**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 | CourseCode | 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 foridentification, characterization and quantification of drugs. Instruments dealt areNMR, Mass spectrometer, IR, HPLC, GC etc.

Objectives

After completion of course student is able to know about chemicals andexcipients

* 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 vibrationalfrequencies and Applications of IR spectroscopy

c. Spectroflourimetry: Theory of Fluorescence, Factorsaffecting fluorescence, Quenchers,

Instrumentation andApplications of fluorescence spectrophotometer.

d. Flame emission spectroscopy and Atomic absorptionspectroscopy: Principle,

Instrumentation, Interferences andApplications.

1. 11hrs

 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-Spincoupling, Coupling constant, Nuclear magnetic double resonance,Brief outline of principles of FT-NMR and 13C NMR. Applicationsof NMR spectroscopy.

1. 11hrs

Mass Spectroscopy: Principle, Theory, Instrumentation of MassSpectroscopy, Different types of ionization like electron impact,chemical, field, FAB and MALDI, APCI, ESI, APPI Analyzers ofQuadrupole and Time of Flight, Mass fragmentation and its rules,Meta stable ions, Isotopic peaks and Applications of Mass spectroscopy

1. 11hrs

Chromatography: Principle, apparatus, instrumentation, chromatographic parameters, factors affecting resolution and applications of the following: a)Paper chromatography b) Thin Layer chromatographyc) Ion exchange chromatography d) Column chromatographye) Gas chromatography f) High Performance Liquidchromatographyg) 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 raydiffraction 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 - Doglas 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, 4thedition, 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, 3rdEdition, CBS Publishers, New Delhi, 1997.
7. Pharmaceutical Analysis- Modern methods – Part B - J W Munson, Volume11, 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 theirapplications to process chemistry as well as drug discovery.

Objectives

Upon completion of course, the student shall be to understand

* The principles and applications of reterosynthesis
* 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, freeradicals, carbenes and nitrenes. Their method offormation, stability and synthetic applications.

2. Types of reaction mechanisms and methods ofdetermining them,

3. Detailed knowledge regarding the reactions,mechanisms and their relative reactivity and orientations.

Addition reactions

a) Nucleophilic uni- and bimolecular reactions (SN1 andSN2)

b) Elimination reactions (E1 & E2; Hoffman &Saytzeff’srule)

c) Rearrangement reaction

2 12Hrs

Study of mechanism and synthetic applications of followingnamed Reactions:

Ugi reaction, Brook rearrangement, Ullmann coupling reactions,Dieckmann Reaction, Doebner-Miller Reaction, SandmeyerReaction, Mitsunobu reaction, Mannich reaction, Vilsmeyer-HaackReaction, Sharpless asymmetric epoxidation, Baeyer-Villigeroxidation, Shapiro & Suzuki reaction, Ozonolysis and Michaeladdition reaction

3 12Hrs

Synthetic Reagents & Applications:

Aluminiumisopropoxide, N-bromosuccinamide, diazomethane,dicyclohexylcarbodimide, Wilkinson reagent, Witting 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-and1,3-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: carbamatesand amides

4 12Hrs

Heterocyclic Chemistry:

Organic Name reactions with their respective mechanism andapplication involved in synthesis of drugs containing five, sixmembered and fused hetrocyclics such as Debus-Radziszewskiimidazole synthesis, Knorr Pyrazole Synthesis Pinner PyrimidineSynthesis, CombesQuinoline Synthesis, BernthsenAcridineSynthesis, Smiles rearrangement and Traube purine synthesis.

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

5 12Hrs

Synthon approach and retrosynthesis applications

i. Basic principles, terminologies and advantages ofretrosynthesis; guidelines for dissection of molecules.Functional group interconvertion and addition (FGI and FGA)

ii. C‐X disconnections; C‐C disconnections – alcohols andcarbonyl compounds; 1,2‐, 1,3‐,1,4‐, 1,5‐, 1,6‐difunctionalizedcompounds

iii. Strategies for synthesis of three, four, five and six‐memberedring.

**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.

**JAWAHARLAL NEHRU TECHNOLOGICAL UNIVERSITY ANANTAPUR**

**M. Pharm – I year I Sem. (Pharmaceutical Chemistry) L T P C**

 **4 0 0 4**

**(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 receptorinteractions, 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 drugsSystematic study, SAR, Mechanism of action and synthesis ofnew generation molecules of following class of drugs:

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

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

4 12Hrs

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

5 12Hrs

PeptidomimeticsTherapeutic values of Peptidomimetics, design ofpeptidomimetics by manipulation of the amino acids, modificationof the peptide backbone, incorporating conformational constraintslocally or globally. Chemistry of prostaglandins, leukotrienesandthromboxones.

**REFERENCES**

1. Medicinal Chemistry by Burger, Vol I –VI.

2. Wilson and Gisvold’s Text book of Organic Medicinal and PharmaceuticalChemistry, 12th Edition, Lppincott Williams & Wilkins, WoltessKluwer(India) Pvt.Ltd, New Delhi.

3. Comprehensive Medicinal Chemistry – Corwin and Hansch.

4. Computational and structural approaches to drug design edited by RobertM 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, IppincottWilliams& Wilkins, Woltess 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 RichardB.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 ofmedicinal compounds from natural origin and general methods of structuralelucidation of such compounds. It also emphasizes on isolation, purification andcharacterization of medicinal compounds from natural origin.

Objectives

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

* 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 pharmaceuticalsfor the following class of drugs

a) Drugs Affecting the Central Nervous System: MorphineAlkaloids

b) Anticancer Drugs: Paclitaxel and Docetaxel, Etoposide, andTeniposide

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, generalmethods of structural determination of alkaloids, structuralelucidation and stereochemistry of ephedrine, morphine, ergot,emetine and reserpine.

b) Flavonoids

Introduction, isolation and purification of flavonoids, Generalmethods of structural determination of flavonoids; Structuralelucidation of quercetin.

c) Steroids

General introduction, chemistry of sterols, sapogenin and cardiacglycosides. 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 ofstructural elucidation of Terpenoids; Structural elucidation ofdrugs belonging to mono (citral, menthol, camphor), di(retinol,Phytol, taxol) and tri terpenoids (Squalene,Ginsenoside)carotinoids (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 discoveryrDNA technology, hybridoma technology, New pharmaceuticalsderived from biotechnology; Oligonucleotide therapy. Genetherapy: Introduction, Clinical application and recent advances ingene therapy, principles of RNA & DNA estimation

b). Active constituent of certain crude drugs used inIndigenous system Diabetic therapy – Gymnemasylvestre,Salacia reticulate, Pterocarpusmarsupiam, Swertiachirata,Trigonellafoenumgraccum; Liver dysfunction – Phyllanthusniruri;Antitumor – Curcuma longa Linn.

5 12Hrs

Structural Characterization of natural compoundsStructural characterization of natural compounds using IR,1HNMR, 13CNMR and MS Spectroscopy of specific drugs e.g.,Penicillin, Morphine, Camphor, Vit-D, Quercetin and Digitalisglycosides.

**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 Nostrant Rein Hld.

3. Recent advances in Phytochemistry Vol. I to IV – ScikelRuneckles,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, Chapmannstall.

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) L T P C**

 **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 techniquesfor identification, characterization and quantification of drugs. Instruments dealtare LC-MS, GC-MS, ATR-IR, DSC etc.

Objectives

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

* 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 importantfunctional groups like alcohols, amines, carbonyl groups andalkanes, 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). Thermalmethods of analysisIntroduction, principle, instrumentation and application of DSC,DTA and TGA.

b). Raman SpectroscopyIntroduction, Principle, Instrumentation and Applications.

c). Radio immunoassayBiologicalstandardization , 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 - Doglas 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 DSethi, 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 theirapplications 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 ofmicrowave, effects of solvents in microwave assistedsynthesis, microwave technology in process optimization, itsapplications in various organic reactions and heterocyclessynthesis

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

d. Continuous flow reactors: Working principle, advantages andsynthetic applications.

2 12Hrs

Chemistry of peptides

a. Coupling reactions in peptide synthesis

b. Principles of solid phase peptide synthesis, t-BOC and FMOCprotocols, various solid supports and linkers: Activationprocedures, peptide bond formation, deprotectionandcleavage from resin, low and high HF cleavage protocols,formation of free peptides and peptide amides, purification andcase studies, site-specific chemical modifications of peptides

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

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

3 12Hrs

Photochemical Reactions

Basic principles of photochemical reactions. Photo-oxidation,photo-addition and photo-fragmentation.PericyclicreactionsMechanism, Types of pericyclic reactions such as cycloaddition,electrocyclic reaction and sigmatrophic rearrangement reactionswith examples

4 12Hrs

Catalysis:

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

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

c. Homogenous catalysis, hydrogenation, hydroformylation,hydrocyanation, Wilkinson catalysts, chiral ligands and chiralinduction, Ziegler‐Natta catalysts, some examples ofhomogenous 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, specificrotation, racemates and resolution of racemates, the Cahn,Ingold, Prelog (CIP) sequence rule, meso compounds, pseudoasymmetric centres, axes of symmetry, Fischers D and Lnotation, cis-trans isomerism, E and Z notation.

b. Methods of asymmetric synthesis using chiral pool, chiralauxiliaries and catalytic asymmetric synthesis, enantiopureseparation 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.

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**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 arttechniques involved in computer assisted drug design.

Objectives

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

* 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: BasicsHistory and development of QSAR: Physicochemical parametersand methods to calculate physicochemical parameters: Hammettequation and electronic parameters (sigma), lipophilicityeffectsand parameters (log P, pi-substituent constant), steric effects(Taft steric and MR parameters) Experimental and theoreticalapproaches for the determination of these physicochemicalparameters.

2 12Hrs

Quantitative Structure Activity Relationships: ApplicationsHansch analysis, Free Wilson analysis and relationship betweenthem, Advantages and disadvantages; Deriving 2D-QSARequations.3D-QSAR approaches and contour map analysis.Statistical methods used in QSAR analysis and importance ofstatistical parameters.

3 12Hrs

Molecular Modeling and Docking

a) Molecular and Quantum Mechanics in drug design.

b) Energy Minimization Methods: comparison between globalminimum conformation and bioactive conformation

c) Molecular docking and drug receptor interactions: Rigiddocking, flexible docking and extra-precision docking.Agents acting on enzymes such as DHFR, HMG-CoAreductase and HIV protease, choline esterase ( AchE&BchE)

4 12Hrs

Molecular Properties and Drug Design

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

b) De novo drug design: Receptor/enzyme-interaction and itsanalysis, Receptor/enzyme cavity size prediction, predictingthe functional components of cavities, Fragment based drugdesign.

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

5 12Hrs

Pharmacophore Mapping and Virtual ScreeningConcept of pharmacophore, pharmacophoremapping,identification of Pharmacophore features and Pharmacophoremodeling; Conformational search used in pharmacophoremapping.InSilico Drug Design and Virtual Screening TechniquesSimilarity based methods and Pharmacophore based screening,structure based In-silico virtual screening protocols.

**REFERENCES**

1. Computational and structural approaches to drug discovery, Robert MStroud 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, ElsevierPublishers.

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, OxfordUniversity Press.

8. Wilson and Gisvold’s Text book of Organic Medicinal and PharmaceuticalChemistry, Ippincott Williams & Wilkins.

9. Comprehensive Medicinal Chemistry – Corwin and Hansch, PergamonPublishers.

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) L T P C**

 **4 0 0 4**

**(17S02204) PHARMACEUTICAL PROCESS CHEMISTRY**

Scope

Process chemistry is often described as scale up reactions, taking them fromsmall quantities created in the research lab to the larger quantities that areneeded for further testing and then to even larger quantities required forcommercial production. The goal of a process chemist is to develop syntheticroutes that are safe, cost-effective, environmentally friendly, and efficient. Thesubject is designed to impart knowledge on the development and optimization ofa synthetic route/s and the pilot plant procedure for the manufacture of ActivePharmaceutical Ingredients (APIs) and new chemical entities (NCEs) for thedrug development phase.

Objectives

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

* 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 strategyStages 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 genotoxicimpurities

2 12Hrs

Unit operations

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

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

c) Distillation: azeotropic and steam distillation

d) Evaporation: Types of evaporators, factors affectingevaporation.

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

3 12Hrs

Unit Processes - I

a) Nitration: Nitrating agents, Aromatic nitration, kineticsand mechanism of aromatic nitration, process equipmentfor technical nitration, mixed acid for nitration,

b) Halogenation: Kinetics of halogenations, typesofhalogenations, catalytic halogenations. Case study onindustrial halogenation process.

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

4 12Hrs

Unit Processes - II

a) Reduction: Catalytic hydrogenation, Heterogeneousand homogeneous catalyst; Hydrogen transfer reactions,Metal hydrides. Case study on industrial reductionprocess.

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 ofcost-effective routes, reagent selection, familiesofreagents useful for scale-up.

5 12Hrs

Industrial Safety

a) MSDS (Material Safety Data Sheet), hazard labels ofchemicals 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(EnvironmentalManagement 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

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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 approachesinvolving (3 experiments)
	1. Oxidationb) Reduction/hydrogenationc) Nitration
2. Comparative study of synthesis of APIs/intermediates by different syntheticroutes (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 Massspectra
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-iodotolene 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 ofselected 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, typeof significance tests, parametric tests(students “t” test, ANOVA, Correlationcoefficient, regression), non-parametric tests (wilcoxan rank tests, analysis ofvariance, correlation, chi square test), null hypothesis, P values, degree offreedom, interpretation of P values.

UNIT – III

Medical Research: History, values in medical ethics, autonomy, beneficence,non-maleficence, double effect, conflicts between autonomy andbeneficence/non-maleficence, euthanasia, informed consent, confidentiality,criticisms of orthodox medical ethics, importance of communication, controlresolution, 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, personalhygiene, 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 medicalresearch, and additional principles for medical research combined withmedical care.

References

1. *C.R.Kothari* “*Research Methodology Methods & Techniques”, Second Edition, New Delhi: New Age International publisher*
2. *Pharmaceutical Statistics 5th edition by Sanford Bolton and Charles Bon.*
3. *Biostatistics by R.S. Shukla and P.S.Chandel-S.Chand.*
4. *Guidelines On The Regulation Of Scientific Experiments On Animals; Government of India June 2007*, <https://www.aaalac.org/resources/SOP_CPCSEA.pdf>.
5. *WMA Declaration of Helsinki - Ethical Principles for Medical Research Involving Human Subjects:* [*http://anesthesia.gr/wp-content/uploads/2012/01/Decleration-of-Helsinki.pdf*](http://anesthesia.gr/wp-content/uploads/2012/01/Decleration-of-Helsinki.pdf)*.*
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