ANDHRA UNIVERSITY
SEMESTER – IV SYLLABUS
M.SC., CHEMISTRY (Organic Chemistry Specialization)
(For the batch admitted during the academic year 2019-2020)

Paper – 1: Modern Synthetic Methodology in Organic Chemistry

UNIT - I

Modern Synthetic Methods: Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction and Ugi reaction. Brook rearrangement; Tebbe olefination. Metal mediated C-C and C-X coupling reactions: Heck, Stille. Suzuki, Negishi and Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann coupling reactions.

Multicomponent Reactions: Passerini, Biginelli, Hantzsch and Mannich reactions.

Metathesis: Grubb's 1st and 2nd generation catalyst, Olefin cross coupling metathesis (OCM), ring closing metathesis(RCM), ring opening metathesis (ROM), applications.

UNIT-II

Oxidation: Metal based and non-metal based oxidations of (a) alcohols to carbonyls (Chromium, Manganese, aluminium, silver, ruthenium. DMSO, hypervalent iodine and TEMPO based reagents). (b) phenols (Fremy's salt, silver carbonate) (c) alkenes to epoxides (peroxides/per acids based), Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation.(d) alkenes to diols (Manganese, Osmium based), Sharpless asymmetric dihydroxylation, Prevost reaction and Woodward modification, (e) alkenes to carbonyls with bond cleavage (Manganese, Osmium, Ruthenium and lead based, ozonolysis) (f) alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation, selenium, chromium based allylic oxidation) (g) ketones to ester/lactones (Baeyer-Villiger)

UNIT-III

Reduction: (a) Catalytic hydrogenation (Heterogeneous: Palladium/Platinum/Rhodium/Nickel etc; Homogeneous: Wilkinson). Noyori asymmetric hydrogenation. (b) Metal based reductions using Li/Na/Ca in liquid ammonia, Sodium, Magnesium, Zinc, Titanium and Samarium (Birch, Pinacol formation, McMurry, Acyloin formation, dehalgenation and deoxygenations) (c) Hydride transfer reagents-$NaBH_4$ triacetoxyborohydride, L-selectride, K-selectride, Luche reduction; $LiAlH_4$, DIBAL-H, and Red-Al.

UNIT-IV
NEWER METHODS IN ORGANIC SYNTHESIS

Green Chemistry-Introduction, principles, atom economy and scope (illustrate with two examples)

Microwave induced reactions: Principle conditions, advantages over conventional heating methods-applications

Ionic liquids: Introduction and applications in organic synthesis (illustrate with two examples).
Nanomaterials: Introduction, methods of preparation, applications in organic synthesis
Phase-transfer catalysis: solid-solid, solid-liquid systems-mechanism of catalytic action, type of catalysts, application in few important reactions

Reference books

1. Some Modern Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge University Press, Cambridge, 1988.
2. F. A. Cary and R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009.
3. M. B. Smith, Organic Synthesis, 2nd Edition, 2005
4. J. Tsuji, Palladium Reagents and Catalysts, New Perspectives for the 21st Century, John Wiley & Sons, 2003.
5. I. Ojima, Catalytic Asymmetric Synthesis, 2nd edition, Wiley–VCH, New York, 2000.
6. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press, 2001.
7. R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons, 1994.
8. L. Kuerti and B. Czako, Strategic Applications of named Reactions in Organic Synthesis, Elsevier Academic Press, 2005.
9. Green chemistry, Theory and Practical, Paul T.Anastas and John C.Warner.
10. New trends in green chemistry By V.K.Ahulwalia and M.Kidwai.
11. Organic Synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal

ANDHRA UNIVERSITY
SEMESTER – IV SYLLABUS
M.SC., CHEMISTRY (Organic Chemistry Specialization)
(From the batch admitted during the academic year 2019-2020)

Paper II- Organic Spectroscopy and Structure determination of natural products

UNIT-I

^{13}C NMR spectroscopy & Heteronuclear couplings
Introduction, ^{13}C-chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and aromatic compounds. Types of 13C NMR spectra: Proton-coupled, proton- decoupled and OFF-resonance decoupled (ORD) spectra, DEPT. ^{13}C-NMR solvents:
Heteronuclear couplings: ^{13}C-^{1}H, ^{13}C-D, ^{13}C-^{19}F, ^{13}C-^{31}P. ^{1}H-D, ^{1}H-^{19}F, ^{1}H-^{31}P, ^{1}H-^{15}N

UNIT-II

NMR Instrumentation, 2D-NMR techniques & ESR:

NMR Instrumentation: Types of NMR Spectrometers-Continuous Wave (CW)-NMR, Fourier Transform (FT)-NMR, NMR solvents, sample preparation
2D-NMR techniques: Principles of 2D NMR, Correlation spectroscopy (COSY) HOMO COSY (1H-1H COSY), Hetero COSY (^{1}H, ^{13}C COSY, HMQC), long range ^{1}H,^{13}C COSY (HMBC), NOESY and 2D-INADEQUATE experiments and their applications.
ESR Spectroscopy: Principles, hyperfine splitting

UNIT-III

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

UNIT-IV

Structure determination of natural products by spectral methods
structure elucidation-Spectroscopic techniques IR, UV, ^{1}H-NMR, ^{13}C-NMR, COSY, HETEROCOSY, and MS- natural products-Examples, flavones-Apigenin, flavanones-Hesperetin, isoflavones-Genistein, coumarins-7-hydroxycoumarin, alkaloids-morphine, quinine, terpenoids-(-) -Menthol, Steroids-stigmasterol. Glycosides-salicin (Alcoholic β-glucoside)

Text books:

1. Spectroscopy, fourth edition, D. L Pavia, G. M Lampman CENGAGE Learning, 2012
2. Spectroscopic Methods in Organic Chemistry. Forth Edition D. M. Williams and I. Fleming Tata - McGraw Hill, New Delhi, 1990. For all spectral methods except ORD and CD and ESR.
3. Organic Spectroscopy, Second Edition, W. Kemp, ELBS Macmillan, 1987 for ORD and CD and ESR.
4. Chemistry of natural products, S. V. Bhat, Narosa Publishing House, 6th reprint 2010 (For IVth unit)

Books in Reference:

1. Applications of absorption spectroscopy of Organic Compounds J.R. Dyer, Prentice Hall of India, New Delhi, 1984.
2. Spectrometric identification of Organic Compounds, Fourth Edition, R.M. Silverstein: G.C.Vassiellr and T.C. Merill, Johne Willey, Singapore, 1981.
3. For ORD and CD "Applications of Optical rotation and Circular Dichroism", G.C. Barret, in "Elucidation of Organic structures by Physical and Chemical Methods" Part I (Eds) K.W. Bentley and G.W.Kirty John Wiley, 1972, Chapter VIII (only those aspects mentioned in the syllabus).

4.

ANDHRA UNIVERSITY
SEMESTER – IV SYLLABUS
M.SC., CHEMISTRY (Organic Chemistry Specialization)
(From the batch admitted during the academic year 2019-2020)

Paper – III: Designing organic synthesis and synthetic applications of organo- boranes and -silanes

UNIT-I

Disconnection approach -Principles

Introduction, Terminology: Retrosynthesis, Target Molecule (TM), synthon, synthetic equivalent, functional group interconversion (FGI). Linear and convergent synthesis. Criteria for selection of target . Order of events in retrosynthesis with reference to Salbutamol, Proparcaine and Dopamine. Chemoselectivity, Regioselectivity, reversal of polarity and cyclizations. Protecting groups-Principles of protection of alcohols, amine, carbonyl and carboxyl groups

UNIT-II

Synthetic Strategies

A) Introduction to one group disconnections: C-C disconnection-alcohols and carbonyl compounds: C-X disconnections- alcohols and carbonyl compounds and sulphides two group C-C and C-X disconnections,
B) Introduction to Two group C-C disconnections; Diels-Alder reaction, 1,5- difunctionalised compounds, Michael addition and Robinson annulation.
Two group C-X disconnections; 1, 1-difunctionalised, 1, 2-difunctionalised and 1, 3-difunctionalised compounds. Control in carbonyl condensations, explanation with examples oxanamide and mevalonic acid.

UNIT –III

Organoboranes: Hydroboration- Preparation of Organoboranes. Reagents -dicylohexyl borane, disiamyl borane, thexyl borane, 9-BBN and mono-, di-isopinocampheyl borane. Functional group transformations of Organo boranes-Oxidation, protonolysis and rearrangements Formation of carbon-carbon-bonds viz organo boranes- carbonylation. cyanoboration.

UNIT –IV

Organo Silanes: Preparation and synthetic applications of trimethylsilyl chloride, dimethyl-t-butylsilyl chloride, trimetthylsilyl cyanide, trimethylsilyl iodide and trimethylsilyl triflate.

Protection of functional groups- Trimethylsilyl ethers, Silyl enol ethers. Synthetic applications of α-silyl carbanions, β-silyl carbonium ions. Peterson's olefination.

Books for Reference:

1. Organic syntheses via boranes / Herbert C. Brown; with techniques by Gary W. Kramer, Alan B. Levy, M. Mark Midland. New York : Wiley, 1975
2. Some Modern Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge University Press, Cambridge, 1988.
3. Organic Synthesis: The disconnection approach, S. Warrant John Wiley & sons, New York, 1984.
4. Modern Synthetic Reactions, Herbert O. House, Second Edition, W.A. Benzamine Inc. Menio Park, California, 1972.
5. Principle of Organic Synthesis- R.O.C. Norman and J. M. Coxon.(ELBS)
6. Organic Synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal.
7. Organic Synthesis by C Willis and M Willis
8. Problems on organic synthesis by Stuart Warren

ANDHRA UNIVERSITY
SEMESTER – IV SYLLABUS
M.SC., CHEMISTRY (Organic Chemistry Specialization)
(For the batch admitted during the academic year 2019-2020

Paper IV-Drug design and drug chemistry

UNIT I

Basic consideration of drugs

General Classification, nomenclature, drug metabolism. **Development of drugs**: Procedure followed in drug design, concepts of lead compound lead modification, concept of prodrugs, Structure Activity Relationship (SAR)-factors affecting bio-activity-resonance, inductive effect, isosterism, bio-isosterism, spatial considerations, Qunatitative Structure Activity Relationships (QSAR)-Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials.

UNIT II

Antineoplastic Agents: Introduction, classification-**alkylating agents**- mechanism and mode of action, nitrogen mustards-synthesis, properties, uses and dosage - Chlorambucil, cyclophosphamide and melphalan. **Antimetobolites**- synthesis, properties, uses and dosage-pyrimidine analogues-5-flurouracil, purine analogues-6-mercaptopurine, folic acid analogues-Methotrexate. **Antibiotics**-structure, properties and dosage-Doxorubicin, Mitomycin. \

UNIT III

Cardiovascular Drugs & Oral Hypoglycemic Drugs

Cardiovascular Drugs: Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators. Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol, oxyprenolol.

Oral Hypoglycemic Drugs: Introduction, Classification, **Sulphonylureas**- synthesis, mode of action, properties, uses and dosage- tolbutamide, glipizide. **Biguanides**- synthesis, mode of action, properties, uses and dosage-Metformin. **α-glucosidage inhibitors**- synthesis, mode of action, properties, uses and dosage- Miglitol. **Dipeptidyl Peptidase-4 (DPP-4) inhibitors**-synthesis, mode of action, properties, uses and dosage-saxagliptin and sitagliptin

UNIT IV

Local Antiinfective Drugs & Antiviral drugs

Local Antiinfective Drugs: Introduction and general mode of action. Synthesis of sulphonamides, ciprofloxacin, norfloxacin, dapsone, amino salicylic acid, isoniazid, fluconazole, econozole and chloroquin.

Antiviral Drugs: Introduction, classification based on mechanism of action, Nucleoside or Nucleotide Reverse Transcriptase Inhibitors (NRTIs)-Synthesis, metabolism, properties and uses and dosage-Acyclovir, Zidovudine (Anti-HIV agent). Non-Nucleoside or Nucleotide Reverse Transcriptase Inhibitors (NNRTIs)-Synthesis, metabolism, properties and uses and dosage-Nevirapine, Efavirenz. Protease Inhibitors (PIs)- Synthesis, metabolism, properties and uses and dosage-Indinavir. CCR5-Inhibitors - Synthesis, metabolism, properties and uses and dosage-Maraviroc

SUGGESTED BOOKS FOR READING

1. **Text book of medicinal chemistry, Volume I & II, Third edition by V Alagarsamy, CBS-publishers**
2. **Introduction to Medicinal Chemistry**, A Gringuage, Wiley-VCH.
3. **Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry**, Ed Robert F. Dorge.
4. An Introduction to Drug Design, S. S. Pandeya and J. R. Dimmock, New Age International.
5. Burger's Medicinal Chemistry and Drug Discovery, Vol-1 (Chapter.-9 and Ch-14), Ed. M. E. Wolff, John Wiley.
6. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
7. The Organic Chemistry of Drug Design and Drug Action, R. B. Silverman, Academic Press.
8. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.