3. Organic Chemistry: Clayden, Greeves, Warren & wother.
4. Organic Chemistry: Stanley H. Pine
5. Organic Synthesis: W. Carruthers
6. Organic Synthesis: Norman and Coxon

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CHEEO-304: Advanced organic chemistry

04 Hrs/Week **Credits: 04** **Marks 100**

UNIT-I: Introduction to Bioorganic chemistry [12 hrs]

Basic concepts, Proximity effects in organic chemistry, Molecular adaptation, Molecular recognition.

UNIT-II: Enzyme Chemistry [12 hrs]

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

UNIT-III: Co-Enzyme Chemistry [12 hrs]

Chemical structures of co-enzymes and cofactors, Oxidoreduction (NAD^+, $NADP^+$), Pyridoxal phosphate (PLP), Thiamine pyrophosphate (TPP), Biotin (CO_2 carrier), Haemoglobin (O_2-carrier), Flavin (FMN, FAD, $FADH_2$), Oxene Reactions, Lipoic acid, Mechanisms of reactions catalyzed by co-factors.

UNIT-IV: Asymmetric Synthesis [12 hrs]

Chiral pool, Chiral auxiliary, Enantio- & Diastereoselective synthesis, Chiral reagent and chiral catalyst including CBS reagent, NADH, Asymmetric hydrogenation including BINAP, Hydroboration- Ipc_2BH, $IpcBH_2$, Asymmetric epoxidation- (+) DET & (-) DET, Sharpless, Jacobson, Asymmetric dihydroxylation- $(DHQD)_2PHAL$ & $(DHQ)_2PHAL$, Felkin-Anh model, Zimmermann-Traxler transition state model, Proline catalyzed asymmetric reactions.

UNIT-V: Name Reactions [12 hrs]

Arndt-Eistert, Hunds-Diecker reaction, Baeyer-Villiager, Dakin, Gabriel synthesis, Michael, Darzen, Prins, Henry, Reimer-Tiemann, Hoffmann–Loffler–Freytag, Dieckmann cyclization, Chichibabin, Vilsmeier, Ene, Ullmann reaction, Mannich, Strecker amino acid synthesis. Bamford-Steven, Baylis-Hillmann, Corey-Fuchs Reaction, Julia olefination, Mukaiyama aldol, Mitsunobu, Peterson olefination, Corey-Winter olefination, Woodward and Prevost

dihydroxylation, Shapiro, Ritter, Stille, Heck, Sonogashira, Suzuki, Duff, Chugaev, Petasis, McMurry reaction and Coupling. Ring closing metathesis (Grubb's metathesis), Aldol-Tishchenko (Evans-Tishchenko reaction), Ugi, Passerini, Biginelli, Hantzsch condensation.

Reference Books:

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

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CHEEO-305: Environmental chemistry

04 Hrs/Week **Credits: 04** **Marks 100**

UNIT-I: Introduction to Environmental Chemistry [12 hrs]

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

UNIT-II: Atmosphere, Hydrosphere and Lithosphere [12 hrs]

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

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

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

UNIT-III: Chemical Toxicology [12 hrs]

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

UNIT-IV: Air Pollution [12 hrs]

Particulates, Aerosols, SOx, NOx, COx and hydrocarbon, Photochemical smog, Air-quality standards

UNIT-V: Water Pollution [12 hrs]

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

Reference Books:

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

CHEEO-306 : Green chemistry

04 Hrs/Week **Credits: 04** **Marks 100**

UNIT-I: Introduction to Green Chemistry

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

UNIT-II: Microwave mediated organic synthesis (MAOS):

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

UNIT-III: Ionic liquids and PTC

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

UNIT-IV: Supported catalysts and bio-catalysts for Green chemistry

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

UNIT-V: Supramolecular Chemistry and Biomimetic Chemistry

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

Reference Books

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

CHELO-307: Laboratory course

06Hrs/Week **Credits: 03** **Marks : 50**

Qualitative analysis of ternary mixtures.

In a mixture at least one liquid one water soluble compound be given.

CHELO-308: Laboratory course

06 Hrs/Week **Credits: 03** **Marks : 50**

Preparations involving at least two stage based on name reactions, condensations, cyclocondensations, reagents and rearrangements (as covered under the theory). Separation purification of the product by column is desired.

CHELO-309: Laboratory course

06 Hrs/Week **Credits: 03** **Marks : 50**

(A) Preparations involving one stage based upon the green synthetic protocols (as covered in theory syllabus).

(B) Structure elucidation of organic compounds by spectral analyses.

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CHECO-401 : Heterocyclic chemistry

02 Hrs/Week **Credits: 02** **Marks 50**

UNIT-I **[12 hrs]**

Nomenclatures of all types of heterocycles, Classification of heterocycles: as aromatics based upon various membered ring systems.

UNIT-II **[18 hrs]**

General synthetic routes based on name reactions, reactivities, utilities and wherever possible spectral analyses of the following class of heterocycles.

Four membered: Azitidines, including β- lactums.

Five membered: Thiazoles, Oxazoles, Pyrazoles and Imidazoles.

Six membered: Pyridines, Pyrimidines.

Fused heterocycles: Flavones, Chromones, Coumarines, Indoles, Quinolines, Benzodiazepines, and Phenothiazines.

Reference Books:

1. Heterocyclic Chemistry: vol. I, II, III: R. R. Gupta, M. Kumar and M. Gupta
2. Heterocyclic Chemistry: Joules and Mills
3. Modern heterocyclic Chemistry: L. A. Paquette (Benjamin)
4. Organic Chemistry: Jonathan Clayden

CHECO-402: Organic synthesis: Retrosynthetic approach

04 Hrs/Week **Credits: 04** **Marks 100**

UNIT-I Disconnection Approach **[18 hrs]**

Introduction to:

(i) Grounding of organic chemistry for understanding retrosynthesis;

(i) Retrosynthetic analysis and designing of the synthesis;

(ii) Disconnection approach: An introduction to synthons, synthetic equivalents, disconnection approach, functional group interconversions, importance of order of events in organic synthesis, one and two group C-X disconnections, selective organic transformations: chemoselectivity, regioselectivity, stereoselectivity, enentioselectivity, Reversal of polarity, cyclization reactions, amine synthesis.

UNIT-II Protecting Groups **[06 hrs]**

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

UNIT-III *C-C Disconnections* **[12 hrs]**

(i) One group C-C Disconnections:

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

(ii) Two group C-C Disconnections:

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

UNIT-IV Ring Synthesis **[12 hrs]**

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

UNIT-V Complex molecules **[12 hrs]**

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

Reference Books:

1. Organic Synthesis: The Disconnection Approach: Stuart Warren
2. Designing Organic Synthesis: Stuart Warren

3. Organic Synthesis: Strategy and Control: Paul Wyatt and Stuart Warren
4. The Logic of Chemical Synthesis: E. J. Corey and Xue-Min Chelg
5. Classics in Total Synthesis I, II and III: K. C. Nicolaou and others
6. Organic Synthesis Concepts, Methods, Starting Materials: J. Fuhrhop, G. Penzlin
7. Some Modern Methods of Organic Synthesis: W. Carruthers
8. Organic Synthesis: M. B. Smith
9. Principles of Organic Synthesis: R. Norman and J. M. Coxan.
10. Advanced Organic Chemistry: Jerry March
11. Organic Chemistry: Clayden, Greeves, Warren and Wothers

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CHECO-403: Chemistry of natural products

04 Hrs/Week **Credits: 04** **Marks 100**

UNIT-I: Terpenoids & Carotenoids **[12 hrs]**

Classification, Nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule, Structure determination, stereochemistry, and synthesis of the following representative molecules: Citral, Geraniol, α-Terpineol, Menthol, Farnesol, Zingiberene, Phytol, Abietic acid and β- Carotene.

UNIT-II: Alkaloids **[12 hrs]**

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry and synthesis of the following: Ephedrine, (+)-coniine, nicotine, atropine, Quinine and Morphine.

UNIT-III: Steroids **[12 hrs]**

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Bile acids, Androsterone, Testosterone, Estrone, Progestrone.

UNIT-IV: Anthocyanins and Flavones **[12 hrs]**

Occurrence, nomenclature and general methods of structure determination. Synthesis of cyanidin chloride, cyanin, Hirsutidin chloride, Flavones (Kostanecki and Baker-Venkataraman approaches), Flavonols, Qurcetin, and Isoflavones.

UNIT-V: Biogenesis **[12 hrs]**

The building blocks and construction mechanisms of the following:

(a) Terpenoids: Mono-, Sesqui-, Di-, Tri-Terpenoids and steroids.

(b) Alkaloids: pyridine alkaloids, Benzyl Isoquinoline alkaloids, morphine alkaloids and Indole alkaloids.

(c) The Shikimic acid pathway.

Reference Books:

1. The Organic Chemistry of Drug Design and Drug Action: R. B. Silverman, Academic press.
2. Natural Products: Chemistry and Biological Significance: J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthrope and J. B.Harborne, Longman, Essex.

3. Organic Chemistry: Vol. II, I. L. Finar, ELBS.
4. Introduction to Flavonoids: B. A. Bohm, Harwood Academic Publishers
5. New Trends in Natural Product Chemistry: Atta-ur-Rahman and M. I. Choudhary, Harwood Academic publishers.
6. Biogenesis of Natural Products: Baldev Kumar and Harishkumar Chopra (Narosa Publication)

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CHEEO-404: Medicinal chemistry

04 Hrs/Week **Credits: 04** **Marks 100**

UNIT-I: Basic consideration of drug activity **[18 hrs]**

Definition and Introduction of following terms-Drug, Prodrug, Hard and Soft drugs, agonists, antagonists, affinity, efficacy, potency, isosterism, bioisosterism, pharmacophores, lead molecule, lethal dose (LD50) and effective dose (ED50) (i) Factors affecting bioactivity, (ii) Theories of drug activity, (iii) Structure activity relationship (SAR), QSAR (2D and 3D method) and Hantzsch equation (iv) Drug receptor mechanism.

UNIT-II Pharmacokinetics **[06 hrs]**

(i) Drug absorption, Distribution and deposition of drugs.

(ii) Excretion and elimination of drugs, Bioavailability.

UNIT-III Pharmacodynamics **[12 hrs]**

(i) Mechanism of drug action: Enzyme stimulation and enzyme inhibition, antimetabolites, membrane active drugs, chelation; (ii) Drug metabolism and inactivation: Factors affecting drug metabolism, pathways of drug metabolism [Metabolic reaction (Phase I) and conjugation reaction (Phase II)].

UNIT-IV Classification of Drugs **[06 hrs]**

The detail contents of the each class of the drugs.

UNIT-V **[18 hrs]**

Synthesis and Utilities of the following drug molecules (at least one convenient synthetic route with possible mechanism) from following classes:

I. Anti inflammatory Drugs: (a) Naproxen (b) Ibuprofen (c) Oxaprozin (d) Diclofenac Sodium (e) Rofecoxib (f) Celecoxib.

II. Anti-hypertensive Drugs: (a) Verapamil (b) Captopril (c) d-sotalol (d) Atenolol (e) Diltiazem (f) Semotiadil fumarate.

III. Drugs acting on CNS: (a) CNS Stimulant : Dextro-amphetamine

(b) Respiratory Stimulant : Doxapram

(c) CNS anti-depressant : (i) Chlorpromazine (Antipsychotic) (ii) Diazepam (Anxiolytic)

(iii) Phenobarbitol (Antiepileptic)

IV Anesthetic Drugs:

(a) General : Ketamine (b) Local : (i) Lidocaine (ii) Procaine

V. Antibiotics: (a) Chloramphenicol (b) Ampicillin (c) Amoxycillin (d) Cefepime (e) Cefpirome (f) Antimycobactrial: Ethambutol (g) Antiviral: Acyclovir (h) Antimicrobial: Sulfamethoxazole

VI. Antidiabetics : (a) Troglitazone (b) Chlorpropamide (c) Tolbutamide

VII. Antineopastic Drugs: (a) Antagonist: Fluorouracil (b) Alkylating agents: i) Chlorambucil (ii) Cis-Platin

Reference Books:

1. FOYE'S Principles of Medicinal Chemistry VIth Edition: Thomas L. Lemke, David A. Williams, Victoria F. Roche and S. William Zito.
2. Introduction of Medicinal Chemistry: A. Gringuage, Wiley-VCH.
3. Synthesis of Essential Drugs: R. S. Vardanyan and V. J. Hruby.
4. Volumes of Burger's Medicinal Chemistry: M. E. Wolf, JohnWiley.
5. Medicinal Chemistry: David J. Triggle.
6. Essentials of Medicinal Chemistry IInd: Andrejus Korolkovas, WileyVCH.

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CHEEO-405 : Organic high polymers

04 Hrs/Week **Credits: 04** **Marks 100**

UNIT-I: Introduction to Polymers [12 hrs]

(i) Introduction to organic polymers and various terms like Monomer, comonomer, mesomer, homopolymer, heteropolymer, co-polymer, degree of polymerization, plastic, resin, fibers et

(ii) Mechanism of polymerizations (Chain and condensation) and methods of polymerizations viz. mass, solution, emulsion and suspension.

UNIT-II: Evaluation of Polymers [12 hrs]

Molecular weight of polymers and their determinations by end group analysis, sedimentation, osmometric and viscometric measurements.

UNIT-III: Natural Polymers [12 hrs]

Isolations, characterizations and regenerations/derivatizations of natural polymers like Cellulose, Rubber and natural silk/ wool.

UNIT-IV: Synthetic Polymers [18 hrs]

Mechanism of polymerization, reactivity, stability, and applications of following polymers:

Polyethylene, polypropylene, polyvinyl chloride, polyvinyl acetate, and polymethyl methacrylate.

Polyethylene terphthalate, alkyd resin, polycarbonate and nylons.

Phenoplast, urea- formaldehyde resin, melamine-formaldehyde resin, polyurethanes, polysiloxane and epoxy resins

UNIT-V: Processing of Polymeric Materials [06 hrs]

Molding, Fiber formation, formation of films, fillers, plasticizers and cross linking agents

Reference Books:

1. Textbook of Polymer Science: Fred W. Billmeyer.
2. Polymer Science: V. R. Gowarikar, N. N. Viswanathan, Jaydeep Sreedhar
3. Organic Polymer Chemistry: K. J. Saunder

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CHEEO-406 : Drug design and drug discovery

04 Hrs/Week **Credits: 04** **Marks 100**

UNIT-I: Principles of Drug design and drug discovery [12 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. Pharmacokinetics (ADME), pharmacodynamics, Nature of drug-receptor interactions and their theories-Occupancy theory, Induced-fit theory, Macromolecular purturbation 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.

UNIT-II: Lead modification and SAR Studies [12 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 SAR studies in sulfa drugs, benzodiazepines, and taxol analogs.

UNIT-III: Quantitative Structure-Activity Relationship (QSAR) studies [12 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 significant analysis. Principles of molecular modeling in drug design.

UNIT-IV: Combinatorial Synthesis [12 hrs]

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. Furkasmix 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.

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 Chemistry 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. Burger's Medicinal Chemistry and Drug Discovery: Principles and Practices. Vol. 1.
19. Medicinal Chemistry by G. Patricks.
20. Text book of Drug Design and Discovery, Edited by Povl Krogsgaard – Larsen Tommy Liljefors.

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CHEOR-407: Research project (Experimental)

24 Hrs/week **Credit : 12** **200 Marks**

CHEOR-408 : Research project (Dissertation, Presentation and Seminars)

6 Hrs/week **Credit : 6** **100 Marks**
