

UTTAR PRADESH UNIVERSITY OF MEDICAL SCIENCES, SAIFAI

FACULTY OF PHARMACY



**REGULATIONS, EXAMINATION SCHEME AND SYLLABUS
FOR
M.PHARM (PHARMACEUTICAL CHEMISTRY)**

**Adapted from Master of Pharmacy (M. Pharm, Pharmaceutical Chemistry)
COURSE REGULATIONS 2014 as per PCI Regulations**

Regulations

1. Short Title and Commencement

These regulations shall be called as “The Regulations for the Master of Pharmacy (Pharmaceutical Chemistry) Degree Program - Credit Based Semester System (CBSS)”. 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 Pharmacy 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 7. 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.

9. Course of study

The course of study for M. Pharm shall include Semester wise Theory & Practical as given in Tables 1-4. The number of hours to be devoted to each theory and practical course in any semester shall not be less than that shown in Tables 1-4.

Table – 1: Course of study for M. Pharm. (Pharmaceutical Chemistry) Sem I & II

Course Code	Course	Credit Hours	Credit Points	Hrs./wk	Marks
MPC 101T	Modern Pharmaceutical Analytical Techniques	4	4	4	100
MPC 102T	Advanced Organic Chemistry -I	4	4	4	100
MPC 103T	Advanced Medicinal chemistry	4	4	4	100
MPC 104T	Chemistry of Natural Products	4	4	4	100
MPC 105P	Pharmaceutical Chemistry Practical I	12	6	12	150
MPC 106	Seminar/ Assignment	7	4	7	100
Total		35	26	35	650
MPC 201T	Advanced Spectral Analysis	4	4	4	100
MPC 202T	Advanced Organic Chemistry -II	4	4	4	100
MPC 203T	Computer Aided Drug Design	4	4	4	100
MPC 204T	Pharmaceutical Process Chemistry	4	4	4	100
MPC 205P	Pharmaceutical Chemistry Practical II	12	6	12	150
MPC 206	Seminar/ Assignment	7	4	7	100
Total		35	26	35	650

Table 2: Course of study for M. Pharm. (Pharmaceutical Chemistry) Sem III & IV

Course Code	Course	Credit Hours	Credit Points
MPC 301T	Research Methodology and Biostatistics*	4	4
MPC 302	Journal club	1	1
MPC 303	Discussion / Presentation (Proposal Presentation)	2	2
MPC 304	Research Work*	28	14
Total		35	21
MPC 401	Journal club	1	1
MPC 402	Research Work	31	16
MPC 403	Discussion / Final Presentation	3	3
Total		35	20

* Non- University Exam

Table – 3: Semester wise credit distribution

Semester	Credit Points
I	26
II	26
III	21
IV	20
Co-curricular Activities (Attending Conference, Scientific Presentations and Other Scholarly Activities)	Minimum = 02 Maximum = 07*
Total Credit Points	Minimum = 95 Maximum = 100*

*Credit Points for Co-curricular Activities

Table – 4: Guidelines for Awarding Credit Points for Co-curricular Activities

Name of the Activity	Maximum Credit Points Eligible / activity
Participation in National Level Seminar/Conference/Workshop /Symposium/ Training Programs (related to the specialization of the student)	01
Participation in international Level Seminar/ Conference/ Workshop /Symposium/ Training Programs (related to the specialization of the student)	02
Academic Award/Research Award from State Level/ National Agencies	01
Academic Award/Research Award from International Agencies	02
Research / Review Publication in National Journals (Indexed in Scopus / Web of Science)	01
Research / Review Publication in International Journals (Indexed in Scopus / Web of Science)	02

Note: International Conference: Held Outside India

International Journal: The Editorial Board outside India

*The credit points assigned for extracurricular and or co-curricular activities shall be given by the principals of the colleges and the same shall be submitted to the University. The criteria to acquire this credit point shall be defined by the institute from time to time.

10. Program Committee

1. The M. Pharm. programme shall have a Programme Committee constituted by the Head of the institution in consultation with all the Heads of the departments.
2. The composition of the Programme Committee shall be as follows:
A teacher at the cadre of Professor shall be the Chairperson; One Teacher from each M. Pharm specialization and four student representatives (two from each academic year), nominated by the Head of the institution.
3. Duties of the Programme Committee:
 - i. Periodically reviewing the progress of the classes.
 - ii. Discussing the problems concerning curriculum, syllabus and the conduct of classes.
 - iii. Discussing with the course teachers on the nature and scope of assessment for the course and the same shall be announced to the students at the beginning of respective semesters.
 - iv. Communicating its recommendation to the Head of the institution on academic matters.
 - v. The Programme Committee shall meet at least twice in a semester preferably at the end of each sessional exam and before the end semester exam.

11. Examinations/Assessments

The schemes for internal assessment and end semester examinations are given in Tables 5 & 6.

11.1. End semester examination

The End Semester Examinations for each theory and practical course through semesters I to IV shall be conducted by the university except for the subject with Asterix symbol (*) for which examinations shall be conducted by the subject experts at college level and the marks/grades shall be submitted to the university.

Tables – 5: Schemes for internal assessments and end semester for I and II Sem for M. Pharm (Pharmaceutical Chemistry).

(Pharmaceutical Chemistry).								
Course Code	Course	Internal Assessment				End Semester Exam		Total Marks
		Continuous Mode	Sessional Exam		Total	Marks	Duration	
			Marks	Duration				
SEMESTER I								
MPC 101T	Modern Pharmaceutical Analytical Techniques	10	15	1 Hr	25	75	3 Hrs	100
MPC 102T	Advanced Organic Chemistry -I	10	15	1 Hr	25	75	3 Hrs	100
MPC 103T	Advanced Medicinal chemistry	10	15	1 Hr	25	75	3 Hrs	100
MPC 104T	Chemistry of Natural Products	10	15	1 Hr	25	75	3 Hrs	100
MPC 105P	Pharmaceutical Chemistry Practical I	20	30	6 Hrs	50	100	6 Hrs	150
MPC 106	Seminar/ Assignment	-	-	-	-	-	-	100
TOTAL								650
SEMESTER II								
MPC 201T	Advanced Spectral Analysis	10	15	1 Hr	25	75	3 Hrs	100
MPC 202T	Advanced Organic Chemistry -II	10	15	1 Hr	25	75	3 Hrs	100
MPC 203T	Computer Aided Drug Design	10	15	1 Hr	25	75	3 Hrs	100
MPC 204T	Pharmaceutical Process Chemistry	10	15	1 Hr	25	75	3 Hrs	100
MPC 205P	Pharmaceutical Chemistry Practical II	20	30	6 Hrs	50	100	6 Hrs	150
MPC 206	Seminar/ Assignment	-	-	-	-	-	-	100
TOTAL								650

Tables – 6: Schemes for internal assessments and End semester Examination for III and IV Sem.

Course Code	Course	Internal Assessment				End Semester Exam		Total Marks
		Continu- ous Mode	Sessional Exam		Total	Marks	Duration	
			Marks	Duratio n				
SEMESTER III								
MPC 301T	Research Methodology and Biostatistics*	10	15	1 Hr	25	75	3 Hrs	100
MPC 302	Journal club	-	-	-	25	-	-	25
MPC 303	Discussion / Presentation (Proposal Presentation)	-	-	-	50	-	-	50
MPC 304	Research work*	-	-	-	-	350	1 Hr	350
TOTAL								525
SEMESTER IV								
MPC 401	Journal club	-	-	-	25	-	-	25
MPC 402	Research work	-	-	-	-	400	1 Hr	400
MPC 403	Discussion /Final Presentation	-	-	-	75	-	-	75
TOTAL								500

*Non-University Examination

11.2. Internal assessment: Continuous mode

The marks allocated for Continuous mode of Internal Assessment shall be awarded as per the scheme given below.

Table – 7: Scheme for awarding internal assessment: Continuous mode

For Theory	
Criteria	Maximum Marks
Attendance	8
Student – Teacher interaction	2
Total	10
For Practical	
Attendance	10
Based on Practical Records, Regular viva voce, etc.	10
Total	20

Table – 8: Guidelines for the allotment of marks for attendance

Percentage of Attendance	Theory	Practical
95 – 100	8	10
90 – 94	6	7.5
85 – 89	4	5
80 – 84	2	2.5
Less than 80	0	0

11.2.1. Sessional Exams

Two sessional exams shall be conducted for each theory / practical course as per the schedule fixed by the college(s). The scheme of question paper for theory and practical sessional examinations is given below. The average marks of two sessional exams shall be computed for internal assessment as per the requirements given in Tables 9-12.

Question paper pattern for theory Sessional examination

I. Multiple Choice Questions (MCQs)	= 10 x 1 = 10
OR	
Objective Type Questions (10 x 1) (Answer all the questions)	= 10 x 1 = 10
II. Short Answers (Answer 2 out of 3)	= 2 x 5 = 10
III. Long Answers (Answer 1 out of 2)	= 1 x 10 = 10
Total	= 30 marks

Question paper pattern for practical sessional examination

I. Experiment(s)	= 20
II. Viva voce	= 10
Total	= 30 marks

12. Promotion and award of grades

A student shall be declared PASS and eligible for getting grade in a course of M. Pharm. program if he/she secures at least 50% marks in that particular course including internal assessment.

13. Carry forward of marks

In case a student fails to secure the minimum 50% in any Theory or Practical course as specified in 12, then he/she shall reappear for the end semester examination of that course. However, his/her marks of the Internal Assessment shall be carried over and he/she shall be entitled for grade obtained by him/her on passing.

14. End Semester Examination

End semester examination shall be conducted as per the schedule given in Table 9. The exact dates of examination shall be notified from time to time.

Table – 9: Tentative schedule of end semester examinations

Semester	For Regular/Carry over Candidates
I and III	December/January
II and IV	May / June

15. Allowed to keep terms (ATKT):

No student shall be admitted to any examination unless he/she fulfils the norms given in Section 6. ATKT rules are applicable as follows: A student shall be eligible to carry forward all the courses of I and II semesters till the III semester examinations. However, he/she shall not be eligible to attend the courses of IV semester until all the courses of I, II and III semesters are successfully completed.

A student shall be eligible to get his/her CGPA upon successful completion of the courses of I to IV semesters within the stipulated time period as per the norms.

Note: Grade AB should be considered as failed and treated as one head for deciding ATKT. Such rules are also applicable for those students who fail to register for examination(s) of any course in any semester.

16. Grading of performances

16.1. Letter grades and grade points allocations:

Based on the performances, each student shall be awarded a final letter grade at the end of the semester for each course. The letter grades and their corresponding grade points are given in Table – 10.

Table –10: Letter grades and grade points equivalent to Percentage of marks and performances

Percentage of Marks Obtained	Letter Grade	Grade Point	Performance
90.00 – 100	O	10	Outstanding
80.00 – 89.99	A	9	Excellent
70.00 – 79.99	B	8	Good
60.00 – 69.99	C	7	Fair
50.00 – 59.99	D	6	Average
Less than 50	F	0	Fail
Absent	AB	0	Fail

A learner who remains absent for any End Semester Examination shall be assigned a letter grade of AB and a corresponding grade point of zero. He/she should reappear for the said evaluation/examination in due course.

17. The Semester grade point average (SGPA)

The performance of a student in a semester is indicated by a number called ‘Semester Grade Point Average’ (SGPA). The SGPA is the weighted average of the grade points obtained in all the courses by the student during the semester. For example, if a student takes five courses (Theory/Practical) in a semester with credits C1, C2, C3 and C4 and the student’s grade points in these courses are G1, G2, G3 and G4, respectively, and then students’ SGPA is equal to:

$$SGPA = \frac{C1G1 + C2G2 + C3G3 + C4G4}{C1 + C2 + C3 + C4}$$

The SGPA is calculated to two decimal points. It should be noted that, the SGPA for any semester shall take into consideration the F and ABS grade awarded in that semester. For example, if a learner has a F or ABS grade in course 4, the SGPA shall then be computed as:

$$SGPA = \frac{C1G1 + C2G2 + C3G3 + C4* ZERO}{C1 + C2 + C3 + C4}$$

18. Cumulative Grade Point Average (CGPA)

The CGPA is calculated with the SGPA of all the IV semesters to two decimal points and is indicated in final grade report card/final transcript showing the grades of all IV semesters and their courses. The CGPA shall reflect the failed status in case of F grade(s), till the course(s) is/are passed. When the course(s) is/are passed by obtaining a pass grade on subsequent examination(s) the CGPA shall only reflect the new grade and not the fail grades earned earlier. The CGPA is calculated as:

$$CGPA = \frac{C1S1 + C2S2 + C3S3 + C4S4}{C1 + C2 + C3 + C4}$$

where C1, C2, C3,.... is the total number of credits for semester I,II,III,.... And S1,S2, S3,....is the SGPA of semester I,II,III,.... .

19. Declaration of class

The class shall be awarded on the basis of CGPA as follows:

First Class with Distinction	= CGPA of. 7.50 and above
First Class	= CGPA of 6.00 to 7.49
Second Class	= CGPA of 5.00 to 5.99

20. Project work

All the students shall undertake a project under the supervision of a teacher in Semester III to IV and submit a report. 4 copies of the project report shall be submitted (typed & bound copy not less than 75 pages).

The internal and external examiner appointed by the University shall evaluate the project at the time of the Practical examinations of other semester(s). The projects shall be evaluated as per the criteria given below.

Evaluation of Dissertation Book:

Objective(s) of the work done	50 Marks
Methodology adopted	150 Marks
Results and Discussions	250 Marks
Conclusions and Outcomes	50 Marks
Total =	<hr/> 500 Marks

Evaluation of Presentation:

Presentation of work	100 Marks
Communication skills	50 Marks
Question and answer skills	100 Marks
Total =	<hr/> 250 Marks

21. Award of Ranks

Ranks and Medals shall be awarded on the basis of final CGPA. However, candidates who fail in one or more courses during the M. Pharm program shall not be eligible for award of ranks. Moreover, the candidates should have completed the M. Pharm program in minimum prescribed number of years, (two years) for the award of Ranks.

22. Award of degree

Candidates who fulfill the requirements mentioned above shall be eligible for award of degree during the ensuing convocation.

23. Duration for completion of the program of study

The duration for the completion of the program shall be fixed as double the actual duration of the program and the students have to pass within the said period, otherwise they have to get fresh Registration.

24. Re-admission after break of study

Candidate who seeks re-admission to the program after break of study has to get the approval from the university by paying a condonation fee.

Program Outcomes (POs)

1. Enable the post graduate students to understand the spectroscopic and chromatographic techniques with their applications.
2. Enable the post graduate students to understand the basic and advanced organic and medicinal chemistry, emphasizing the reactions with their mechanism.
3. Enable the post graduate students to understand the chemistry of natural products.
4. Enable the post graduate students to understand the Computer aided drug design with their applications in search of new entities.

PROGRAM SPECIFIC OUTCOMES (PSOs)

1. Knowledge: Enable post graduates to understand the core and basic knowledge in different subjects of pharmaceutical chemistry as per the requirement of pharmaceutical sectors.
2. Employment and Entrepreneurship: Enable post graduates to succeed in technical or professional careers in pharmaceutical industry/ Academic institutes or in health care system.
3. Professional Practice: Enable post graduates to practice profession and adapt themselves to the constantly developing global pharmaceutical trends.
4. Lifelong Learning & Professional Ethics: Enable the post graduates to be a lifelong learner in terms of personal and professional growth with ethics and self-esteem.

Syllabus
M.PHARM PHARMACEUTICAL CHEMISTRY (MPC)
Semester I and II

Semester I

MODERN PHARMACEUTICAL ANALYTICAL TECHNIQUES (MPC 101T)

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.

Course Outcomes: Through this course students should be able to

CO1: Demonstrate the principle, theory, instrumentation and applications of UV-Visible spectroscopy, IR spectroscopy, Spectrofluorimetry, Flame emission spectroscopy and Atomic absorption spectroscopy.

CO2: Demonstrate the principle, theory, instrumentation and applications of NMR spectroscopy and Mass Spectroscopy.

CO3: Illustrate the principle, apparatus, instrumentation and applications of various chromatographic techniques.

CO4: Discuss the principle, instrumentation, and applications of electrophoresis and X ray techniques.

CO5: Explain the principle, instrumentation, and applications of potentiometry and thermal techniques.

THEORY:60 Hrs **10 hours**

Unit 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.
- 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. Spectrofluorimetry: Theory of Fluorescence, Factors affecting fluorescence (Characteristics of drugs that can be analysed by fluorimetry), Quenchers, Instrumentation and Applications of fluorescence spectrophotometer.
- d. Flame emission spectroscopy and Atomic absorption spectroscopy: Principle, Instrumentation, Interferences and Applications.

Unit 2

10 hours

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,

Unit 3

10 hours

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.

Unit 4

10 hours

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

- 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.

Unit 5

10 hours

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 methods, Bragg's law, Rotating crystal technique, X ray powder technique, Types of crystals and applications of X-ray diffraction.

Unit 6

10 hours

a. Potentiometry: Principle, working, Ion selective Electrodes and Application of potentiometry.
 b. 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. Differential Thermal Analysis (DTA): Principle, instrumentation and advantage and disadvantages, pharmaceutical applications, derivative differential thermal analysis (DDTA). 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 - 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, Vol 11, Marcel. Dekker Series
8. Spectroscopy of Organic Compounds, 2nd Edn., P.S/Kalsi, Wiley Eastern Ltd., Delhi.
9. Textbook of Pharmaceutical Analysis, KA. Connors, 3rd Edition, John Wiley & Sons, 1982. 37

ADVANCED ORGANIC CHEMISTRY – I (MPC 102T)

Scope

This course 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.

Course Outcomes: Through this course students should be able to

CO1: Analyze the generation and stability, reactivity of various synthetic process intermediates.

CO2: Understand the concepts of substitution, elimination and rearrangement reactions.

CO3: Understand and implement suitable role of name reactions during chemical synthesis.

CO4: Examine and demonstrate the practical application of several synthetic reagents and protecting groups during organic synthesis.

CO5: Apply the disconnection strategy to develop synthetic routes for small target molecule to process chemistry as well as drug discovery.

THEORY:60 Hrs

Unit 1

12 hours

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

Unit 2

12 hours

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.

Unit 3

12 hours

Synthetic Reagents & Applications:

Aluminium isopropoxide, N-bromosuccinimide, diazomethane, dicyclohexylcarbodiimide, Wilkinson reagent, Wittig reagent. Osmium tetroxide, titanium chloride, diazopropane, diethyl azodicarboxylate, Triphenylphosphine, Benzotriazol-1-yloxy tris (dimethylamino) phosphonium hexafluoro-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

Unit 4

12 hours

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, Berntsen Acridine Synthesis, Smiles rearrangement and Traube purine synthesis.

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

Unit 5

12 hours

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”, 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 Wothers., Oxford University Press 2001.
4. “Organic Chemistry” Vol I and II. I.L. Finar. ELBS, Pearson Education Ltd. Dorling Kindersley India) Pvt. Ltd.
5. A guide to mechanisms in Organic Chemistry, Peter Skyes (Orient Longman, New Delhi).
6. Reactive Intermediates in Organic Chemistry, Tandon and Gowell, 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, Wiley India
10. Principles of Organic Synthesis, ROC Norman and JM Coxan, Nelson Thornes.
11. Organic Synthesis - Special Techniques. VK Ahluwalia and R Agarwal, Narosa Publishers.
12. Organic Reaction Mechanisms IVth Ed, VK Ahluwalia and RK Parashar, Narosa Publishers. 39

ADVANCED MEDICINAL CHEMISTRY (MPC 103T)

Scope: This course 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.

Course Outcomes: Through this course students should be able to

CO1: Understand the fundamental concepts of drug discovery and biological drug targets.

CO2: Understand the fundamental concepts of prodrug design, analog design and combating drug resistance.

CO3: Discuss the medicinal chemistry aspects of various classes of drugs.

CO4: Analyze the stereochemistry and drug action.

CO5: Determine the kinetics, design and uses of enzyme inhibitors.

CO6: Explain the design and uses of peptidomimetics and chemistry of eicosanoids.

THEORY 60 Hrs

Unit 1

12 hours

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 versus antagonists, artificial enzymes.

Unit 2

12 hours

Prodrug Design and Analog design:

a) Prodrug 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 considerations 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, position isomers, design of stereo isomers and geometric isomers, fragments of a lead molecule, variation in inter atomic distance.

Unit 3

12 hours

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:

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 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.

Unit 4

12 hours

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

Unit 5

12 hours

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. 40

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. Brahmkar, 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 (MPC 104T)

Scope: This course 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.

Course Outcomes: Through this course students should be able to

CO1: Understand importance and chemistry of different types of natural products as lead compounds in new pharmaceutical drug design.

CO2: Remember and understand general methods of structural elucidation of structurally diverse natural products of flavonoids, alkaloids, steroidal and terpenoids class.

CO3: Understand the concept of recombinant DNA technology and its applications in new drug discovery.

CO4: Develop knowledge of spectroscopy techniques for structural characterization of natural compounds.

CO5: Apply different methods of extraction, isolation and purification for compounds from natural source.

THEORY 60 Hrs

12 hours

Unit 1

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

- Drugs affecting the central nervous system: Morphine Alkaloids
- Anticancer drugs: Paclitaxel and Docetaxel, Etoposide, and Teniposide
- Cardiovascular drugs: Lovastatin, Teprotide and Dicoumarol
- Neuromuscular blocking drugs: Curare alkaloids
- Anti-malarial drugs and analogues
- Chemistry of macrolide antibiotics (Erythromycin, Azithromycin, Roxithromycin, and Clarithromycin) and β -Lactam antibiotics (Cephalosporins and Carbapenem)

Unit 2

12 hours

- 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.
- Flavonoids: Introduction, isolation and purification of flavonoids, General methods of structural determination of flavonoids; Structural elucidation of quercetin.
- 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 (Vitamin D).

Unit 3

12 hours

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

Unit 4

12 hours

- 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
- Active constituent(s) 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.

Unit 5**12 hours**

Structural characterization of natural compounds using IR, ¹HNMR, ¹³CNMR and MS Spectroscopy of specific drugs e.g., Penicillin, Morphine, Camphor, Vitamin D, Quercetin and Digitalis glycosides

REFERENCES

1. Modern Methods of Plant Analysis, Peech and MV 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, Chapmanstall.
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 (MPC 105P)

Scope: This course is designed to provide hand-on practice for analysis of pharmacopoeial compounds and reactions of synthetic importance. It also includes performing isolation, purification and characterization of medicinal compounds.

Course Outcomes: Through this course students should be able to

CO1: Outline the principles involved in pharmaceutical analysis

CO2: Apply appropriate techniques for the qualitative and quantitative analysis of chemicals in laboratories and in industries

CO3: Illustrate both basics and practical aspects of various separation techniques including chromatographic methods.

CO4: Illustrate both theory and practical aspects of various name reactions and synthesis of medicinally important compounds.

CO5: Interpret NMR, IR, MS, UV-Vis spectroscopic techniques in solving structure of organic molecules and in determination of their stereochemistry

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-Schmidt 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

Seminar/Assignment (MPC106)

Scope: This course provides path to acquire skills and focuses on work in a professional digital format online/offline towards specific job goals and so forth. It also provides an opportunity to re-address previous projects, assignments for inclusion in their portfolios.

Course Outcomes: Through this course students should be able to

CO1: Analyze the knowledge gained during degree program to generate new skills and present it in a scientific manner

CO2: Develop the presentation proficiency

CO3: Develop specific communication skills associated with reporting technical information

CO4: Apply substantive argumentation, utilizing personal views that are based on critical analysis of works of various field of analysis

CO5: Outline how to cite the different information sources and previous reports related to specific area of the study

CO6: Develop good scientific and writing skills in paper presentation

M. Pharm II Sem

ADVANCED SPECTRAL ANALYSIS (MPC 201T)

Scope: This course 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.

Course Outcomes: Through this course students should be able to

CO1: Understand and apply different spectroscopic techniques for interpretation of various organic compounds spectra.

CO2: Understand theoretical and practical skill of the hyphenated instruments.

CO3: Develop skill to analyse and evaluate organic compounds.

CO4: Learn principles, instrumentation and application of different chromatographic techniques.

CO5: Understand different methods of analysis.

THEORY 60Hrs

Unit 1

12 hours

1. 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.

Unit 2

12 hours

NMR spectroscopy:

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

Unit 3

12 hours

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.

Unit 4

12 hours

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) Flash chromatography

Unit 5

12 hours

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 immuno assay: Biological standardization, bioassay, ELISA, Radioimmuno assay of digitalis and insulin.

REFERENCES

1. Spectrometric Identification of Organic compounds - Robert M Silverstein, Sixth edition, John Wiley & Sons, 2004. 46
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

ADVANCED ORGANIC CHEMISTRY – II (MPC 202T)

Scope: This course is designed to provide in-depth knowledge about recent advances in organic chemistry, different techniques of organic synthesis and their applications to process chemistry as well as drug discovery.

Course Outcomes: Through this course students should be able to

CO1: Understand the principles and applications of Green chemistry in microwave assisted and ultrasound assisted reactions.

CO2: Explain the concept of peptide chemistry.

CO3: Examine the concept of photochemical and pericyclic reactions.

CO4: Determine the various catalysts used in organic reactions.

CO5: Understand the concept of stereochemistry and develop the knowledge of carrying out asymmetric synthesis.

THEORY 60 Hrs

12 hours

Unit 1

1. Green Chemistry:

- Introduction, principles of green chemistry
- 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
- Ultrasound assisted reactions: Types of sonochemical reactions, homogenous, heterogeneous liquid-liquid and liquid-solid reactions, synthetic applications
- Continuous flow reactors: Working principle, advantages and synthetic applications.

Unit 2

12 hours

Chemistry of peptides

- Coupling reactions in peptide synthesis
- 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
- Segment and sequential strategies for solution phase peptide synthesis with any two case studies
- Side reactions in peptide synthesis: Deletion peptides, side reactions initiated by proton abstraction, protonation, overactivation and side reactions of individual amino acids.

Unit 3

12 hours

Photochemical reactions:

Basic principles of photochemical reactions, Photo-oxidation, photo addition and photo-fragmentation.

Pericyclic reactions:

Mechanism, Types of pericyclic reactions such as cyclo addition, electrocyclic reaction and sigmatropic rearrangement reactions with examples

Unit 4

12 hours

Catalysis:

- Types of catalysis, heterogeneous and homogeneous catalysis, advantages and disadvantages
- Heterogeneous catalysis – preparation, characterization, kinetics, supported catalysts, catalyst deactivation and regeneration, some examples of heterogeneous catalysis used in synthesis of drugs.
- 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
- 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

Unit 5

12 hours

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, pseudo asymmetric centres, axes of symmetry, Fischers 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”, 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 Wothers., 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, ROC Norman and JM Coxan, 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.

COMPUTER AIDED DRUG DESIGN (MPC 203T)

Scope: This course is designed to impart knowledge on the current state of the art techniques involved in computer assisted drug design.

Course Outcomes: Through this course students should be able to

CO1: Illustrate the role of CADD, QSAR and discuss various physicochemical parameters in drug discovery

CO2: Generating 2D and 3D QSAR models.

CO3: Discuss Molecular modeling and docking including Quantum Mechanics, energy minimization methods and drug receptor interactions.

CO4: Understanding prediction and analysis of ADMET properties, De novo drug design, homolog modelling.

CO5: Understanding pharmacophore mapping, virtual screening and In Silico Drug Design.

THEORY 60 Hrs

Unit 1

12 hours

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.

Unit 2

12 hours

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.

Unit 3

12 hours

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, cholinesterase (AChE & BchE)

Unit 4

12 hours

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.

Unit 5

12 hours

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 Robert M Stroud and Janet. F Moore.

PHARMACEUTICAL PROCESS CHEMISTRY (MPC 204T)

Scope: This course 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.

Course Outcomes: Through this course students should be able to

CO1: Understand the fundamental concepts of process chemistry including synthetic strategy, scale up process, in process control and case studies.

CO2: Discuss the various unit operations including extraction, filtration, distillation, evaporation and crystallization.

CO3: Analyze the reaction mechanism and methods of nitration, halogenation and oxidation.

CO4: Understand the process of reduction, fermentation, reaction progress kinetics and expedient routes.

CO5: Illustrate the industrial safety.

**Theory : 60 Hrs
12 hours**

Unit 1

Process chemistry: Introduction, Synthetic strategy

Stages of scale up process: Bench, pilot and largescale process.

In-process control and validation of largescale process.

Case studies of some scale up process of APIs.

Impurities in API, types and their sources including genotoxic impurities

Unit 2

12 hours

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, non-aqueous solutions factors affecting crystallization, nucleation. Principle and general methods of preparation of polymorphs, hydrates, solvates and amorphous APIs.

Unit 3

12 hours

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. Non-metallic oxidizing agents such as H₂O₂, sodium hypochlorite, Oxygen gas, ozonolysis.

Unit 4

12 hours

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.

Unit 5

12 hours

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 chemical engineering, 7th edition, McGraw 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 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 53

PHARMACEUTICAL CHEMISTRY PRACTICALS – II (MPC 205P)

Scope: This course is designed to provide hand-on practice for synthesis of APIs/intermediates by different synthetic routes and interpretation of organic compounds by spectroscopic techniques.

Course Outcomes: Through this course students should be able to

CO1: Analyze the drug-protein interactions using molecular docking software

CO2: Relate the conventional and advanced synthetic methods of organic synthesis

CO3: Interpret the spectra of different organic compounds

CO4: Determine the purity of pharmaceuticals by differential scanning calorimetry

CO5: Make use of different routes for synthesis of organic compounds

CO6: Utilize various software's of drug design

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
11. Preparation of 4-chlorobenzhydrylpiperazine. (an intermediate for cetirizine HCl).
12. Preparation of 4-iodotoluene from p-toluidine.
13. NaBH₄ 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 (Any two)
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

Seminar Assignment (MPC206)

Scope: This course provides path to acquired skills and focuses on work in a professional digital format online/offline towards specific job goals and so forth. It also provides an opportunity to re-address previous projects, assignments for inclusion in their portfolios.

Course Outcomes: Through this course students should be able to

CO1: Discuss the methods in the major subject/field of study

CO2: Apply substantive argumentation, utilizing personal views that are based on critical analysis of works from various fields of knowledge

CO3: Assess and critically analyze different solutions

CO4: Demonstrate professional competence by identifying and analyzing emerging issues

CO5: Prioritize professional competence by identifying and analyzing emerging issues

CO6: Apply foundational research skills to address a research question

M. Pharmacy (Pharmaceutical Chemistry) III Sem

RESEARCH METHODOLOGY & BIOSTATISTICS (MPC 301T)

The subject trains the user in statistical methods to see the significance in the data derived from research experiments.

Course Outcomes: After completion of course, the student will be able to

CO1: Understand different experimental designs required in research

CO2: Understand applications of parametric and non-parametric tests in research

CO3: Understand the values and ethics of medical research

CO4: Understand the purpose of control and supervision of experiments on animals

Unit 1

12 Hours

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 2

12 hours

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 (Wilcoxon rank tests, analysis of variance, correlation, chi square test), null hypothesis, P values, degree of freedom, interpretation of P values.

Unit 3

12 Hours

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 4

12 Hours

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 5

12 Hours

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

REFERENCES

1. Kothari C.R., Research Methodology Methods and Techniques, Vishwa Prakashan, New Delhi.
2. Lokesh K., Methodology of Educational research, Vikash Publishing House Pvt. Ltd., New Delhi.
3. Kumar R., Research Methodology, Dorling Kindersley (India) Pvt. Ltd., New Delhi.
4. Rao G.N., Research Methodology and Qualitative Methods, B.S. Publications, Hyderabad.
5. Saunders M., Lewis P. and Thornhill A., Research Methods for Business Students, Dorling

Kindersley (India) Pvt. Ltd., New Delhi.

6. Bolton S. and Bon C., Pharmaceutical Statistics: Practical and Clinical Applications, Marcel Dekker, New York.

7. Garg, B.L., Karadia, R., Agarwal, F. and Agarwal, An introduction to Research Methodology, RBSA Publishers, Jaipur.

8. Fisher R.A. Statistical Methods for Research Works, Oliver and Boyd, Edinburgh.

9. Chow S.S. and Liu J.P., Statistical Design and Analysis in Pharmaceutical Sciences, Marcel Dekker, New York.

10. Buncher C.R., Statistics in the Pharmaceutical Industry, Marcel Dekker, New York.

JOURNAL CLUB (MPC 302)

Scope: It provides a platform to enhance the research aptitude, reading capabilities and presenting capabilities of researcher by using various published articles.

Course Outcomes: After completion of course, the student will be able to

CO1: Identify the various recent studies in the field of pharmaceutical research

CO2: Illustrate professional competence by identifying and analyzing emerging issues

CO3: Analyze ability of self-learning and professional development

CO4: Develop a capacity to communicate research results clearly, comprehensively and persuasively

CO5: Understand the journal guidelines/instructions for writing manuscripts.

DISCUSSION/PRESENTATION (MPC 303)

Scope: This course helps the students to analyze the research done and search its future perspective

Course Outcomes: After completion of course, the student will be able to

CO1: Outline possible strategies to deal with research problems

CO2: Analyze the research problem and evaluate alternative solutions

CO3: Propose scientific argumentation based on critical analysis of work

CO4: Integrate their knowledge and practical skills during problem solving

CO5: Develop the key skills required to facilitate a scientific discussion

RESEARCH WORK (MPC 304)

Scope: This course involves the students to use rigorous methods to solve problems related to a substantive area of the study.

Course Outcomes: After completion of course, the student will be able to

CO1: Ability to identify the research problem.

CO2: Understand methodologies to solve the research problem.

CO3: Generation of result, arrangement and analysis.

CO4: Create substantive argumentation, utilizing personal views that are based on critical analysis of works from various fields of knowledge.

CO5: Demonstrate different tools employed in arranging **REFERENCES** in manuscripts

M. Pharm IV Sem

JOURNAL CLUB (MPC 401)

Scope: It provides a platform to enhance the research aptitude, reading capabilities and presenting capabilities of researcher by using various published articles.

Course Outcomes: After completion of course, the student will be able to

CO1: Identify the various recent studies in the field of pharmaceutical research

CO2: Illustrate professional competence by identifying and analyzing emerging issues

CO3: Analyze ability of self-learning and professional development

CO4: Develop a capacity to communicate research results clearly, comprehensively and persuasively

CO5: Understand the journal guidelines/instructions for writing manuscripts.

RESEARCH WORK (MPC 402)

Scope: This course involves the students to use rigorous methods to solve problems related to a substantive area of the study.

Course Outcomes: After completion of course, the student will be able to

CO1: Ability to identify the research problem.

CO2: Understand methodologies to solve the research problem.

CO3: Generation of result, arrangement and analysis.

CO4: Create substantive argumentation, utilizing personal views that are based on critical analysis of works from various fields of knowledge.

CO5: Demonstrate different tools employed in arranging **REFERENCES** in manuscripts

DISCUSSION/ FINAL PRESENTATION (MPC 403)

Scope: This course helps the students to analyze the research done and search its future perspective

Course Outcomes: After completion of course, the student will be able to

CO1: Outline possible strategies to deal with research problems

CO2: Analyze the research problem and evaluate alternative solutions

CO3: Propose scientific argumentation based on critical analysis of work

CO4: Integrate their knowledge and practical skills during problem solving

CO5: Develop the key skills required to facilitate a scientific discussion