GANDHI INSTITUTE OF TECHNOLOGY AND MANAGEMENT (GITAM)
(Deemed to be University)
VISAKHAPATNAM * HYDERABAD * BENGALURU

Accredited by NAAC with A^+ Grade

REGULATIONS AND SYLLABUS

OF

MASTER OF PHARMACY (M. Pharm. Pharmaceutical Chemistry)

(w.e.f. 2020-21 admitted batch)

A University Committed to Excellence

MASTER OF PHARMACY (M. Pharm. Pharmaceutical Chemistry)
REGULATIONS as per PCI
(w.e.f. 2020-2021 admitted batch)

1.0 ADMISSIONS

1.1 Admissions into M. Pharmacy programme of GITAM University are governed by GITAM University admission regulations.

2.0 MINIMUM QUALIFICATION FOR ADMISSION

A Pass in the following examinations

2.1 B. Pharm. Degree examination of an Indian University established by law in India from an institution approved by Pharmacy Council of India (PCI) and has scored not less than 50 % of the maximum marks (aggregate of 4 years of B. Pharm.)

2.2 Every student, selected for admission to post graduate pharmacy programme 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.

2.3 Admissions into M. Pharm. will be based on All India Entrance Test (GAT - PGP) conducted by GITAM University and the rule of reservation is followed wherever applicable.

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 PROGRAMME

The programme of study for M. Pharm. shall extend over a period of four semesters (two academic years).

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 November/December to April/May 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. PROGRAMME/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.** These credits are divided into theory courses, practical, seminars, assignments, research work, discussions with the supervisor and journal club over the duration of four semesters. The credits are distributed semester-wise as shown in Table 8. 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. specialization shall include semester wise theory & practical as given in Table –1 to 3. The number of hours to be devoted to each theory and practical course in any semester shall not be less than that shown in Table –1 to 3.

Table – 1: Course of study for M. Pharm. (Pharmaceutical Chemistry)

Course Code	Course	Credit Hours	Credit Points	Hrs./wk	Marks
Semester I					
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 106P	Seminar/Assignment	7	4	7	100
	Total	35	26	35	650
Semester II					
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 206P	Seminar/Assignment	7	4	7	100
	Total	35	26	35	650

Table – 2: Course of study for M. Pharm. III Semester

Course Code	Course	Credit Hours	Credit points
MRM 301T	Research Methodology and Biostatistics*****	4	4
MPR 301T	Journal club	2	2
MPR 302T	Discussion/Presentation (Proposal presentation)	2	2
MPR 303P	Research Work (Proposed project work, Literature survey, Plan of work, Methodology)	28	14
Total		36	22

* Non University Exam

Table – 3: Course of study for M. Pharm. IV Semester

Course Code	Course	Credit Hours	Credit points
MPR 401T	Discussion/ Final Presentation (Presentation of work, communication skills, question and answers)	3	3
MPR 402P	Research work and colloquium (Objective(s) of the work done, Methodology adopted, Results & Discussions, Conclusions & Outcomes)	36	18
Total		39	21

Table – 4: Semester wise credits distribution

Semester	Credit points
I	26
II	26
III	22
IV	21
Total Credit Points	**95**

10. PROGRAMME 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 Table –5 to 6.

11.1. **End semester examinations**

The End Semester Examinations for each theory and practical course through semesters I to IV shall be conducted by the respective University except for the subject with asterix symbol (*) in table 6 for which examinations shall be conducted by the subject experts at college level and the marks/grades shall be submitted to the University.

Table – 5: Schemes for internal assessments and end semester (Pharmaceutical Chemistry– MPC)

Course code	Course	Internal Assessment				End Semester Exams		Total Marks
		Continuous mode	Sessional Exams		Total	Marks	Duration	
			Marks	Duration				
Semester I								
MPC 101T	Modern Pharmaceutical Analytical Techniques	10	15	1 Hr	25	75	3 Hr	100
MPC 102T	Advanced Organic Chemistry - I	10	15	1 Hr	25	75	3 Hr	100
MPC 103T	Advanced Medicinal Chemistry	10	15	1 Hr	25	75	3 Hr	100
MPC 104T	Chemistry of Natural Products	10	15	1 Hr	25	75	3 Hr	100
MPC 105P	Pharmaceutical Chemistry Practical – I	20	30	6 Hr	50	100	6 Hr	150
MPC 106P	Seminar/Assignment	-	-	-	-	100	-	100
Total								650
Semester II								
MPC 201T	Advanced Spectral Analysis	10	15	1 Hr	25	75	3 Hr	100
MPC 202T	Advanced Organic Chemistry – II	10	15	1 Hr	25	75	3 Hr	100
MPC 203T	Computer Aided Drug Design	10	15	1 Hr	25	75	3 Hr	100
MPC	Pharmaceutical Process	10	15	1 Hr	25	75	3 Hr	100

204T	Chemistry							
MPC 205P	Pharmaceutical Chemistry Practical – II	20	30	6 Hr	50	100	6 Hr	150
MPC 206P	Seminar/Assignment	-	-	-	-	100	-	100
Total								650

Table – 6: Schemes for internal assessments and end semester examinations

(Semester III & IV)

Course code	Course	Internal Assessment				End Semester Exams		Total Marks
		Continuous mode	Sessional Exams		Total	Marks	Duration	
			Marks	Duration				
Semester III								
MRM 301T	Research Methodology and Biostatistics*	10	15	1 Hr	25	75	3 Hr	100
MPR 301T	Journal club	-	-	-	100	-	-	100
MPR 302T	Discussion/Presentation (Proposal presentation)	-	-	-	100	-	-	100
MPR 303P	Research Work (proposed project work, Literature survey, Plan of work, Methodology)	-	-	-	-	100	1 Hr	100
Total								400
Semester IV								
MPR 401T	Discussion/ Presentation (Presentation of work, communication skills, question and answers)	-	-	-	100	-	-	100
MPR 402P	Research Work and colloquium (Objective(s) of the work done, Methodology adopted, Results & Discussions, Conclusions & Outcomes)	-	-	-	-	100	1 Hr	100
Total								200

* Non University Examination

11.2. **Internal assessment: Continuous mode**

The marks allocated for Continuous mode of Internal Assessment shall be awarded as follows.

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

Criteria	Maximum Marks
Theory	
Attendance (Refer Table -5)	8
Student – Teacher interaction	2
Total	10
Practical	
Attendance (Refer Table – 5)	10
Based on Practical Records, Regular viva voce, etc.	10

Total	20

Table – 8: Guidelines for 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 **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 in the tables 5 – 6. The average marks of two sessional exams shall be computed for internal assessment as per the requirements given in tables.

12. PROMOTION AND AWARD OF GRADES

A student shall be declared PASS and eligible for getting grade in a course of M. Pharm. programme 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. IMPROVEMENT OF INTERNAL ASSESSMENT

A student shall have the opportunity to improve his/her performance only once in the sessional exam component of the internal assessment. The re-conduct of the sessional exam shall be completed before the commencement of next end semester theory examinations.

15. REEXAMINATION OF END SEMESTER EXAMINATIONS

Reexamination of end semester examination shall be conducted as per the schedule given in table 9. The exact dates of examinations shall be notified from time to time.

Table – 9: Tentative schedule of end semester examinations

Semester	For Regular candidates	For Failed Candidates
I and III	November/December	April/May
II and IV	April/May	November/December

16. ALLOWED TO KEEP TERMS (ATKT):

No student shall be admitted to any examination unless he/she fulfills the norms given in 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.

17. GRADING OF PERFORMANCES

17.1. 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.

18. 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:

$$\mathbf{SGPA} = \frac{\mathbf{C_1G_1 + C_2G_2 + C_3G_3 + C_4G_4}}{\mathbf{C_1 + C_2 + C_3 + C_4}}$$

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 AB grade awarded in that semester. For example, if a learner has a F or AB grade in course 4, the SGPA shall then be computed as:

$$\mathbf{SGPA} = \frac{\mathbf{C_1G_1 + C_2G_2 + C_3G_3 + C_4 \times ZERO}}{\mathbf{C_1 + C_2 + C_3 + C_4}}$$

19. 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:

$$\mathbf{CGPA} = \frac{\mathbf{C_1S_1 + C_2S_2 + C_3S_3 + C_4S_4}}{\mathbf{C_1 + C_2 + C_3 + C_4}}$$

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, …. …….

20. 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

21. 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).

22. 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. programme shall not be eligible for award of ranks. Moreover, the candidates should have completed the M. Pharm. programme in minimum prescribed number of years, (two years) for the award of Ranks.

23. AWARD OF DEGREE

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

24. DURATION FOR COMPLETION OF THE PROGRAMME OF STUDY

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

25. REVALUATION/RETOTALING OF ANSWER PAPERS

There is no provision for revaluation of the answer papers in any examination. However, the candidates can apply for retotaling by paying a prescribed fee.

26. RE-ADMISSION AFTER BREAK OF STUDY

Candidates who seeks re-admission to the programme after break of study has to get the approval from the University by paying a condonation fee.

27. PROGRAMME EDUCATIONAL OBJECTIVES (PEO)

PEO1: To provide a comprehensive and advanced pharmaceutical education leading to M. Pharm. Degree.

PEO2: To integrate pharmacy knowledge and skills with pharmaceutical research.

PEO3: To develop pharmacists to contribute effectively in the social health care system.

PEO4: To provide hands on training through state of art infrastructure to inculcate research aptitude in pharmaceutical sciences.

PEO5: To inculcate leadership and entrepreneurship capabilities in future pharmacy professionals.

28. PROGRAM OUTCOMES (PO)

PO 1: Graduates are acquaintance with mechanisms for reactions in organic chemistry, polymer chemistry and biochemistry and to develop synthetic route for small molecules.

PO 2: Capability of understanding and up gradation of an organic reaction including isolating, purifying and characterizing the product.

PO 3: Acquire a detailed understanding of the processes involved in the design, development and discovery of medicinal compounds.

PO 4: Graduates will receive knowledge of numerous hyphenated analytical instrumental procedures as well as the ability to interpret the data obtained from them.

PO 5: Gain a full understanding of how novel pharmaceuticals were created using pharmacophore modeling and docking techniques.

29. PROGRAM SPECIFIC OUTCOMES:

PSO 1: Graduates are competent to conduct independent research, investigation, and development new chemical entities, as well as synthetic techniques and drug design.

PSO 2: Graduates can use software and technology to conduct research and design products and processes.

PSO3: Graduates with the understanding of numerous identified reactions, processes, and properties of distinct chemical groups, as well as drug synthesis optimization can contribute to drug discovery.

PSO 4: Graduates with their understanding of cost-effective and environmentally friendly mechanisms by lowering the number of stages and limiting waste by following green chemistry principles can minimize the pollution.

PSO 5: Gain knowledge of practical techniques and advanced techniques to solve the problems in isolation, separation, purification and confirmation of chemical entities.

SEMESTER – I

PHARMACEUTICAL CHEMISTRY (MPC)

MPC 101T. MODERN PHARMACEUTICAL ANALYTICAL TECHNIQUES

Hours per week: 4L — End Examination: 75 Marks
Credit: 4 — Midsem: 25 Marks

Course Description: This course is designed to provide the student with basic information about various instrumental techniques covering spectroscopy, chromatography and thermal analysis. During the course the student will be learning the concepts and applications of various absorption (UV-Visible, IR) and emission (Spectrofluorimetry, Flame photometry) spectroscopic techniques along with X-ray crystallography, NMR and Mass spectroscopy. The student will also gain knowledge on the significance of various basic to complex chromatographic (TLC, HPLC, GC, Affinity chromatography) and electrophoresis (Gel, Moving boundary) techniques.

Course objectives: 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.

UNIT – I **12 Hrs**

a. UV-Visible spectroscopy: Introduction, Theory, laws, instrumentation associated with UV-Visible spectroscopy, choice of solvents and solvent effect and applications of UV-Visible spectroscopy, 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 analyzed by fluorimetry), quenchers, instrumentation and applications of fluorescence spectrophotometer.
d. Flame emission spectroscopy and Atomic absorption spectroscopy: Principle, instrumentation, interferences and applications.

UNIT – II **12 Hrs**

NMR spectroscopy: Quantum numbers and their role in NMR, principle, instrumentation, solvent requirement in NMR, relaxation process, NMR signals in various compounds, chemical shift, factors influencing chemical shift, spin-spin coupling, coupling constant, nuclear magnetic double resonance, brief outline of principles of FT-NMR and 13C NMR. Applications of NMR spectroscopy.

UNIT – III **12 Hrs**

Mass Spectroscopy: Principle, theory, instrumentation of mass spectroscopy, different types of ionization like electron impact, chemical, field, FAB and MALDI, APCI, ESI, APPI. Analyzers of quadrupole and time of flight, mass fragmentation and its rules, meta stable ions, isotopic peaks and applications of mass spectroscopy.

UNIT – IV **12 Hrs**

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 – V **12 Hrs**

a. Principle, instrumentation and applications of gel electrophoresis and moving boundary electrophoresis

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

c. Thermal Techniques:

Differential Scanning Calorimetry (DSC): 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).

Thermogravimetric Analysis (TGA): Principle, instrumentation, factors affecting results, advantages and disadvantages, pharmaceutical applications.

Course outcomes: After completion of course student is able to know,

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

References

1. Spectrometric Identification of Organic compounds - Robert M Silverstein, 6th 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 – A H Beckett and J B 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 edition, P.S/Kalsi, Wiley Eastern Ltd., Delhi.
9. Textbook of Pharmaceutical Analysis, K A Connors, 3rd edition, John Wiley & Sons, 1982.

MPC 102T. ADVANCED ORGANIC CHEMISTRY – I

Hours per week: 4L | End Examination: 75 Marks
Credit: 4 | Midsem: 25 Marks

Course description:

This course covers the fundamentals of organic chemistry, including the application of named reactions, the study of organic reaction mechanisms, as well as synthetic reagents, protecting groups, and the synthesis of drugs containing five, six, and fused heterocycles, including the synthon approach.

Course objectives: 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.

UNIT – I **12 Hrs**

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

1. Nucleophilic uni- and bimolecular reactions (SN1 and SN2)
2. Elimination reactions (E1 & E2; Hoffman & Saytzeff's rule)
3. Rearrangement reaction

UNIT – II **12 Hrs**

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

UNIT – III **12 Hrs**

1. Synthetic Reagents & Applications

Aluminiumisopropoxide, 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).

2. Protecting groups

a. Role of protection in organic synthesis
b. Protection for the hydroxyl group, including 1,2-and1,3-diols: ethers, esters, carbonates, cyclic acetals & ketals
c. Protection for the carbonyl group: Acetals and ketals
d. Protection for the carboxyl group: Amides and hydrazides, esters

e. Protection for the amino group and amino acids: Carbamates and amides

UNIT – IV **12 Hrs**

Heterocyclic Chemistry:

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

Synthesis of few representative drugs containing these heterocyclic nuclei 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.

UNIT – V **12 Hrs**

Synthon approach and retrosynthesis applications

(i) Basic principles, terminologies and advantages of retrosynthesis; guidelines for dissection of molecules. Functional group interconvertion 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.

Course outcomes: 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

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 4th edition, VK Ahluwalia and RK Parashar, Narosa

Publishers.

MPC 103T. ADVANCED MEDICINAL CHEMISTRY

Hours per week: 4L | End Examination: 75 Marks
Credit: 4 | Midsem: 25 Marks

Course description:

The course focuses on fundamental aspects of contemporary medicinal chemistry. Introduces design and development of drug candidates to cure diseases based on the modulation of current drug targets, including proteins, nucleic acids, and other receptor-based functionalities. Focuses on Stereochemistry, structure-activity relationships, pharmacokinetics, and pharmacodynamics.

Course objectives: 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.

UNIT – I **12 Hrs**

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, agonist's vs antagonists, and artificial enzymes.

UNIT – II **12 Hrs**

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 consideration of prodrug design.

(b) Combating drug resistance: Causes for drug resistance, strategies to combat drug resistance in antibiotics and anticancer therapy,

(**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.

UNIT – III **12 Hrs**

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 – IV **12 Hrs**

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

UNIT – V **12 Hrs**

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.

Course outcomes: 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

References

1. Medicinal Chemistry by Burger, Vol I –VI.
2. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, 12th edition, Lippincott Williams & Wilkins, 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, 3rd edition, Oxford University Press, USA.
11. Biopharmaceutics and pharmacokinetics, D M. Brahmankar, Sunil B. Jaiswal II Edition, 2014, Vallabh Prakashan, New Delhi.
12. Peptidomimetics in Organic and Medicinal Chemistry by Antonio Guarna and Andrea Trabocchi, 1st edition, Wiley publishers.

MPC 104T. CHEMISTRY OF NATURAL PRODUCTS

Hours per week: 4L — End Examination: 75 Marks
Credit: 4 — Midsem: 25 Marks

Course description:

The course provides a brief introduction to natural products as leads for new pharmaceuticals, significant medicinal plants will be discussed. Important classes of compounds (secondary metabolites) like alkaloids, flavonoids, terpinoids, vitamins and steroids from nature will be emphasised, and stress will be put on classification, isolation, purification, molecular modification and structural analysis and pharmaceutical perspectives.

Course objectives: 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.

UNIT – I **12 Hrs**

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

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

UNIT – II **12 Hrs**

(a) Alkaloids

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

(b) Flavonoids

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

(c) Steroids

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

UNIT – III

(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).

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

UNIT – IV **12 Hrs**

(a) Recombinant DNA technology and drug discovery

rDNA technology, hybridoma technology, new pharmaceuticals derived from biotechnology; Oligonucleotide therapy. Gene therapy: Introduction, clinical application and recent advances in gene therapy, principles of RNA & DNA estimation.

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

UNIT – V **12 Hrs**

Structural Characterization of natural compounds

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

Course outcomes: 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

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

MPC 105P. PHARMACEUTICAL CHEMISTRY PRACTICAL – I

Hours per week: 12 End Examination: 100 Marks
Credit: 6 Midsem: 50 Marks

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

SEMESTER – II

MPC 201T. ADVANCED SPECTRAL ANALYSIS

Hours per week: 4L — End Examination: 75 Marks
Credit: 4 — Midsem: 25 Marks

Course description:

This course covers the fundamentals and in-depth knowledge of hyphenated analytical instrumental techniques such as LC-MS, GC-MS, ATR-IR, DSC, and others for drug identification, characterization, and quantification. Different chromatographic methods are taught, as well as other key topics, to help students comprehend and apply the principles involved in the identification of various bulk medicines and their formulations.

Course objectives: 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.

UNIT – I **12 Hrs**

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 – II **12 Hrs**

NMR spectroscopy:

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

UNIT – III **12 Hrs**

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 – IV **12 Hrs**

Chromatography:

Principle, Instrumentation and Applications of the following:

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

UNIT – V **12 Hrs**

(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.

Course outcomes: 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

References

1. Spectrometric Identification of Organic compounds - Robert M Silverstein, Sixth edition, John Wiley & Sons, 2004.
2. Principles of Instrumental Analysis - Doglas A Skoog, F. James Holler, Timothy A. Nieman, 5th edition, Eastern press, Bangalore, 1998
3. Instrumental methods of analysis – Willards, 7th edition, CBS publishers.
4. Organic Spectroscopy - William Kemp, 3rd edition, ELBS, 1991.
5. Quantitative analysis of Pharmaceutical formulations by HPTLC - P 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

MPC 202T. ADVANCED ORGANIC CHEMISTRY – II

Hours per week: 4L End Examination: 75 Marks

Credit: 4 Midsem: 25 Marks

Course description:

This course discusses the necessity of clean and sustainable technology as well as the application of green chemistry. Introduces new synthesis concepts such as microwave and ultrasonic assisted synthesis, peptide chemistry, photochemical and pericyclic reactions, and the utilization of bio catalysts, as well as Asymmetric synthesis understanding.

Course objectives: 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.

UNIT – I **12 Hrs**

Green Chemistry:

(a) Introduction, principles of green chemistry

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

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

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

UNIT – II **12 Hrs**

Chemistry of peptides

(a) Coupling reactions in peptide synthesis

(b) Principles of solid phase peptide synthesis, t-BOC and FMOC protocols, various solid supports and linkers: Activation procedures, peptide bond formation, deprotection and cleavage from resin, low and high HF cleavage protocols, formation of free peptides and peptide amides, purification and case studies, site-specific chemical modifications of peptides

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

(d) Side reactions in peptide synthesis: Deletion peptides, side reactions initiated by proton abstraction, protonation, over- activation and side reactions of individual amino acids.

UNIT – III **12 Hrs**

(a) Photochemical reactions

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

(b) Pericyclic reactions: Mechanism, Types of pericyclic reactions such as cyclo addition, electrocyclic reaction and sigmatrophic rearrangement reactions with examples.

UNIT – IV **12 Hrs**

Catalysis:

(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

UNIT – V **12 Hrs**

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.

Course outcomes: 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

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, 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, R O C Norman and J M Coxan, Nelson thorns
8. Organic synthesis- Special techniques V K Ahluwalia and R Aggarwal, Narosa Publishers.
9. Organic reaction mechanisms IV edition, V K Ahluwalia and R K Parashar, Narosa Publishers.

MPC 203T. COMPUTER AIDED DRUG DESIGN

Hours per week: 4L — End Examination: 75 Marks
Credit: 4 — Midsem: 25 Marks

Course description:

This Computer Aided Drug Design course covers all of the major computational approaches used in drug development and provides a foundational understanding of the topic. The course will cover structure and target-based design, molecular modelling, quantum physics, drug

similarity characteristics, QSAR, and pharmacokinetics and dynamics utilising a variety of open-source applications.

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

UNIT – I **12 Hrs**

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 – II **12 Hrs**

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 – III **12 Hrs**

Molecular Modeling and Docking

(a) Molecular and quantum mechanics in drug design.

(b) Energy Minimization Methods: Comparison between global minimum conformation and bioactive conformation**.**

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

UNIT – IV **12 Hrs**

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 – V **12 Hrs**

(a) Pharmacophore Mapping and Virtual Screening

Concept of pharmacophore, pharmacophore mapping, identification of pharmacophore features and pharmacophore modeling; conformational search used in pharmacophore mapping.

(b) In Silico Drug Design and Virtual Screening Techniques

Similarity based methods and pharmacophore based screening, structure based in-silico virtual screening protocols.

Course outcomes: 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

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

MPC 204T. PHARMACEUTICAL PROCESS CHEMISTRY

Hours per week: 4L — End Examination: 75 Marks
Credit: 4 — Midsem: 25 Marks

Course description:

This course aims to impart knowledge on safe, cost-effective, environmentally friendly, and efficient synthetic routes, as well as industrial safety measures, by providing a detailed description on the handling of most important industrial unit operations, scale up process processes for APIs.

Course objectives: 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.

UNIT – I **12 Hrs**
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.

UNIT – II **12 Hrs**

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 – III **12 Hrs**

Unit Processes - I

(a) Nitration: Nitrating agents, aromatic nitration, kinetics and mechanism of aromatic nitration, process equipment for technical nitration, mixed acid for nitration.
(b) Halogenation: Kinetics of halogenations, types of halogenations, catalytic halogenations. Case study on industrial halogenation process.
(c) Oxidation: Introduction, types of oxidative reactions, liquid phase oxidation with oxidizing agents. Nonmetallic Oxidizing agents such as H_2O_2, sodium hypochlorite, oxygen gas, ozonolysis.

UNIT – IV **12 Hrs**

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 – V **12 Hrs**

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.

Course outcomes: 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

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 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

MPC 205P. PHARMACEUTICAL CHEMISTRY PRACTICALS – II

Hours per week: 12 — End Examination: 100 Marks
Credit: 6 — Midsem: 50 Marks

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-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 (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

SEMESTER – III

MRM 301T. RESEARCH METHODOLOGY & BIOSTATISTICS

Hours per week: 4L — End Examination: 75 Marks
Credit: 4 — Midsem: 25 Marks

Course Description: This introductory course of research methodologies and biostatistics will give students an overview of the many study designs and statistical tests that are used in the medical industry to answer research issues. This course focuses on the CPCSEA guidelines and prerequisites for performing animal experiments, categorising research projects, developing a study, experimental design, measuring and interpreting data, and conducting ethical research.

Course objectives: Impart knowledge on statistical principles that can be applied to design experiments and help in the interpretation of the results.

UNIT – I **12 Hrs**

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

UNIT – II **12 Hrs**

Biostatistics: Definition, application, sample size, importance of sample size, factors influencing sample size, dropouts.
Measures of central tendency: Computation of means, median and mode from grouped and ungrouped data. Measure of dispersion: Computation of variance, standard deviation, standard error and their coefficients.

UNIT – III **12 Hrs**

Regression and correlation: Method of least squares, Correlation Coefficient, rank correlation and multiple regressions.
Probability rules: Binomial, poison and normal distribution.

UNIT – IV **12 Hrs**

Tests of significance: Testing hypotheses- principle and applications of Z, t-, F- ratio and chi-square tests in pharmaceutical and medical research. Analysis of Variance: 1-way, 2-way and 3-way classification. Non-parametric tests: Sign test, Wilcoxon signed rank test, Wilcoxon rank sum test, Kruskal Wallis test, run test and median tests.

UNIT – V **12 Hrs**

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.

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

Course Outcomes: Upon completion of the course the student is able to select appropriate statistical methods required for a particular research design and develop appropriate research hypothesis for a research project. Develop appropriate framework for research studies. Gain knowledge regarding CPCSEA guidelines and prerequisites for conducting animal experiments.

References

1. Santosh Gupta: "Research Methodology and Statistical Techniques", Deep & Deep Publication, 2001

2. C. R. Kothari: "Research Methodology – Methods & Techniques", 2nd edition, Wishwa Prakashan, 2000.

3. K. P. C. Swain:"A Text book of Research Methodology", 1st edition, Kalyani Publishers, 2007.

4. "Research Methodology and Statistical Techniques" Indira Gandhi National Open University.

5. M. N. Ghosh: "Fundamentals of Experimental Pharmacology", 2nd edition, Scientific Book Agency, Calcutta, India, 1984.

6. H. G. Vogel: "Drug Discovery and Evaluation-Pharmacological Assays", 2nd edition, Springer Verlag, Berlin, Germany, 2002.