

SEMESTER -3 (OrganicChemistry)

CHE(O) 501

Natural Products and Biomolecules

Unit I : Natural pigment

Natural colouring matter, general classification, method of synthesis, biosynthesis studies of anthocyanins (cyanine) flavones (chrysin) and flavanol (Quercetin)

Porphyrin-structure, spectral properties and synthesis, general and structure determination of Haemoglobin, chlorophyll and Bilirubin.

Unit II : Alkaloids and vitamins

Alkaloids: General biogenetic studies of alkaloids, chemistry of quinine, morphine , reserpine and colchicine

Vitamins : Introduction, synthesis and biochemical function of vitamin B(Thiamine), Vitamin H and α -tocopherol (Vitamin E), vitamin C.

Unit III: Steroids and hormones

General biosynthesis studies of steroids, structure of cholesterol and ergosterol (No synthesis). Stereochemistry of steroids, chemistry of bile acids.

Chemistry of androgens, oestrogens and gestrogens, their synthesis and biochemical role. Adrenocortical hormones, partial synthesis of cortisone.

Unit IV: Terpenoids and carotenoids

Classification, nomenclature, general methods of structure determination, chemistry and synthesis of abietic acid and gibberellic acid (gibberllin-A), farnesol, zingiberine and squalene. Biosynthetic studies on triterpenoids and tetraterpenoides.

Reference books:

1. *Organic chemistry vol I & II (sixth edition) I.L.Finar*
2. *Chemistry of vitamins-S.F.Dyke*
3. *Chemistry of natural products by Bantely, Vol 1-10*
4. *L.J.Wade Jr. Organic chemistry, Prentice hall, England cliffs, 1987*
5. *Chemistry of Natural products vol I & II by O.P.Agrawal*

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Medicinal Chemistry

General classification, structural variations, synthesis and medicinal uses of the following classes of drugs. In addition to the above structure Activity Relationships and Mode of Action should be discussed in classes wherever it is mentioned.

Unit I : Antibiotics

Antibiotics that interfere with the biosynthesis of bacterial cell wall.

- A. The β -lactum antibiotics : Penicillin and cephalosporin
- B. Non lactum antibiotics (only name and structures)
- C. Bacitracin, vancomycin and cycloserine (only name and structures)

Antibiotics that interfere with the protien biosynthesis in microorganisms : non lactum antibiotics, tetracycline, chloroamphenicol

Structure actively relationship (SAR) among penicillinis and tetracyclins

Non classifiable antibiotics (only structure and therapeutic uses)

Synthesis of pencillin V, ampicillin, cephalosporin and chloroamphenicol.

Unit II : Psychoactive drugs

CNS depressant:

- A. General and local anaesthetics
- B. Sedative and hypnotics

Antipsychotic drugs

- A. Antidepressant
- B. Neuroleptics

Synthesis of the following

Thiopental, amobarbital, diazepam, chlorzoxipron, alprazolam, glutethimide, nikethamide, procaine, lidocaine and dibucaine, Ibuprofen, meclizine sodium, novalgine, pethidine

Unit III: Antimalarial and Antituberculosis drugs

Antimalarials: Modern chemotherapy of malaria, 4-amino and 8-amino quinolins, 9-amino acridine.

Synthesis of mefloquine, chloroquine, primaquine and daraprim

Mode of action of antimalarial agents

SAR of antimalarial agents

Anti tuberculosis: Synthesis of only the following drugs:

Isoniazid (INH), Ethionamide, Ethambutol, DDS (Dapsone)

Unit IV :Cardiovascular, diuretics and hypoglycemic agents

Synthesis of amyl nitrate, diltiazem, atenolol, methyl dopa, tolbutamide, chlorpropamide, glibenclamide, acetazolamide, chlorothiazide, furosemide and ethacrynic acid

Reference books:

1. *Burger's medicinal chemistry and drug design (5/e) 1997, vol 1 to 5 edited by Manfred E.Woltt (John Wiley and Sons Inc. New York)*
2. *Principles of medicinal chemistry by William A. Foye (ed), Lea and Febiger (Philadelphia)*
3. *Principles of medicinal chemistry vol I & II (5/e) F.S.Kadam, K.R. Mahadik and K.G. Bohra (Nirali publication)*
4. *Medicinal chemistry by Ashutosh Kar*
5. *The organic chemistry of drug synthesis vol I, II and III (1980) ed by D. Lednicer and L.A. Mitscher (John Wiley and Sons, New York)*
6. *Wilson and Gisvold text book of organic medicinal and pharmaceutical chemistry (5/e, 1982) by Robert Doerge (J.B. Lippincott Company, Philadelphia/ Toppan Co. Ltd, Tokyo)*
7. *Topics in medicinal chemistry vol I & II by Rabinowitz Myerson (Interscience 1968)*
8. *The pharmaceutical basis of therapeutics by Geoman and Gilman (McMillan Co.)*

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Organic Spectroscopy

Unit I :UV & IR

UV: Electronic transitions, chromophores, auxochromes, bathochromic and hypsochromic shifts, solvent effects, Woodward-Fieser rules for dienes, enones and aromatic compounds applications of UV., instrumentation.

I.R. Vibrational transitions, important group frequencies, factors affecting I.R. group frequency, applications of I.R. instrumentation

Unit II : NMR

Elementary ideas of NMR integration, chemical shifts, Factors affecting, chemical shifts, coupling (first order, analysis) instrumentation and principles and instrumentation, FT, chemical shifts, spin-spin coupling different spin systems, mechanism of spin coupling. E.g. AB, ABX, factors affecting vicinal and geminal couplings, rate processes, long range couplings, spin decoupling, shift reagents, solvent shifts, nuclear Overhauser effect. 2D NMR (COSY and HETCOR) applications.

Unit III: C¹³ NMR and Mass spectrometry

C13 NMR: elementary ideas, instrumental problems, chemical shift features of hydrocarbons, effect of substituent on chemical shifts olefinic, acetylenic, aromatic and carbonyl carbons, effects of coupling
Mass spectrometry: theory, instrumentation, modes of ionization, types of detectors, modes of fragmentation. Different types of ions, molecular ions, isotopic peaks, factors controlling fragmentation, hyphenated mass spectroscopy techniques.

Unit IV:

Structural elucidation of drug molecules based on joint application of UV, IR, PMR, CMR and mass spectroscopy.

Reference books:

1. *Spectroscopic methods in organic chemistry*, D.H. Williams and Tan Fleming
2. *Spectrometric identification of organic compounds*, T.C. Morrill R.M. Silverstein and G. Bassler, 6th edition, John Wiley and sons
3. *Introduction to spectroscopy*, D.L. Pavia, G.M. Lampman and G.S. Kriz, 3rd edn, Harcourt college publishers.
4. *Organic spectroscopy* by W. Kemp
5. *Organic spectroscopy* by P.S. Kalsi

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Industrial Chemistry

Unit I : Basic principles

Basic chemical data, batch versus continuous operation, design, flow charts, chemical process selection, safety, hazardous, fire toxic materials, research and development patents, good manufacturing practice and laboratory practice.

Unit II: Unit processes in organic chemistry

Nitration, sulfonation, halogenation, amination and alkylation methods and industrial chemicals derived from benzene, naphthalene and anthracene using unit process.

Unit III

Green chemistry -12 principles of green chemistry

Green solvents- aqueous phase reactions Wurtz reaction, Wittig-Horner reaction,

Michael reaction

- Solid phase reactions: halogenation, aldol condensation, Grignard reaction.

- Ionic liquid as green solvent- hydrogenation, Diels-Alder reaction, o-alkylation and N-alkylation

Green catalysts of green reagents (introduction)

Unit IV

Manufacture and uses of

- Agrochemicals (insecticides, fungicides, plant nutrients and plant hormones, Weedicides, pesticides)

- Unit operations

Reference books:

1. *Unit processes in organic synthesis* by P.H. Groggin
2. *Industrial Chemical process* by R.N. Shreve
3. *Riegels handbook of industrial chemistry* ed by James and Kent
4. *Dryden's outlines of chemical Technology* M. Gopal Rao

SEMESTER -3
Organic Chemistry - Practicals
CHE(O) 505 & 506 PR

Preparation of industrially important compounds by following name reactions (mechanism, purification and characterization of the synthesized compounds)

1. Sandmeyer reaction
2. Pechmann reaction
3. Skraup synthesis
4. Riemer-Tiemann reaction
5. Kolbe-smith reaction
6. Claisen-smith synthesis
7. Hoffman reaction
8. Diels-alder reaction
9. Green –bromination

Estimation

1. Drug assay (estimation of sulpha drug)
2. Non-aqueous titration
3. Nitrite value
4. Drug dissolution

Reference books:

1. *Quantitative analysis by Arther I.Vogel*
2. *Quantitative analysis by V.K.Ahluwalia*
3. *Quantitative analysis by Mann and sanders*

SEMESTER -4 (Organic Chemistry)

CHE(O) 507

Advanced Organic Chemistry

Unit I : Pericyclic reactions

Introduction, classification of pericyclic reactions, stereochemistry, molecular orbital symmetry, frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system, F.M.O. and PMO approach to cycloaddition and electrocyclic reactions: Generalisation of Woodward-Hoffmann rule, sigmatropic rearrangement-suprafacial and antarafacial shifts of H. Stereoselectivity in sigmatropic rearrangement, enantioselectivity in pericyclic reactions.

Unit II : Conformational analysis

Confirmation at cyclic systems: Confirmation of cyclohexane, mono and disubstituted cyclohexane, heterocyclic compounds, five and six membered heterocycles, stereoelectronic effects, fused bicyclic system, decalin, dodecalin, polycyclic system, perhydrophenanthrene, bridged systems-conformation of sugars, steric strains due to unavoidable crowding, stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

Unit III : Oxidation

Introduction, different oxidation processes, hydrocarbons-alkenes, aromatic rings, saturated C-H group (activated and unactivated), alcohols, diols, aldehydes, ketones, amines, hydrazine and sulphides.

Unit IV: Reduction

Introduction, different reductive processes, hydrocarbons-alkanes, alkenes, alkynes and aromatic rings
Carbonyl compounds- aldehydes, ketones, acids and their derivatives, epoxides, nitro, nitroso, azo and oxime groups,

Preparation and properties and application of Pd and Ti compounds as organometallic agents

Reference books

1. *Advance organic chemistry by Jerry March*
2. *Advance organic chemistry by Carey and Sundberg,*
3. *Advance organic chemistry by Francis A. Carey*

SEMESTER -4 (Organic Chemistry)

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Advanced Organic Synthesis

Unit I : Protection of groups

Principle of protection of hydroxyl, amino, carbonyl, carboxylic acid with different reagents and their deprotection, synthetic equivalent groups, synthetic analysis and planning, control of stereochemistry.

Unit II : Disconnection approach

An introduction to synthesis, and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis one group C-X and two group C-X disconnections, chemo-selectivity, reversal and polarity.

Unit III : One group C-C disconnections

Alcohols and carbonyl compounds, region-selectivity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

Unit IV: Ring synthesis

Saturated heterocycles, synthesis of 3, 4, 5, and 6-membered rings, aromatic heterocycles in organic synthesis

Reference books

1. *Organic synthesis : the disconnection approach by stuart Warren (wiley student edition)*
2. *Organic chemistry- clayden, greeves, warren and wothers, (oxford press)*

SEMESTER -4 (Organic Chemistry)

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Bio organic Chemistry

Unit I : Water and vitamins

Water –interaction among biomolecules in aqueous systems, buffering against pH changes, in biological systems, participation of water in biological reactions.

Vitamins-classification, introduction, chemistry, absorption transport, mobilization and biochemical functions of Vitamins A, D, E, K, C, B, B2, B6, H and folic acid

Unit II : Proteins and enzymes

Proteins: properties and conventions of common amino acids, stereoisomerism in α -amino acid, peptides: formation, compositions and sizes of protein separation, purification and characterization, sequencing of peptides, sanger's method, edman degradation, outline of other methods, protein sequences and evolution. Oxygen binding proteins, haemoglobin and myoglobin in oxygen transport and storage.

Enzymes: classification, nomenclature and extraction factors affecting catalytic activity and specificity in action, regulation of enzyme activity, enzyme inhibition, illustrative enzymatic reactions using chymotrypsin, hexokinase, enolase and lysozyme

Unit III: Carbohydrates and nucleic acid

Carbohydrates: classification and stereochemistry, biologically important hexose derivatives, nomenclature of disaccharides, structure and role of some homo and hetero polysaccharides, glucoconjugates : proteoglycans, glycoproteins and glycolipids

Nucleic acid: compounds of nucleic acids, nomenclature of nucleotides, nucleosides, structure of DNA and structure of RNA

Unit IV: Lipids

Nomenclature, structure and physical properties of some naturally occurring fatty acids, triacylglycerol and waxes as sources of stored energy, insulation of water repellants, types of membrane lipids, introduction to glycerophospho lipids, galactolipids, sphingo lipids, phospholipids and sterols, bile acids.

Reference books:

1. *Principles of biochemistry –Donald J.Voet, Judith G.Voet, charlotte w. pratt (John willey and sons)*
2. *Lehninger principles of biochemistry- David L.Nelson and Michael M.wx (Palgrave Macmillan / w.h. freeman company new york)*
3. *Biochemistry – U.Satyanaarayana Baro and allied P.Ltd., kolkata*

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Selected topics in Medicinal Chemistry

Unit I : Drug design:

Introduction, naming of organic medicinal compounds, literature of medicinal chemistry, development of new drugs, procedure followed in drug design, concept of lead compound and lead modification, pro drugs, soft drugs, phase I, II and III clinical trials, structure activity relationship, theories of drug activity : occupational theory, rate theory, induced fit theory, quantitative structure activity relationship, history and development of QSAR. Concept of drug receptors, elementary treatment of drug receptor interactions, physio chemical parameters lipophilicity, partition coefficient, electronic ionization constant, concept of 3-D QSAR.

Unit II : Pharmacokinetic and pharmacodynamics

Pharmacokinetics : introduction to drug absorption, distribution, metabolism, elimination. important pharmacokinetic parameters in defining drug deposition and in therapeutics, uses of pharmaceuticals in drug development process

Pharmacodynamics: Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, drug metabolism, biotransformation, significance of drug metabolism in medicinal chemistry.

Unit III :

A. Dosage forms, Quality control and application of computers in chemistry

Dosage forms, types of dosages, different routes of administration, quality control of drugs pharmacopias, modern methods of pharmaceutical analysis.

B. Computer in chemistry

Use of computer in chemistry and industry

Important websites for data search chemistry

Information about online journals for chemistry

Unit IV:Medicine

Overview, Medicinal use of nanomaterials-Drug delivery

Protein and peptide delivery –cancer, surgery, visualization, nanoparticle targeting

Medical application of molecular nanotechnology-nanorobots, cell repair machines, nanonephrology.

References Books:

1. *Burger's Medicinal Chemistry and Drug Discovery (5/e), 1997, Vol. 1, 2, 3, 4,5, Edited by ManFred E. Wolff (John Wiley & Sons, inc., New York).*
2. *Wilson and Gisvold's Text-book of Organic Medicinal and Pharmaceutical Chemistry (5/e, 1982) by Robert F. Doerge (J. B. Lippincott Company, Philadelphia/Toppan Co. Ltd., Tokyo).*
3. *Principles of Medicinal Chemistry, Vol. I & II (5/e), by S. S. Kadam, K. R. Mahadik, K. G. Bothra (Nirali Prakashan).*
4. *QSAR: quantitative structure-activity relationships in drug design by Jean-Luc Fauchère. ISBN:084515141X, 9780845151419*
5. *QSAR : Hansch analysis and related approaches By Hugo Kubinyi*

SEMESTER -4 (Organic Chemistry)
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dissertation/industrial training