

JAWAHARLAL NEHRU TECHNOLOGICAL UNIVERSITY ANANTAPUR
Course Structure and Syllabi for M.Pharm-Pharmaceutical Chemistry
(JNTUA-Affiliated Pharmacy Colleges 2017-18)

I YEAR - I Semester

S. No	Course Code	Subjects	L	T	P	C
1	17S01101	Modern Pharmaceutical Analytical Techniques	4	-	-	4
2	17S02101	Advanced Organic Chemistry -I	4	-	-	4
3	17S02102	Advanced Medicinal chemistry	4	-	-	4
4	17S02103	Chemistry of Natural Products	4	-	-	4
5	17S02104	Pharmaceutical Analysis Practical for Pharmaceutical Chemistry	-	-	6	3
6	17S02105	Pharmaceutical Chemistry Practical I	-	-	6	3
7	17S02106	Seminar/Assignment	-	-	7	4
Total			16	-	19	26

I YEAR II Semester

S. No	Course Code	Subject	L	T	P	C
1	17S02201	Advanced Spectral Analysis	4	-	-	4
2	17S02202	Advanced Organic Chemistry -II	4	-	-	4
3	17S02203	Computer Aided Drug Design	4	-	-	4
4	17S02204	Pharmaceutical Process Chemistry	4	-	-	4
5	17S02205	Pharmaceutical Chemistry Practical II	-	-	6	3
6	17S02206	Pharmaceutical Chemistry Practical III	-	-	6	3
7	17S02207	Seminar/Assignment	-	-	7	4
Total			16	-	19	26

III SEMESTER

S.No	Subject Code	Subject	L	T	P	C
1.	17S01301	Research Methodology and Biostatistics	4	-	-	4
2.	17S02301	Journal Club	1	-	-	1
3.	17S02302	Teaching Assignment	10	-	-	2
4.	17S02303	Comprehensive viva voce	-	-	-	2
5.	17S02304	Discussion / Presentation (Proposal presentation)	-	-	2	2
6.	17S02305	Research Work	-	-	28	14
Total			15	-	30	25

IV SEMESTER

S.No	Subject Code	Subject	L	T	P	C
1.	17S02401	Journal Club	1	-	-	1
2.	17S02402	Research work	31	-	-	16
3.	17S02403	Discussion/ Final Presentation	3	-	-	3
Total			35	-	-	20

JAWAHARLAL NEHRU TECHNOLOGICAL UNIVERSITY ANANTAPUR

M. Pharm – I year I Sem. (Pharmaceutical Chemistry)

L T P C
4 0 0 4

(17S01101) MODERN PHARMACEUTICAL ANALYTICAL TECHNIQUES

Scope

This subject deals with various advanced analytical instrumental techniques for identification, characterization and quantification of drugs. Instruments dealt are NMR, Mass spectrometer, IR, HPLC, GC etc.

Objectives

After completion of course student is able to know about chemicals and excipients

- The analysis of various drugs in single and combination dosage forms
- Theoretical and practical skills of the instruments

THEORY

60 HOURS

1. 11 hrs
 - a. UV-Visible spectroscopy: Introduction, Theory, Laws, Instrumentation associated with UV Visible spectroscopy, Choice of solvents and solvent effect and Applications of UV Visible spectroscopy.
 - b. IR spectroscopy: Theory, Modes of Molecular vibrations, Sample handling, Instrumentation of Dispersive and Fourier -Transform IR Spectrometer, Factors affecting vibrational frequencies and Applications of IR spectroscopy
 - c. Spectrofluorimetry: Theory of Fluorescence, Factors affecting fluorescence, Quenchers, Instrumentation and Applications of fluorescence spectrophotometer.
 - d. Flame emission spectroscopy and Atomic absorption spectroscopy: Principle, Instrumentation, Interferences and Applications.
2. 11 hrs

NMR spectroscopy: Quantum numbers and their role in NMR, Principle, Instrumentation, Solvent requirement in NMR, Relaxation process, NMR signals in various compounds, Chemical shift, Factors influencing chemical shift, Spin-Spin coupling, Coupling constant, Nuclear magnetic double resonance, Brief outline of principles of FT-NMR and ¹³C NMR. Applications of NMR spectroscopy.
3. 11 hrs

Mass Spectroscopy: Principle, Theory, Instrumentation of Mass Spectroscopy, Different types of ionization like electron impact, chemical, field, FAB and MALDI, APCI, ESI, APPI Analyzers

of Quadrupole and Time of Flight, Mass fragmentation and its rules, Meta stable ions, Isotopic peaks and Applications of Mass spectroscopy

4. 11hrs
Chromatography: Principle, apparatus, instrumentation, chromatographic parameters, factors affecting resolution and applications of the following: a) Paper chromatography b) Thin Layer chromatography c) Ion exchange chromatography d) Column chromatography e) Gas chromatography f) High Performance Liquid chromatography g) Affinity chromatography
5 11hrs

- a. Electrophoresis: Principle, Instrumentation, Working conditions, factors affecting separation and applications of the following:
- a) Paper electrophoresis b) Gel electrophoresis c) Capillary electrophoresis
 - d) Zone electrophoresis e) Moving boundary electrophoresis f) Iso electric focusing
- b. X ray Crystallography: Production of X rays, Different X ray diffraction methods, Bragg's law, Rotating crystal technique, Xray powder technique, Types of crystals and applications of Xray diffraction.
- c. Immunological assays: RIA (Radio immuno assay), ELISA, Bioluminescence assays. 5hrs

REFERENCES

1. Spectrometric Identification of Organic compounds - Robert M Silverstein, Sixth edition, John Wiley & Sons, 2004.
2. Principles of Instrumental Analysis - Douglas A Skoog, F. James Holler, Timothy A. Nieman, 5th edition, Eastern press, Bangalore, 1998.
3. Instrumental methods of analysis – Willards, 7th edition, CBS publishers.
4. Practical Pharmaceutical Chemistry – Beckett and Stenlake, Vol II, 4th edition, CBS Publishers, New Delhi, 1997.
5. Organic Spectroscopy - William Kemp, 3rd edition, ELBS, 1991.
6. Quantitative Analysis of Drugs in Pharmaceutical formulation - P D Sethi, 3rd Edition, CBS Publishers, New Delhi, 1997.
7. Pharmaceutical Analysis- Modern methods – Part B - J W Munson, Volume 11, Marcel Dekker Series

JAWAHARLAL NEHRU TECHNOLOGICAL UNIVERSITY ANANTAPUR

M. Pharm – I year I Sem. (Pharmaceutical Chemistry)

L T P C
4 0 0 4

(17S02101) ADVANCED ORGANIC CHEMISTRY - I

SCOPE

The subject is designed to provide in-depth knowledge about advances inorganic chemistry, different techniques of organic synthesis and their applications to process chemistry as well as drug discovery.

Objectives

Upon completion of course, the student shall be to understand

- The principles and applications of retrosynthesis
- The mechanism & applications of various named reactions
- The concept of disconnection to develop synthetic routes for small target molecule.
- The various catalysts used in organic reactions
- The chemistry of heterocyclic compounds

THEORY

60 Hrs

1.

12Hrs

Basic Aspects of Organic Chemistry:

1. Organic intermediates: Carbocations, carbanions, free radicals, carbenes and nitrenes. Their method of formation, stability and synthetic applications.
2. Types of reaction mechanisms and methods of determining them,
3. Detailed knowledge regarding the reactions, mechanisms and their relative reactivity and orientations.

Addition reactions

- a) Nucleophilic uni- and bimolecular reactions (SN1 and SN2)
- b) Elimination reactions (E1 & E2; Hoffman & Saytzeff's rule)
- c) Rearrangement reaction

2

12Hrs

Study of mechanism and synthetic applications of following named Reactions:

Ugi reaction, Brook rearrangement, Ullmann coupling reactions, Dieckmann Reaction, Doebner-Miller Reaction, Sandmeyer Reaction, Mitsunobu reaction, Mannich reaction, Vilsmeier-Haack Reaction, Sharpless asymmetric epoxidation, Baeyer-Villiger oxidation, Shapiro & Suzuki reaction, Ozonolysis and Michael addition reaction

3

12Hrs

Synthetic Reagents & Applications:

Aluminiumisopropoxide, N-bromosuccinamide, diazomethane, dicyclohexylcarbodiimide, Wilkinson reagent, Wittig reagent, Osmium tetroxide, titanium chloride, diazopropane, diethylazodicarboxylate, Triphenylphosphine, Benzotriazol-1-yloxy) tris(dimethylamino) phosphoniumhexafluoro-phosphate (BOP).

Protecting groups

- a. Role of protection in organic synthesis
- b. Protection for the hydroxyl group, including 1,2- and 1,3-diols: ethers, esters, carbonates, cyclic acetals & ketals
- c. Protection for the Carbonyl Group: Acetals and Ketals
- d. Protection for the Carboxyl Group: amides and hydrazides, esters
- e. Protection for the Amino Group and Amino acids: carbamates and amides

4

12Hrs

Heterocyclic Chemistry:

Organic Name reactions with their respective mechanism and application involved in synthesis of drugs containing five, six-membered and fused heterocyclics such as Debus-Radziszewski imidazole synthesis, Knorr Pyrazole Synthesis, Pinner Pyrimidine Synthesis, Combes Quinoline Synthesis, Bernthsen Acridine Synthesis, Smiles rearrangement and Traube purine synthesis.

Synthesis of few representative drugs containing these heterocyclic nucleus such as Ketoconazole, Metronidazole, Miconazole, celecoxib, antipyrin, Metamizole sodium, Terconazole, Alprazolam, Triamterene, Sulfamerazine, Trimethoprim, Hydroxychloroquine, Quinine, Chloroquine, Quinacrine, Amsacrine, Prochlorperazine, Promazine, Chlorpromazine, Theophylline, Mercaptopurine and Thioguanine.

5

12Hrs

Synthon approach and retrosynthesis applications

- i. Basic principles, terminologies and advantages of retrosynthesis; guidelines for dissection of molecules. Functional group interconversion and addition (FGI and FGA)
- ii. C-X disconnections; C-C disconnections – alcohols and carbonyl compounds; 1,2-, 1,3-, 1,4-, 1,5-, 1,6-difunctionalized compounds
- iii. Strategies for synthesis of three, four, five and six-membered ring.

REFERENCES

1. "Advanced Organic chemistry, Reaction, Mechanisms and Structure", JMarch, John Wiley and Sons, New York.
2. "Mechanism and Structure in Organic Chemistry", ES Gould, Hold Rinchartand Winston, New York.
3. "Organic Chemistry" Clayden, Greeves, Warren and Woihers.,OxfordUniversity Press 2001.
4. "Organic Chemistry" Vol I and II. I.L. Finar. ELBS, Pearson Education Lts,Dorling Kindersley 9India) Pvt. Ltd.,.
5. A guide to mechanisms in Organic Chemistry, Peter Skyes (OrientLongman, New Delhi).
6. Reactive Intermediates in Organic Chemistry, Tandom and Gowel, Oxford& IBH Publishers.
7. Combinational Chemistry – Synthesis and applications – Stephen RWilson& Anthony W Czarnik, Wiley – Blackwell.
8. Carey, Organic Chemistry, 5th Edition (Viva Books Pvt. Ltd.)
9. Organic Synthesis - The Disconnection Approach, S. Warren, Wily India
10. Principles of Organic Synthesis, ROC Norman and JM Coxan, NelsonThorns.
11. Organic Synthesis - Special Techniques. VK Ahluwalia and R Agarwal,Narosa Publishers.
12. Organic Reaction Mechanisms IVthEdtn, VK Ahluwalia and RK Parashar,Narosa Publishers.

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M. Pharm – I year I Sem. (Pharmaceutical Chemistry)

L T P C
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(17S02102) ADVANCED MEDICINAL CHEMISTRY

SCOPE

The subject is designed to impart knowledge about recent advances in the field of medicinal chemistry at the molecular level including different techniques for the rational drug design.

Objectives

At completion of this course it is expected that students will be able to understand

- Different stages of drug discovery
- Role of medicinal chemistry in drug research
- Different techniques for drug discovery
- Various strategies to design and develop new drug like molecules for biological targets
- Peptidomimetics

THEORY

60 Hrs

1.

12Hrs

Drug discovery: Stages of drug discovery, lead discovery; identification, validation and diversity of drug targets. Biological drug targets: Receptors, types, binding and activation, theories of drug receptor interaction, drug receptor interactions, agonists vs antagonists, artificial enzymes.

2

12Hrs

Prodrug Design and Analog design:

a) Prodrug design: Basic concept, Carrier linked prodrugs/Bioprecursors, Prodrugs of functional group, Prodrugstoimprove patient acceptability, Drug solubility, Drugabsorption and distribution, site specific drug deliveryand sustained drug action. Rationale of prodrugdesignand practical consideration of prodrug design.

b) Combating drug resistance: Causes for drugresistance, strategies to combat drug resistance inantibiotics and anticancer therapy, Genetic principles of drug resistance.

c) Analog Design: Introduction, Classical & Non classical,Bioisosteric replacement strategies, rigid analogs,alteration of chain branching, changes in ring size, ringposition isomers, design of stereo isomers andgeometric isomers, fragments of a lead molecule,variation in inter atomic distance.

3

12Hrs

Medicinal chemistry aspects of the following class of drugs Systematic study, SAR, Mechanism of action and synthesis of new generation molecules of following class of drugs:

a) Anti-hypertensive drugs, Psychoactive drugs, Anticonvulsant drugs, H₁ & H₂ receptor antagonist, COX1 & COX2 inhibitors, Adrenergic & Cholinergic agents, Antineoplastic and Antiviral agents.

b) Stereochemistry and Drug action: Realization that stereoselectivity is a pre-requisite for evolution. Role of chirality in selective and specific therapeutic agents. Case studies, Enantio selectivity in drug adsorption, metabolism, distribution and elimination.

4

12Hrs

Rational Design of Enzyme Inhibitors Enzyme kinetics & Principles of Enzyme inhibitors, Enzyme inhibitors in medicine, Enzyme inhibitors in basic research, rational design of non-covalently and covalently binding enzyme inhibitors.

5

12Hrs

Peptidomimetics Therapeutic values of Peptidomimetics, design of peptidomimetics by manipulation of the amino acids, modification of the peptide backbone, incorporating conformational constraints locally or globally. Chemistry of prostaglandins, leukotrienes and thromboxones.

REFERENCES

1. Medicinal Chemistry by Burger, Vol I –VI.
2. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, 12th Edition, Lippincott Williams & Wilkins, Wolters Kluwer (India) Pvt.Ltd, New Delhi.
3. Comprehensive Medicinal Chemistry – Corwin and Hansch.
4. Computational and structural approaches to drug design edited by Robert M Stroud and Janet. F Moore
5. Introduction to Quantitative Drug Design by Y.C. Martin.
6. Principles of Medicinal Chemistry by William Foye, 7th Edition, Lippincott Williams & Wilkins, Wolters Kluwer (India) Pvt.Ltd, New Delhi.
7. Drug Design Volumes by Arienes, Academic Press, Elsevier Publishers, Noida, Uttar Pradesh..
8. Principles of Drug Design by Smith.
9. The Organic Chemistry of the Drug Design and Drug action by Richard B. Silverman, II Edition, Elsevier Publishers, New Delhi.
10. An Introduction to Medicinal Chemistry, Graham L. Patrick, III Edition, Oxford University Press, USA.

11. Biopharmaceutics and pharmacokinetics, DM.Brahmankar, Sunil B.Jaiswal II Edition, 2014, VallabhPrakashan, New Delhi.

12. Peptidomimetics in Organic and Medicinal Chemistry by Antonio Guarnaand Andrea Trabocchi, First edition, Wiley publishers.

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M. Pharm – I year I Sem. (Pharmaceutical Chemistry)

L T P C
4 0 0 4

(17S02103) CHEMISTRY OF NATURAL PRODUCTS

SCOPE

The subject is designed to provide detail knowledge about chemistry of medicinal compounds from natural origin and general methods of structural elucidation of such compounds. It also emphasizes on isolation, purification and characterization of medicinal compounds from natural origin.

Objectives

At completion of this course it is expected that students will be able to understand-

- Different types of natural compounds and their chemistry and medicinal importance
- The importance of natural compounds as lead molecules for new drug discovery
- The concept of rDNA technology tool for new drug discovery
- General methods of structural elucidation of compounds of natural origin
- Isolation, purification and characterization of simple chemical constituents from natural source

THEORY

60 Hrs

1.

12Hrs

Study of Natural products as leads for new pharmaceuticals for the following class of drugs

- a) Drugs Affecting the Central Nervous System: Morphine Alkaloids
- b) Anticancer Drugs: Paclitaxel and Docetaxel, Etoposide, and Teniposide
- c) Cardiovascular Drugs: Lovastatin, Teprotide and Dicoumarol
- d) Neuromuscular Blocking Drugs: Curare alkaloids
- e) Anti-malarial drugs and Analogues
- f) Chemistry of macrolid antibiotics (Erythromycin, Azithromycin, Roxithromycin, and Clarithromycin) and β - Lactam antibiotics (Cephalosporins and Carbapenem)

2

12Hrs

a) Alkaloids

General introduction, classification, isolation, purification, molecular modification and biological activity of alkaloids, general methods of structural determination of alkaloids, structural elucidation and stereochemistry of ephedrine, morphine, ergot, emetine and reserpine.

b) Flavonoids

Introduction, isolation and purification of flavonoids, General methods of structural determination of flavonoids; Structural elucidation of quercetin.

c) Steroids

General introduction, chemistry of sterols, sapogenin and cardiac glycosides. Stereochemistry and nomenclature of steroids, chemistry of contraceptive agents male & female sex hormones (Testosterone, Estradiol, Progesterone), adrenocorticoids (Cortisone), contraceptive agents and steroids (Vit – D).

3

12Hrs

a) Terpenoids

Classification, isolation, isoprene rule and general methods of structural elucidation of Terpenoids; Structural elucidation of drugs belonging to mono (citral, menthol, camphor), di (retinol, Phytol, taxol) and tri terpenoids (Squalene, Ginsenoside) carotenoids (β carotene).

b) Vitamins

Chemistry and Physiological significance of Vitamin A, B1, B2, B12, C, E, Folic acid and Niacin.

4

12Hrs

a). Recombinant DNA technology and drug discovery rDNA technology, hybridoma technology, New pharmaceuticals derived from biotechnology; Oligonucleotide therapy. Gene therapy: Introduction, Clinical application and recent advances in gene therapy, principles of RNA & DNA estimation

b). Active constituent of certain crude drugs used in Indigenous system Diabetic therapy – *Gymnema sylvestre*, *Salacia reticulata*, *Pterocarpus marsupium*, *Swertia chirata*, *Trigonella foenum-graecum*; Liver dysfunction – *Phyllanthus niruri*; Antitumor – *Curcuma longa* Linn.

5

12Hrs

Structural Characterization of natural compounds Structural characterization of natural compounds using IR, ¹H NMR, ¹³C NMR and MS Spectroscopy of specific drugs e.g., Penicillin, Morphine, Camphor, Vit-D, Quercetin and Digitalis glycosides.

REFERENCES

1. Modern Methods of Plant Analysis, Peech and M.V. Tracey, Springer – Verlag, Berlin, Heidelberg.
2. Phytochemistry Vol. I and II by Miller, Jan Nostrand Rein Hld.
3. Recent advances in Phytochemistry Vol. I to IV – Scikel Runeckles, Springer Science & Business Media.

4. Chemistry of natural products Vol I onwards IWPAC.
5. Natural Product Chemistry Nakanishi Gggolo, University Science Books, California.
6. Natural Product Chemistry "A laboratory guide" – Rapheal Khan.
7. The Alkaloid Chemistry and Physiology by RHF Manske, Academic Press.
8. Introduction to molecular Phytochemistry – CHJ Wells, Chapmanstall.
9. Organic Chemistry of Natural Products Vol I and II by GurdeepandChatwall, Himalaya Publishing House.
10. Organic Chemistry of Natural Products Vol I and II by O.P. Agarwal, KrishanPrakashan.
11. Organic Chemistry Vol I and II by I.L. Finar, Pearson education.
12. Elements of Biotechnology by P.K. Gupta, Rastogi Publishers.
13. Pharmaceutical Biotechnology by S.P.Vyas and V.K.Dixit, CBS Publishers.
14. Biotechnology by Purohit and Mathur, Agro-Bios, 13th edition.
15. Phytochemical methods of Harborne, Springer, Netherlands.
16. Burger's Medicinal Chemistry.

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M. Pharm – I year I Sem. (Pharmaceutical Chemistry)

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0	0	6	3

(17S02104) PHARMACEUTICAL ANALYSIS PRACTICAL FOR PHARMACEUTICAL CHEMISTRY

1. Analysis of Pharmacopoeial compounds and their formulations by UV Visspectrophotometer, RNA & DNA estimation
2. Simultaneous estimation of multi component containing formulations by UVspectrophotometry
3. Experiments based on Column chromatography
4. Experiments based on HPLC
5. Experiments based on Gas Chromatography
6. Estimation of riboflavin/quinine sulphate by fluorimetry
7. Estimation of sodium/potassium by flame photometry

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M. Pharm – I year I Sem. (Pharmaceutical Chemistry)

L	T	P	C
0	0	6	3

(17S02105) PHARMACEUTICAL CHEMISTRY PRACTICAL - I

To perform the following reactions of synthetic importance

1. Purification of organic solvents, column chromatography
2. Claisen-schimidt reaction.
3. Benzyllic acid rearrangement.
4. Beckmann rearrangement.
5. Hoffmann rearrangement
6. Mannich reaction
7. Synthesis of medicinally important compounds involving more than one step along with purification and Characterization using TLC, melting point and IR spectroscopy (4 experiments)
8. Estimation of elements and functional groups in organic natural compounds
9. Isolation, characterization like melting point, mixed melting point, molecular weight determination, functional group analysis, co-chromatographic technique for identification of isolated compounds and interpretation of UV and IR data.
10. Some typical degradation reactions to be carried on selected plant constituents
11. Oxidation and free radical coupling
12. Fries rearrangement
13. Perkins reaction

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M. Pharm – I year II Sem. (Pharmaceutical Chemistry)

L T P C
4 0 0 4

(17S02201) ADVANCED SPECTRAL ANALYSIS

Scope

This subject deals with various hyphenated analytical instrumental techniques for identification, characterization and quantification of drugs. Instruments dealt are LC-MS, GC-MS, ATR-IR, DSC etc.

Objectives

At completion of this course it is expected that students will be able to understand-

- Interpretation of the NMR, Mass and IR spectra of various organic compounds
- Theoretical and practical skills of the hyphenated instruments
- Identification of organic compounds

THEORY

60Hrs

1.

12Hrs

UV and IR spectroscopy:

Wood ward – Fieser rule for 1,3- butadienes, cyclic dienes and α,β -carbonyl compounds and interpretation compounds of enones. ATR-IR, IR Interpretation of organic compounds.

2

12Hrs

NMR spectroscopy: 1-D and 2-D NMR, NOESY and COSY, HECTOR, INADEQUATE techniques, Interpretation of organic compounds.

3

12Hrs

Mass Spectroscopy

Mass fragmentation and its rules, Fragmentation of important functional groups like alcohols, amines, carbonyl groups and alkanes, Meta stable ions, Mc Lafferty rearrangement, Ring rule, Isotopic peaks, Interpretation of organic compounds.

4

12Hrs

Chromatography:

Principle, Instrumentation and Applications of the following :

a) GC-MS b) GC-AAS c) LC-MS d) LC-FTIR e) LC-NMR f) CEMSg) High Performance Thin Layer chromatography h) Supercritical fluid chromatography i) Ion Chromatography j) I-EC (Ion-Exclusion Chromatography) k) Flash chromatography

5

12Hrs

a). Thermal methods of analysis Introduction, principle, instrumentation and application of DSC, DTA and TGA.

b). Raman Spectroscopy Introduction, Principle, Instrumentation and Applications.

c). Radio immunoassay Biological standardization , bioassay, ELISA, Radioimmunoassay of digitalis and insulin.

REFERENCES

1. Spectrometric Identification of Organic compounds - Robert M Silverstein, Sixth edition, John Wiley & Sons, 2004.

2. Principles of Instrumental Analysis - Douglas A Skoog, F. James Holler, Timothy A. Nieman, 5th edition, Eastern press, Bangalore, 1998.

3. Instrumental methods of analysis – Willards, 7th edition, CBS publishers.

4. Organic Spectroscopy - William Kemp, 3rd edition, ELBS, 1991.

5. Quantitative analysis of Pharmaceutical formulations by HPTLC - P D Sethi, CBS Publishers, New Delhi.

6. Quantitative Analysis of Drugs in Pharmaceutical formulation - P D Sethi, 3rd Edition, CBS Publishers, New Delhi, 1997.

7. Pharmaceutical Analysis- Modern methods – Part B - J W Munson, Volume 11, Marcel Dekker Series

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M. Pharm – I year II Sem. (Pharmaceutical Chemistry)

L T P C
4 0 0 4

(17S02202) ADVANCED ORGANIC CHEMISTRY - II

Scope

The subject is designed to provide in-depth knowledge about advances inorganic chemistry, different techniques of organic synthesis and their applications to process chemistry as well as drug discovery.

Objectives

Upon completion of course, the student shall able to understand

- The principles and applications of Green chemistry
- The concept of peptide chemistry.
- The various catalysts used in organic reactions
- The concept of stereochemistry and asymmetric synthesis.

THEORY

60 Hrs

1.

12Hrs

Green Chemistry:

a. Introduction, principles of green chemistry

b. Microwave assisted reactions: Merit and demerits of its use, increased reaction rates, mechanism, superheating effects of microwave, effects of solvents in microwave assisted synthesis, microwave technology in process optimization, its applications in various organic reactions and heterocyclic synthesis

c. Ultrasound assisted reactions: Types of sonochemical reactions, homogenous, heterogeneous liquid-liquid and liquid-solid reactions, synthetic applications

d. Continuous flow reactors: Working principle, advantages and synthetic applications.

2

12Hrs

Chemistry of peptides

a. Coupling reactions in peptide synthesis

b. Principles of solid phase peptide synthesis, t-BOC and FMOC protocols, various solid supports and linkers: Activation procedures, peptide bond formation, deprotection and cleavage from resin, low and high

HF cleavage protocols, formation of free peptides and peptide amides, purification and case studies, site-specific chemical modifications of peptides

c. Segment and sequential strategies for solution phase peptide synthesis with any two case studies

d. Side reactions in peptide synthesis: Deletion peptides, side reactions initiated by proton abstraction, protonation, overactivation and side reactions of individual amino acids.

3

12Hrs

Photochemical Reactions

Basic principles of photochemical reactions. Photo-oxidation, photo-addition and photo-fragmentation. Pericyclic reactions Mechanism, Types of pericyclic reactions such as cycloaddition, electrocyclic reaction and sigmatropic rearrangement reactions with examples

4

12Hrs

Catalysis:

a. Types of catalysis, heterogeneous and homogeneous catalysis, advantages and disadvantages

b. Heterogeneous catalysis – preparation, characterization, kinetics, supported catalysts, catalyst deactivation and regeneration, some examples of heterogeneous catalysis used in synthesis of drugs.

c. Homogeneous catalysis, hydrogenation, hydroformylation, hydrocyanation, Wilkinson catalysts, chiral ligands and chiral induction, Ziegler-Natta catalysts, some examples of homogeneous catalysis used in synthesis of drugs

d. Transition-metal and Organo-catalysis in organic synthesis: Metal-catalyzed reactions

e. Biocatalysis: Use of enzymes in organic synthesis, immobilized enzymes/cells in organic reaction.

f. Phase transfer catalysis - theory and applications

5

12Hrs

Stereochemistry & Asymmetric Synthesis

a. Basic concepts in stereochemistry – optical activity, specific rotation, racemates and resolution of racemates, the Cahn, Ingold, Prelog (CIP) sequence rule, meso compounds, pseudoasymmetric centres, axes of symmetry, Fischer's D and L notation, cis-trans isomerism, E and Z notation.

b. Methods of asymmetric synthesis using chiral pool, chiral auxiliaries and catalytic asymmetric synthesis, enantiopure separation and Stereo selective synthesis with examples.

REFERENCES

1. "Advanced Organic chemistry, Reaction, mechanisms and structure", JMarch, John Wiley and sons, New York.
2. "Mechanism and structure in organic chemistry", ES Gould, Hold RinchartandWinston,NewYork.
3. "Organic Chemistry" Clayden, Greeves, Warren and Woihers.,OxfordUniversity Press 2001.
4. "Organic Chemistry" Vol I and II. I.L. Finar. ELBS, Sixth ed., 1995.
5. Carey, Organic chemistry, 5th edition (Viva Books Pvt. Ltd.)
6. Organic synthesis-the disconnection approach, S. Warren, Wily India
7. Principles of organic synthesis, ROCNorman and JMCoxan, Nelson thorns
8. Organic synthesis- Special techniques VK Ahluwalia and R Aggarwal,Narosa Publishers.
9. Organic reaction mechanisms IV edtn, VK Ahluwalia and RK Parashar,Narosa Publishers.

JAWAHARLAL NEHRU TECHNOLOGICAL UNIVERSITY ANANTAPUR

M. Pharm – I year II Sem. (Pharmaceutical Chemistry)

L	T	P	C
4	0	0	4

(17S02203) COMPUTER AIDED DRUG DESIGN

Scope

The subject is designed to impart knowledge on the current state of the art techniques involved in computer assisted drug design.

Objectives

At completion of this course it is expected that students will be able to understand

- Role of CADD in drug discovery
- Different CADD techniques and their applications
- Various strategies to design and develop new drug like molecules.
- Working with molecular modeling softwares to design new drug molecules
- The in silico virtual screening protocols

Theory

60 Hrs

1.

12Hrs

Introduction to Computer Aided Drug Design (CADD) History, different techniques and applications. Quantitative Structure Activity Relationships: Basics History and development of QSAR: Physicochemical parameters and methods to calculate physicochemical parameters: Hammett equation and electronic parameters (σ), lipophilicity effects and parameters ($\log P$, π -substituent constant), steric effects (Taft steric and MR parameters) Experimental and theoretical approaches for the determination of these physicochemical parameters.

2

12Hrs

Quantitative Structure Activity Relationships: Applications Hansch analysis, Free Wilson analysis and relationship between them, Advantages and disadvantages; Deriving 2D-QSAR equations. 3D-QSAR approaches and contour map analysis. Statistical methods used in QSAR analysis and importance of statistical parameters.

3

12Hrs

Molecular Modeling and Docking

a) Molecular and Quantum Mechanics in drug design.

b) Energy Minimization Methods: comparison between global minimum conformation and bioactive conformation

c) Molecular docking and drug receptor interactions: Rigid docking, flexible docking and extra-precision docking. Agents acting on enzymes such as DHFR, HMG-CoA reductase and HIV protease, choline esterase (AChE & BChE)

4

12Hrs

Molecular Properties and Drug Design

a) Prediction and analysis of ADMET properties of new molecules and its importance in drug design.

b) De novo drug design: Receptor/enzyme-interaction and its analysis, Receptor/enzyme cavity size prediction, predicting the functional components of cavities, Fragment based drug design.

c) Homology modeling and generation of 3D-structure of protein.

5

12Hrs

Pharmacophore Mapping and Virtual Screening Concept of pharmacophore, pharmacophore mapping, identification of Pharmacophore features and Pharmacophore modeling; Conformational search used in pharmacophore mapping. In Silico Drug Design and Virtual Screening Techniques Similarity based methods and Pharmacophore based screening, structure based In-silico virtual screening protocols.

REFERENCES

1. Computational and structural approaches to drug discovery, Robert M Stroud and Janet. F Moore, RCS Publishers.
2. Introduction to Quantitative Drug Design by Y.C. Martin, CRC Press, Taylor & Francis group..
3. Drug Design by Ariens Volume 1 to 10, Academic Press, 1975, Elsevier Publishers.
4. Principles of Drug Design by Smith and Williams, CRC Press, Taylor & Francis.
5. The Organic Chemistry of the Drug Design and Drug action by Richard B. Silverman, Elsevier Publishers.
6. Medicinal Chemistry by Burger, Wiley Publishing Co.
7. An Introduction to Medicinal Chemistry – Graham L. Patrick, Oxford University Press.
8. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, Ippincott Williams & Wilkins.
9. Comprehensive Medicinal Chemistry – Corwin and Hansch, Pergamon Publishers.

10. Computational and structural approaches to drug design edited by RobertM Stroud and Janet. F Moore

JAWAHARLAL NEHRU TECHNOLOGICAL UNIVERSITY ANANTAPUR

M. Pharm – I year II Sem. (Pharmaceutical Chemistry)

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(17S02204) PHARMACEUTICAL PROCESS CHEMISTRY

Scope

Process chemistry is often described as scale up reactions, taking them from small quantities created in the research lab to the larger quantities that are needed for further testing and then to even larger quantities required for commercial production. The goal of a process chemist is to develop synthetic routes that are safe, cost-effective, environmentally friendly, and efficient. This subject is designed to impart knowledge on the development and optimization of a synthetic route/s and the pilot plant procedure for the manufacture of Active Pharmaceutical Ingredients (APIs) and new chemical entities (NCEs) for the drug development phase.

Objectives

At completion of this course it is expected that students will be able to understand

- The strategies of scale up process of APIs and intermediates
- The various unit operations and various reactions in process chemistry

THEORY

60 Hrs

1.

12Hrs

Process chemistry

Introduction, Synthetic strategy Stages of scale up process: Bench, pilot and large scale process.

In-process control and validation of large scale process. Case studies of some scale up process of APIs. Impurities in API, types and their sources including genotoxic impurities

2

12Hrs

Unit operations

a) Extraction: Liquid equilibria, extraction with reflux, extraction with agitation, counter current extraction.

b) Filtration: Theory of filtration, pressure and vacuum filtration, centrifugal filtration,

c) Distillation: azeotropic and steam distillation

d) Evaporation: Types of evaporators, factors affecting evaporation.

e) Crystallization: Crystallization from aqueous, nonaqueous solutions factors affecting crystallization, nucleation. Principle and general methods of Preparation of polymorphs, hydrates, solvates and amorphous APIs.

3

12Hrs

Unit Processes - I

a) Nitration: Nitrating agents, Aromatic nitration, kinetics and mechanism of aromatic nitration, process equipment for technical nitration, mixed acid for nitration,

b) Halogenation: Kinetics of halogenations, types of halogenations, catalytic halogenations. Case study on industrial halogenation process.

c) Oxidation: Introduction, types of oxidative reactions, Liquid phase oxidation with oxidizing agents. Nonmetallic Oxidizing agents such as H₂O₂, sodium hypochlorite, Oxygen gas, ozonolysis.

4

12Hrs

Unit Processes - II

a) Reduction: Catalytic hydrogenation, Heterogeneous and homogeneous catalyst; Hydrogen transfer reactions, Metal hydrides. Case study on industrial reduction process.

b) Fermentation: Aerobic and anaerobic fermentation. Production of

i. Antibiotics; Penicillin and Streptomycin,

ii. Vitamins: B₂ and B₁₂

iii. Statins: Lovastatin, Simvastatin

c) Reaction progress kinetic analysis

i. Streamlining reaction steps, route selection,

ii. Characteristics of expedient routes, characteristics of cost-effective routes, reagent selection, families of reagents useful for scale-up.

5

12Hrs

Industrial Safety

a) MSDS (Material Safety Data Sheet), hazard labels of chemicals and Personal Protection Equipment (PPE)

b) Fire hazards, types of fire & fire extinguishers

c) Occupational Health & Safety Assessment Series 1800 (OHSAS-1800) and ISO-14001 (Environmental Management System), Effluents and its management

REFERENCES

1. Process Chemistry in the Pharmaceutical Industry: Challenges in an Ever-Changing Climate-An Overview; K. Gadamasetti, CRC Press.
2. Pharmaceutical Manufacturing Encyclopedia, 3rd edition, Volume 2.
3. Medicinal Chemistry by Burger, 6th edition, Volume 1-8.
4. W.L. McCabe, J.C Smith, Peter Harriott. Unit operations of chemicalengineering, 7th edition, McGraw Hill
5. Polymorphism in Pharmaceutical Solids .Dekker Series Volume 95 Ed: HG Brittain (1999)
6. Regina M. Murphy: Introduction to Chemical Processes: Principles,Analysis, Synthesis
7. Peter J. Harrington: Pharmaceutical Process Chemistry for Synthesis:Rethinking the Routes to Scale-Up
8. P.H.Groggins: Unit processes in organic synthesis (MGH)
9. F.A.Henglein: Chemical Technology (Pergamon)
10. M.Gopal: Dryden's Outlines of Chemical Technology, WEP East-WestPress
11. Clausen,Mattson: Principle of Industrial Chemistry, Wiley Publishing Co.,
12. Lowenheim& M.K. Moran: Industrial Chemicals
13. S.D. Shukla & G.N. Pandey: A text book of Chemical Technology Vol. II,Vikas Publishing House
14. J.K. Stille: Industrial Organic Chemistry (PH)
15. Shreve: Chemical Process, Mc Grawhill.
16. B.K.Sharma: Industrial Chemistry, Goel Publishing House
17. ICH Guidelines
18. United States Food and Drug Administration official website www.fda.gov

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M. Pharm – I year II Sem. (Pharmaceutical Chemistry)

L	T	P	C
0	0	6	3

(17S02205) PHARMACEUTICAL CHEMISTRY PRACTICALS – II

1. Synthesis of organic compounds by adapting different approaches involving (3 experiments)
 - a) Oxidation
 - b) Reduction/hydrogenation
 - c) Nitration
2. Comparative study of synthesis of APIs/intermediates by different synthetic routes (2 experiments)
3. Assignments on regulatory requirements in API (2 experiments)
4. Comparison of absorption spectra by UV and Wood ward – Fieser rule
5. Interpretation of organic compounds by FT-IR
6. Interpretation of organic compounds by NMR
7. Interpretation of organic compounds by MS
8. Determination of purity by DSC in pharmaceuticals
9. Identification of organic compounds using FT-IR, NMR, CNMR and Mass spectra
10. To carry out the preparation of following organic compounds

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M. Pharm – I year II Sem. (Pharmaceutical Chemistry)

L	T	P	C
0	0	6	3

(17S02206) PHARMACEUTICAL CHEMISTRY PRACTICALS – III

1. Preparation of 4-chlorobenzhydrylpiperazine. (an intermediate for cetirizineHCl).
2. Preparation of 4-iodotoluene from p-toluidine.
3. NaBH₄ reduction of vanillin to vanillyl alcohol
4. Preparation of umbelliferone by Pechhman reaction
5. Preparation of triphenyl imidazole
6. To perform the Microwave irradiated reactions of synthetic importance(Any two)
7. Determination of log P, MR, hydrogen bond donors and acceptors of selected drugs using softwares
8. Calculation of ADMET properties of drug molecules and its analysis using softwares
Pharmacophore modeling
9. 2D-QSAR based experiments
10. 3D-QSAR based experiments
11. Docking study based experiment
12. Virtual screening based experiment
13. Synthesis purification and identification of the following compounds employing some medicinal compounds.

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M. Pharm – III Sem. (Pharmaceutical Chemistry)

L	T	P	C
4	0	0	4

(17S01301) RESEARCH METHODOLOGY & BIostatISTICS

UNIT – I

General Research Methodology: Research, objective, requirements, practical difficulties, review of literature, study design, types of studies, strategies to eliminate errors/bias, controls, randomization, crossover design, placebo, blinding techniques.

UNIT – II

Biostatistics: Definition, application, sample size, importance of sample size, factors influencing sample size, dropouts, statistical tests of significance, types of significance tests, parametric tests (students “t” test, ANOVA, Correlation coefficient, regression), non-parametric tests (wilcoxon rank tests, analysis of variance, correlation, chi square test), null hypothesis, P values, degree of freedom, interpretation of P values.

UNIT – III

Medical Research: History, values in medical ethics, autonomy, beneficence, non-maleficence, double effect, conflicts between autonomy and beneficence/non-maleficence, euthanasia, informed consent, confidentiality, criticisms of orthodox medical ethics, importance of communication, control resolution, guidelines, ethics committees, cultural concerns, truth telling, online business practices, conflicts of interest, referral, vendor relationships, treatment of family members, sexual relationships, fatality.

UNIT – IV

CPCSEA guidelines for laboratory animal facility: Goals, veterinary care, quarantine, surveillance, diagnosis, treatment and control of disease, personal hygiene, location of animal facilities to laboratories, anesthesia, euthanasia, physical facilities, environment, animal husbandry, record keeping, SOPs, personnel and training, transport of lab animals.

UNIT – V

Declaration of Helsinki: History, introduction, basic principles for all medical research, and additional principles for medical research combined with medical care.