GURU NANAK INSTITUTE OF PHARMACEUTICAL SCIENCE & TECHNOLOGY

(An autonomous institute under MAKAUT)

M.PHARM SYLLABUS

Regulation 2020

2020-21

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Table : Course of Study for M. Pharm. (Pharmaceutical Chemistry)

SEMESTER I

Course Code	Name of the course	Credit hours	Credit points	Hrs./wk	Full Marks
THEORY					
R20_MPT1031T	Modern Pharmaceutical Analytical Techniques	4	4	4	100
R20_MPT1032T	Advanced Organic Chemistry - I	4	4	4	100
R20_MPT1033T	Advanced Medicinal Chemistry	4	4	4	100
R20_MPT1034T	Chemistry of Natural Products	4	4	4	100
PRACTICAL					
R20_MPT1935P	Pharmaceutical Chemistry Practical I	12	6	12	200
R20_MPT1936	Seminar/Assignment	7	4	7	100
Total		**35**	**26**	**35**	**700**

SEMESTER II

Course Code	Name of the course	Credit hours	Credit points	Hrs./wk	Full Marks
THEORY					
R20_MPT2031T	Advanced Spectral Analysis	4	4	4	100
R20_MPT2032T	Advanced Organic Chemistry - II	4	4	4	100
R20_MPT2033T	Computer Aided Drug Design	4	4	4	100
R20_MPT2034T	Pharmaceutical Process Chemistry	4	4	4	100
PRACTICAL					
R20_MPT2935P	Pharmaceutical Chemistry Practical II	12	6	12	200
R20_MPT2936	Seminar/Assignment	7	4	7	100
Total		**35**	**26**	**35**	**700**

SEMESTER III

Course Code	Name of the course	Credit hours	Credit points	Hrs./wk	Full Marks
THEORY					
R20_MPT384T	Research Methods and Biostatistics	4	4	4	100
R20_MPT381	Journal Club	1	1	1	100
R20_MPT391	Discussion/Presentation	2	2	2	100
R20_MPT392	Research Work	28	14		100
Total		**35**	**21**	**7**	**400**

SEMESTER IV

Course Code	Name of the course	Credit hours	Credit points	Hrs./wk	Full Marks
R20_MPT481	Journal Club	1	1	1	100
R20_MPT491	Discussion/Final Presentation	3	3	3	100
R20_MPT492	Research Work	31	16		100
R20_MPT482	Co-curricular Activities	3	3	3	100
Total		**38**	**23**	**7**	**400**

Table - Semester wise credits distribution

Semester	Credit Points
I	26
II	26
III	21
IV	23
Total Credit Points	96

REGULATIONS

1. Short Title and Commencement

These regulations shall be called as "The Revised Regulations for the Master of Pharmacy (M. Pharm.) Degree Program - Credit Based Semester System (CBSS) of the Pharmacy Council of India, New Delhi". They shall come into effect from the Academic Year 2016-17. The regulations framed are subject to modifications from time to time by the authorities of the university.

2. Minimum qualification for admission

A Pass in the following examinations

a) B. Pharm Degree examination of an Indian university established by law in India from an institution approved by Pharmacy Council of India and has scored not less than 55 % of the maximum marks (aggregate of 4 years of B.Pharm.)

b) Every student, selected for admission to post graduate pharmacy program in any PCI approved institution should have obtained registration with the State Pharmacy Council or should obtain the same within one month from the date of his/her admission, failing which the admission of the candidate shall be cancelled.

Note: It is mandatory to submit a migration certificate obtained from the respective university where the candidate had passed his/her qualifying degree (B.Pharm.)

3. Duration of the program

The program of study for M.Pharm. shall extend over a period of four semesters (two academic years). The curricula and syllabi for the program shall be prescribed from time to time by Phamacy Council of India, New Delhi.

4. Medium of instruction and examinations

Medium of instruction and examination shall be in English.

5. Working days in each semester

Each semester shall consist of not less than 100 working days. The odd semesters shall be conducted from the month of June/July to November/December and the even semesters shall be conducted from the month of December/January to May/June in every calendar year.

6. Attendance and progress

A candidate is required to put in at least 80% attendance in individual courses considering theory and practical separately. The candidate shall complete the prescribed course satisfactorily to be eligible to appear for the respective examinations.

7. Program/Course credit structure

As per the philosophy of Credit Based Semester System, certain quantum of academic work viz. theory classes, practical classes, seminars, assignments, etc. are measured in terms of credits. On satisfactory completion of the courses, a candidate earns credits. The amount of credit associated with a course is dependent upon the number of hours of instruction per week in that course. Similarly the credit associated with any of the other academic, co/extracurricular activities is dependent upon the quantum of work expected to be put in for each of these activities per week/per activity.

7.1. Credit assignment

7.1.1. Theory and Laboratory courses

Courses are broadly classified as Theory and Practical. Theory courses consist of lecture (L) and Practical (P) courses consist of hours spent in the laboratory. Credits (C) for a course is dependent on the number of hours of instruction per week in that course, and is obtained by using a multiplier of one (1) for lecture and a multiplier of half (1/2) for practical (laboratory) hours.Thus, for example, a theory course having four lectures per week throughout the semester carries a credit of 4. Similarly, a practical having four laboratory hours per week throughout semester carries a credit of 2. The contact hours of seminars, assignments and research work shall be treated as that of practical courses for the purpose of calculating credits. i.e., the contact hours shall be multiplied by 1/2. Similarly, the contact hours of journal club, research work presentations and discussions with the supervisor shall be considered as theory course and multiplied by 1.

7.2. Minimum credit requirements

The minimum credit points required for the award of M. Pharm. degree is 95. However based on the credit points earned by the students under the head of co-curricular activities, a student shall earn a maximum of 100 credit points. These credits are divided into Theory courses, Practical, Seminars, Assignments, Research work, Discussions with the supervisor, Journal club and Co-Curricular activities over the duration of four semesters. The credits are distributed semester-wise as shown in Table 14. Courses generally progress in sequence, building competencies and their positioning indicates certain academic maturity on the part of the learners. Learners are expected to follow the semester-wise schedule of courses given in the syllabus.

8. Academic work

A regular record of attendance both in Theory, Practical, Seminar, Assignment, Journal club, Discussion with the supervisor, Research work presentation and Dissertation shall be maintained by the department / teaching staff of respective courses.

SYLLABUS

Semester I

PHARMACEUTICAL CHEMISTRY

1ST SEMESTER

MODERN PHARMACEUTICAL ANALYTICAL TECHNIQUES

(R20_MPT1031T)

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
- Theoritical and practical skills of the instruments

THEORY 60 Hrs

1. (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, Difference/ Derivative spectroscopy. 10 Hrs

(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, Data Interpretation.

(c) Spectroflourimetry: Theory of Fluorescence, Factors affecting fluorescence (Characterestics of drugs that can be analysed by flourimetry), Quenchers, Instrumentation and Applications of fluorescence spectrophotometer.

(d) Flame emission spectroscopy and Atomic absorption spectroscopy: Principle, Instrumentation, Interferences and Applications.

2. 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 10 Hrs

resonance, Brief outline of principles of FT-NMR and 13C NMR. Applications of NMR spectroscopy.

3. 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. 10 Hrs

4. Chromatography: Principle, apparatus, instrumentation, chromatographic parameters, factors affecting resolution, isolation of drug from excipients, data interpretation and applications of the following: 10 Hrs

(a) Thin Layer chromatography
(b) High Performance Thin Layer Chromatography
(c) Ion exchange chromatography
(d) Column chromatography
(e) Gas chromatography
(f) High Performance Liquid chromatography
(g) Ultra High Performance Liquid chromatography
(h) Affinity chromatography
(i) Gel Chromatography

5. Electrophoresis: Principle, Instrumentation, Working conditions, factors affecting separation and applications of the following: 10 Hrs

(a) Paper electrophoresis (b) Gel electrophoresis (c) Capillary electrophoresis
(d) Zone electrophoresis (e) Moving boundary electrophoresis (f) Iso electric focusing X ray Crystallography: Production of X rays, Different X ray methods, Bragg's law, Rotating crystal technique, X ray powder technique, Types of crystals and applications of X-ray diffraction.

6. Potentiometry: Principle, working, Ion selective Electrodes and Application of potentiometry. 10 Hrs

(a) Thermal Techniques: Principle, thermal transitions and Instrumentation (Heat flux and power compensation and designs), Modulated DSC, Hyper DSC, experimental parameters (sample preparation, experimental conditions, calibration, heating and cooling rates, resolution, source of errors) and their influence, advantage and disadvantages, pharmaceutical applications.

(b) Differential Thermal Analysis (DTA): Principle, instrumentation and advantage and disadvantages, pharmaceutical applications, derivative differential thermal analysis (DDTA).

(c) TGA: Principle, instrumentation, factors affecting results, advantage and disadvantages, pharmaceutical applications

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, 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, Vol 11, Marcel. Dekker Series

8. Spectroscopy of Organic Compounds, 2nd edn., P.S/Kalsi, Wiley estern Ltd., Delhi.

9. Textbook of Pharmaceutical Analysis, KA. Connors, 3rd Edition, John Wiley & Sons, 1982.

ADVANCED ORGANIC CHEMISTRY-I

(R20_MPT1032T)

SCOPE

The subject is designed to provide in-depth knowledge about advances in organic 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 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. Basic Aspects of Organic Chemistry: 12 Hrs

(i) Organic intermediates: Carbocations, carbanions, free radicals, carbenes and nitrenes. Their method of formation, stability and synthetic applications.

(ii) 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 (SN1and SN2)

(b) Elimination reactions (E1 & E2; Hoffman & Saytzeff's rule)

(c) Rearrangement reaction

2. 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, Vilsmeyer-Haack Reaction, Sharpless 12 Hrs

asymmetric epoxidation, Baeyer-Villiger oxidation, Shapiro & Suzuki reaction, Ozonolysis and Michael addition reaction.

3. Synthetic Reagents & Applications: Aluminium isopropoxide, N-bromosuccinamide, diazomethane, dicyclohexylcarbodimide, Wilkinson reagent, Witting reagent. Osmium tetroxide, titanium chloride, diazopropane, diethyl azodicarboxylate, Triphenylphosphine, Benzotriazol-1-yloxy) tris (dimethylamino) phosphonium hexafluoro-phosphate (BOP). 12 Hrs

Protecting groups

(a) Role of protection inorganic 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. Heterocyclic Chemistry: 12 Hrs

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

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

5. Synthon approach and retrosynthesis applications 12 Hrs

(i) Basic principles, terminologies and advantages of retrosynthesis; guidelines for dissection of molecules. Functional group inter convertion 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", J March, John Wiley and Sons, New York.

2. "Mechanism and Structure in Organic Chemistry", ES Gould, Hold Rinchart and Winston, New York.

3. "Organic Chemistry" Clayden, Greeves, Warren and Woihers., Oxford University 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 (Orient Longman, New Delhi).

6. Reactive Intermediates in Organic Chemistry, Tandom and Gowel, Oxford & IBH Publishers.

7. Combinational Chemistry – Synthesis and applications – Stephen R Wilson & 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, Nelson Thorns.

11. Organic Synthesis - Special Techniques. VK Ahluwalia and R Agarwal, Narosa Publishers.

12. Organic Reaction Mechanisms IVth Edtn, VK Ahluwalia and RK Parashar, Narosa Publishers.

ADVANCED MEDICINAL CHEMISTRY

(R20_MPT1033T)

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. (i) Drug discovery : Stages of drug discovery, lead discovery; identification, validation and diversity of drug targets. 12 Hrs

(ii) Biological drug targets: Receptors, types, binding and activation, theories of drug receptor interaction, drug receptor interactions, agonists vs antagonists, artificial enzymes.

2. Pro drug Design and Analog design : 12 Hrs

a) Pro drug design: Basic concept, Carrier linked prodrugs/Bioprecursors, Prodrugs of functional group, Prodrugs to improve patient acceptability, Drug solubility, Drug absorption and distribution, site specific drug delivery and sustained drug action. Rationale of prodrug design and practical consideration of prodrug design.

b) Combating drug resistance : Causes for drug resistance, strategies to combat drug resistance in antibiotics 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, ring position isomers, design of stereo isomers and geometric isomers, fragments of a lead molecule, variation in inter atomic distance.

3. (a) 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: 12 Hrs

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

ii) Stereochemistry and Drug action: Realization that stereo selectivity 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. Rational Design of Enzyme Inhibitors 12 Hrs

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. Peptidomimetics 12 Hrs

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, Lppincott Williams & Wilkins, Woltess 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, Ippincott Williams & 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 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, Vallabh Prakashan, New Delhi.

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

CHEMISTRY OF NATURAL PRODUCTS

(R20_MPT1034T)

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. Study of Natural products as leads for new pharmaceuticals for the following class of drugs 12 Hrs

a) Drugs Affecting the Central Nervous System : Morphine Alkaloids

b) Anti cancer 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 macrolide antibiotics (Erythromycin, Azithromycin, Roxithromycin and Clarithromycin) and β- Lactam antibiotics (Cephalosporins and Carbapenem)

2. (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. 12 Hrs

(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 (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) carotinoids (β carotene). 12 Hrs

(b) Vitamins - Chemistry and Physiological significance of Vitamin A, B1, B2, B12, C, E, Folic acid and Niacin.

4.(a) Recombinant DNA technology and drug discovery r DNA 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 12 Hrs

(b) Active constituent of certain crude drugs used in Indigenous system Diabetic therapy – Gymnema sylvestre, Salacia reticulate, Pterocarpus marsupiam, Swertia chirata,Trigonella foenum graccum; Liver dysfunction – Phyllanthus niruri; Antitumor – Curcuma longa Linn.

5. Structural Characterization of natural compounds Structural characterization of natural compounds using IR,1HNMR,13C NMR and MS Spectroscopy of 12 Hrs

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 Nostrant 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, Chapmannstall.
9. Organic Chemistry of Natural Products Vol I and II by Gurdeep and Chatwall, Himalaya Publishing House.
10. Organic Chemistry of Natural Products Vol I and II by O.P. Agarwal, Krishan Prakashan.
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.

PHARMACEUTICAL CHEMISTRY PRACTICAL – I

(R20_MPT1935P)

1. Analysis of Pharmacopoeial compounds and their formulations by UV Vis spectrophotometer, RNA & DNA estimation
2. Simultaneous estimation of multi component containing formulations by UV spectrophotometry
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

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

SYLLABUS

Semester II

PHARMACEUTICAL CHEMISTRY

2ND SEMESTER

ADVANCED SPECTRAL ANALYSIS

(R20_MPT2031T)

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 60 Hrs

1. UV and IR spectroscopy : Woodward–Fieser rule for 1,3-butadienes, cyclicdienes and α, β-carbonyl compounds and interpretation compounds of enones. ATR-IR, IR Interpretation of organic compounds. 12 Hrs

2. NMR spectroscopy : 1-D and 2-D NMR, NOESY and COSY, HECTOR, INADEQUATE techniques, Interpretation of organic compounds. 12 Hrs

3. 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. 12 Hrs

4. Chromatography: Principle, Instrumentation and Applications of the following : (a) GC-MS (b) GC-AAS (c) LC-MS (d) LC-FTIR (e)LC-NMR (f) CEMS (g) High Performance Thin Layer chromatography (h) Super critical fluid chromatography (i) Ion Chromatography (j) I-EC (Ion-Exclusion Chromatography) (k) Flashchromatography — 12 Hrs

5. (a) Thermal methods of analysis: Introduction, principle, instrumentation and application of DSC, DTA and TGA. — 12 Hrs

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

(c) Radio immune assay : Biological standardization, bioassay, ELISA, Radio immun o assay 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 –PD Sethi, CBS Publishers, New Delhi.

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

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

ADVANCED ORGANIC CHEMISTRY - II

(R20_MPT2032T)

SCOPE

The subject is designed to provide in-depth knowledge about advances in organic 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. Green Chemistry: 12 Hrs

(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 heterocycles synthesis

(c) Ultra sound 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. Chemistry of peptides 12 Hrs

(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. (i) Photochemical Reactions –** Basic principles of photo chemical reactions. Photo-oxidation, photo-addition and photo- fragmentation. 12 Hrs

(ii) Pericyclic reactions - Mechanism, Types of pericyclic reactions such as cyclo addition, electrocyclic reaction and sigma trophic rearrangement reactions with examples

4. Catalysis: 12 Hrs

(a) Types of catalysis, heterogeneous and homogenous 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) Homogenous catalysis, hydrogenation, hydroformylation, hydrocyanation, Wilkinson catalysts, chiral ligands and chiral induction, Ziegler-Natta catalysts, some examples of homogenous 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. Stereochemistry & Asymmetric Synthesis 12 Hrs

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

(b) Methods of a symmetric 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", J March, John Wiley and sons, New York.

2. "Mechanism and structure in organic chemistry", E S Gould, Hold Rinchart and Winston, NewYork.

3. "Organic Chemistry" Clayden, Greeves,Warren and Woihers, Oxford University 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 V K Ahluwalia and R Aggarwal, Narosa Publishers.

9. Organic reaction mechanisms IV edtn, V K Ahluwalia and R K Parashar, Narosa Publish

COMPUTER AIDED DRUG DESIGN

(R20_MPT2033T)

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. 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 (sigma), lipophilicity effects and parameters (log P, pi-substituent constant), steric effects (Taft steric and MR parameters) Experimental and theoretical approaches for the determination of these physicochemical parameters. 12 Hrs

2. 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. 12 Hrs

3. Molecular Modeling and Docking 12 Hrs

(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. Molecular Properties and Drug Design 12 Hrs

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

(b) Denovo 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.(i) Pharmacophore Mapping and Virtual Screening Concept of pharmacophore, pharmacophore mapping, identification of Pharmacophore features and Pharmacophore modeling; Conformational search used in pharmacophore mapping. 12 Hrs

(ii) In Silico Drug Design andVirtual 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,WileyPublishingCo.

7. An Introduction to Medicinal Chemistry– Graham L. Patrick ,Oxford University Press.

8. Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, Ippincott Williams & Wilkins.

9. Comprehensive Medicinal Chemistry–Corwinand Hansch, Pergamon Publishers.

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

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PHARMACEUTICAL PROCESS CHEMISTRY

(R20_MPT2034T)

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. The 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. 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 12 Hrs

2. Unit operations 12 Hrs

(a) Extraction : Liquid equilibria, extraction with reflux, extraction with agitation,countercurrent 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, non aqueous solutions factors affecting crystallization, nucleation. Principle and general methods of Preparation of polymorphs, hydrates, solvates and amorphousAPIs.

3. Unit Processes - I 12 Hrs

(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. Unit Processes - II 12 Hrs

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) Stream lining reaction steps, route selection,

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

5. Industrial Safety 12 Hrs

(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. Mc Cabe, J. C Smith, Peter Harriott. Unit operations of chemical engineering, 7th edition, Mc Graw Hill
5. Polymorphism in Pharmaceutical Solids. Dekker Series Volume 95 Ed: H G 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-West Press
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 textbook 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

PHARMACEUTICAL CHEMISTRY PRACTICALS – II

(R20_MPT2935P)

1. Synthesis of organic compounds by adapting different approaches involving (3experiments)

(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 (2experiments)

4. Comparison of absorption spectra by UV and Woodward–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

11. Preparation of 4-chlorobenzhydrylpiperazine (an intermediate for cetirizine HCl).

12. Preparation of 4-iodotolene from p-toluidine.

13. $NaBH_4$ reduction of vanillin to vanillyl alcohol

14. Preparation of umbelliferone by Pechhman reaction

15. Preparation of triphenyl imidazole

16. To perform the Microwave irradiated reactions of synthetic importance (Anytwo)

17. Determination of log P, MR, hydrogen bond donors and acceptors of selected drugs using softwares

18.Calculation of ADMET properties of drug molecules and its analysis using softwares Pharmacophore modeling

19. 2D-QSAR based experiments

20. 3D-QSAR based experiments

21. Docking study based experiment

22. Virtual screening based experiment

SYLLABUS

Semester III

PHARMACEUTICAL CHEMISTRY

3RD SEMESTER

RESEARCH METHODOLOGY & BIOSTATISTICS

(R20_MPT384T)

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, cross over design, placebo, blinding techniques.

UNIT–II

Biostatistics : Definition, application, sample size, importance of sample size, factors influencing sample size, dropouts, statistical tests of significance, type of significance tests, parametric tests (students "t" test, ANOVA, Correlation coefficient, regression), non-parametric tests (wilcoxan 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.