

Semester-I	Semester-II	Semester-III	Semester-IV
PC-601: Foundation Course in Inorganic Chemistry ④	PC-602: Conformational Analysis and Asymmetric Synthesis ④	PC-701: Advanced Organic Chemistry ④	PC-702: Drug Synthesis and Mechanism of Action ④
PC-603: Foundation Course in Organic Chemistry ④	PC-604: Synthetic Methods in Medicinal Chemistry ④	PC-703: Bioenergetics and Metabolism ④	PC-704: Pharmacology ③ Molecular
PC-605: Foundation Course in Physical Chemistry ④	PC-606: Spectroscopic Studies ④	PC-705(A1): Separation Science ② PC-705(A2): Molecular Spectroscopy ②	PC-706: Medicinal Chemistry ④
PC-607: Introduction to Biomolecules ③	PC-608: Enzymes ② PC-610: Green Chemistry ②	PC-707: Introduction to Microbiology ③ PC-709: Concepts in Drug Design ②	PC-708(A1): Formulation Chemistry ② PC-708(A2): Heat and Mass Transfer ② PC-710(A1): Bio-Statistics ② PC-710(A2): Bio-Ethics ② PC-710(A3): Intellectual Property Right ②
PC-651: Foundation Course Practical-I (Organic Chemistry) ⑧	PC-612: History and Philosophy of Science ⑩	PC-711: Developing Entrepreneurial Mindset ②	PC-712: Systemic Pharmacology ②
PC-653: Foundation Course Practical-II (Physico-Inorganic Chemistry) ⑧	PC-652: Medicinal Chemistry Practical ⑧	PC-751: Computational Drug Design Practical ④	PC-800: Project/Dissertation ⑩
PC-655: Introduction to Computational Chemistry ②	PC-654: Enzymology Practical ⑧	PC-753: Microbiology Practical ④ PC-799: Project/Dissertation ⑧	

CC: Core Course

DCE: Discipline Centric Elective

SEC: Skill Enhancement Course

CFC/AECC: Compulsory Foundation Course/Ability Enhancement Compulsory Course

GE: Generic Elective Course

NUES: Non University Examinational Subject (Entitled for credit and not to be considered for the purpose of declaration of Result)

\*Note: Student would have to opt one course each from 705A1/705A2, 708A1/708A2 and 710A1/710A2/710A3

o : Depicts Hours



*Signature*

*Beepa Devanil Ravi*

**MASTER OF SCIENCE  
(MEDICINAL CHEMISTRY AND DRUG DESIGN)**



**CENTRE FOR EXCELLENCE IN PHARMACEUTICAL SCIENCES  
GURU GOBIND SINGH INDRAPRASTHA UNIVERSITY  
SECTOR-16C, DWARKA, NEW DELHI-110078**

*Deepa Suman*  
*Asst. Prof.*

*Paul*

*Fulw*



## CENTRE FOR EXCELLENCE IN PHARMACEUTICAL SCIENCES

### II- INTRODUCTION TO CBCS (CHOICE BASED CREDIT SYSTEM)

The CBCS provides an opportunity for the students to choose courses from the prescribed courses comprising core, elective/minor or skill-based courses. The courses can be evaluated following the grading system, which is considered to be better than the conventional marks system.

Grading system provides uniformity in the evaluation and computation of the Cumulative Grade Point Average (CGPA) based on student's performance in examinations which enables the student to move across institutions of higher learning. The uniformity in evaluation system also enables the potential employers in assessing the performance of the candidates.

#### Definitions:

- (i) 'Academic Programme' means an entire course of study comprising its programme structure, course details, evaluation schemes etc. designed to be taught and evaluated in a teaching Centre/School or jointly under more than one such Department/Centre.
- (ii) 'Course' means a segment of a subject that is part of an Academic Programme.
- (iii) 'Programme Structure' means a list of courses (Core, Elective, Open Elective) that makes up an Academic Programme, specifying the syllabus, credits, hours of teaching, evaluation and examination schemes, minimum number of credits required for successful completion of the programme etc. prepared in conformity to University rules, eligibility criteria for admission.
- (iv) 'Core Course' (CC) means a course that a student admitted to a particular programme must successfully complete to receive the degree and which cannot be substituted by any other course.
- (v) 'Discipline Centric Elective' (DCE) means an elective course which is available for students of the programme in which student is studying.
- (vi) 'Skill enhancement Course' (SEC) courses are the courses based upon the content that leads to knowledge enhancement and are skill-based which are aimed at providing hands-on-training, competencies, skills etc.
- (vii) 'Compulsory Foundation Course'/'Ability Enhancement Compulsory Course' (CFC/AECC) courses are the courses based upon the content that leads to knowledge enhancement and these courses are value-based.
- (viii) 'Generic Elective Course' (GE) means an optional course to be selected by a student out of such courses offered in the same or any other School/Centre.
- (ix) 'Open Elective' means an elective course which is available for students of all programmes, including students of same School/Centre. Students of other School/Centre will opt these courses subject to fulfilling of eligibility of criteria as laid down by the School/Centre offering the course.

Deepa Desmal

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- (x) 'Credit' means the value assigned to a course which indicates the level of instruction: One-hour lecture per week equals 1 credit, 2 hours practical class per week equals 1 credit. Credit for a practical could be proposed as part of a course or as a separate practical courses.
- (xi) 'SGPA' means Semester Grade Point Average calculated for individual semester.
- (xii) 'CGPA' is Cumulative Grade Points Average calculated for all courses completed by the students at any point of time. CGPA is calculated each year for both the semesters clubbed together.
- (xiii) 'Grand CGPA' is calculated in the last year of the course by clubbing together of CGPA of two years, i.e., four semesters. Grand CGPA is being given in transcript form. To benefit the student a formula for conversation of Grand CGPA into %age marks is given in the transcript.

Deepa Deswal

Bechgal

Techni

Paul

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## CENTRE FOR EXCELLENCE IN PHARMACEUTICAL SCIENCES

### III-Programme Details: Master of Science (M.Sc.) in Medicinal Chemistry and Drug Design Programme Educational Objective (PEO):

- Medicinal Chemistry emphasizes the study of chemical and biochemical rationales for the design and development of drugs. It involves the application of a number of specialized disciplinary approaches and draw from a spectrum of sciences, including analytical chemistry, biochemistry, molecular biology, organic chemistry, and pharmacology through the application of modern techniques and all focused on the ultimate goal of drug synthesis and discovery.
- Drug target identification and validation, rational (target-based) drug design, structural biology, computational-based drug design, methods development (chemical, biochemical, and computational), and "Hit-to-lead" development are all aspects of medicinal chemistry.
- The techniques and approaches of chemical biology, synthetic organic chemistry, combinatorial (bio) chemistry, mechanistic enzymology, computational chemistry, chemical genomics, and high-throughput screening are all used and applied by medicinal chemists towards drug discovery.

#### Programme Objective (PO):

- To provide a broad foundation in Medicinal Chemistry and Drug Design that stresses scientific reasoning and analytical problem solving with a molecular perspective in the development of new drugs.
- To make the Center as Center of Excellence in teaching, cutting-edge research, curriculum development and focusing on interdisciplinary area of research.
- To provide students with the skills required to succeed in drug discovery programme in industry.
- To make international collaborations for students and faculty exchange and research cooperation.
- The Centre would like to attain worldwide recognition in Medicinal Chemistry and allied area of research and teaching.
- To expose the students to a breadth of experimental techniques using modern instrumentation and technologies.
- The Centre also endeavors to contribute to Pharmaceutical Industry, computational-based drug design and address problems of societal importance.
- The Centre also aims at Medicinal Chemistry outreach in the form of books, online courses, and other educational activities.

Deepa Sasmal  
Biswal  
Fulhi  
Parul



## CENTRE FOR EXCELLENCE IN PHARMACEUTICAL SCIENCES

### Programme Outcomes (PSOs):

At the completion of the M.Sc. Medicinal Chemistry and Drug Design program, the students of Centre will be able to:

- **PSO1:** Work in the interdisciplinary areas of chemical sciences, biological sciences, computational methods and its applications.
- **PSO2:** Have sound knowledge about the fundamentals and applications of chemical and allied scientific theories.
- **PSO3:** Apply appropriate techniques for the synthetic methodology in laboratories and in industries.
- **PSO4:** Carry out experiments in the area of organic synthesis, catalysis, separation science, estimation and characterization.
- **PSO5:** Apply appropriate techniques for the qualitative and quantitative analysis of chemicals in laboratories and in industries.
- **PSO6:** Acquires the ability to synthesize, separate and characterize compounds using laboratory and instrumentation techniques.
- **PSO7:** Analyze the data obtained from sophisticated instruments (like FTIR, NMR, GC, GC-MS, HPLC, LC-MS, UV-Vis, and Fluorescence) for the structure determination and chemical analysis.
- **PSO8:** Understands the background of organic reaction mechanisms, complex chemical structures, and instrumental method of chemical analysis, molecular rearrangements and separation techniques.
- **PSO9:** Understand drug target identification and validation, rational (target-based) drug design, structural biology, computational-based drug design, methods development (chemical, biochemical, and computational), and "Hit-to-lead" development for drug discovery.
- **PSO10:** Understand structure-activity relationships to understand the mechanisms of drug action.
- **PSO11:** Apply green/sustainable chemistry approach in frontier areas of synthetic pathways.
- **PSO12:** Students will be able to clearly communicate the results of scientific work in oral, written and electronic formats to both scientists and the public at large.

Deepa Deswal Patel

Shuchi Verma



## CENTRE FOR EXCELLENCE IN PHARMACEUTICAL SCIENCES

### Program Structure:

The Master of Science in Medical Chemistry and Drug Design Chemistry Course is a Two Year Full-Time Course consisting of four Semester, viz. Semester-I, Semester-II, Semester-III and Semester-IV.

First Year	Part-I	First Semester	Second Semester
Second Year	Part-II	Third Semester	Fourth Semester

### Course Credit Scheme at a Glance:

#### First Semester

Course Code	Nomenclature of the Paper		M.M.	C.E.	E.E.	No. of Hours		Credits
						Th.	Pr.	
PC-601	Foundation Course in Inorganic Chemistry	CFC	100	40	60	4		4
PC-603	Foundation Course in Organic Chemistry	CFC	100	40	60	4		4
PC-605	Foundation Course in Physical Chemistry	CFC	100	40	60	4		4
PC-607	Introduction to Bio-molecules	SEC	100	40	60	3		3
PC-651	Foundation Course Practical-I (Organic Chemistry)	AECC	100	40	60		8	4
PC-653	Foundation Course Practical-II (Physico-Inorganic Chemistry)	AECC	100	40	60		8	4
PC-655	Introduction to Computational Chemistry	NUES	100				2	1
			700			15	18	24

\*NUES: (Entitled for credit and not to be considered for the purpose of declaration of Result)

#### Second Semester

Course Code	Nomenclature of the Paper		M.M.	C.E.	E.E.	No. of Hours		Credits
						Th.	Pr.	
PC-602	Conformational Analysis and Asymmetric Synthesis	CC	100	40	60	4		4
PC-604	Synthetic Methods in Medicinal Chemistry (Organic Synthesis)	CC	100	40	60	4		4
PC-606	Spectroscopic Studies	SEC	100	40	60	4		4
PC-608	Enzymes	AECC	100	40	60	2		2
PC-610	Green Chemistry	SEC	100	40	60	2		2
PC-612	History and Philosophy of Science	NUES*	100			1		1
PC-652	Medicinal Chemistry (Practical)	CC	100	40	60		8	4
PC-654	Enzymology (Practical)	AECC	100	40	60		8	4
			800			17	16	25

\*NUES: (Entitled for credit and not to be considered for the purpose of declaration of Result)

*Pandey*  
*Deepa Dussan*  
*Archer*  
*Rehgal*  
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## CENTRE FOR EXCELLENCE IN PHARMACEUTICAL SCIENCES

### Third Semester

Course Code	Nomenclature of the Paper		M.M.	C.E.	E.E.	No. of Hours		Credits
						Th.	Pr.	
PC-701	Advanced Organic Chemistry	CFC	100	40	60	4		4
PC-703	Bioenergetics and Metabolism	SEC	100	40	60	4		4
PC-705 (A1)*	Separation Science	DCE	100	40	60	2		2
PC-705 (A2)*	Molecular Spectroscopy							
PC-707	Introduction to Microbiology	AECC	100	40	60	3		3
PC-709	Concepts in Drug Design	CC	100	40	60	2		2
PC-711**	Developing an Entrepreneurial Mindset	NUES	100			2		2
PC-751	Computational Drug Design (Practical)	CC	100	40	60		4	2
PC-753	Microbiology (Practical)	SEC	100	40	60		4	2
PC-799#	Project/Dissertation						8	4
			800			17	16	25

\*One course to be selected (705A1/705A2) and to be offered with a minimum of seven students.

\*\*NUES: (Entitled for credit and not to be considered for the purpose of declaration of Result)



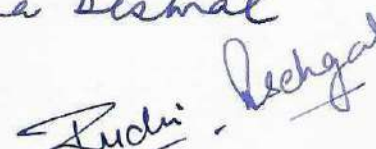
#To be evaluated at the end of the fourth semester.

### Fourth Semester

Course Code	Nomenclature of the Paper		M.M.	C.E.	E.E.	No. of Hours		Credits
						Th.	Pr.	
PC-702	Drug Synthesis and Mechanism of Action	CC	100	40	60	4		4
PC-704	Molecular Pharmacology	AECC	100	40	60	3		3
PC-706	Medicinal Chemistry	CC	100	40	60	4		4
PC-708 (A1)**	Formulation Chemistry	DCE	100	40	60	2		2
PC-708 (A2)**	Heat and Mass Transfer							
PC-710 (A1)***	Bio-Statistics	GE	100	40	60	2		2
PC-710 (A2)***	Bio-Ethics							
PC-710 (A3)***	Intellectual Property Rights (IPR)							
PC-712	Systemic Pharmacology	AECC	100	40	60	2		2
PC-800	Project/Dissertation	CC	100		100		16	8
			700			17	16	25

\*\* One course to be selected (708A1/708A2)

\*\*\*One course to be chosen (710A1/710A2/710A3) and to be offered with a minimum of seven students for both 708 and 710 course

  
 Deepa Desmal  
 Ruchi  
 Deepa



## CENTRE FOR EXCELLENCE IN PHARMACEUTICAL SCIENCES

### Elective Papers

#### For the Students of M.Sc. (Medicinal Chemistry and Drug Design)

A student will earn six credits by choosing any two papers out of the Discipline Centric Elective and one from General Elective offered by the Centre.

Course Code	Course Title	Credits	Teaching Hours per week	Maximum Marks			
				Continuous Evaluation	Mid-Semester Examination	End-Semester Examination	Total
705A1	Discipline Centric Elective	2	2	15	25	60	100
705A2	Discipline Centric Elective	2	2	15	25	60	100
708A1	Discipline Centric Elective	2	2	15	25	60	100
708A2	Discipline Centric Elective	2	2	15	25	60	100
Total Credits/Marks		04					200

#### General Elective

The Center or any other school offers the following open elective papers to the students of fourth semester.

Course Code	Course Title	Credits	Teaching Hours per week	Maximum Marks			
				Continuous Assessment*	Mid-Semester Examination	End-Semester Examination	Total
710A1	Bio-Statistics	2	2	15	25	60	100
710A2	Bio-Ethics	2	2	15	25	60	100
710A3	Intellectual Property Right (IPR)	2	2	15	25	60	100
Total Credits/Marks		02					100

\*Code, will be provided by the respective School opted by the student.

*Deepa Sasmal*  
*Ruchi*  
*Bengal*  
*Parul*



## CENTRE FOR EXCELLENCE IN PHARMACEUTICAL SCIENCES

### First Semester

Course Code	Nomenclature of the Paper	Credits	Teaching hours per week	Maximum Marks			Total
				Continuous Evaluation	Mid-Semester Examination	End-Semester Examination	
PC-601	Foundation Course in Inorganic Chemistry	4	4	15	25	60	100
PC-603	Foundation Course in Organic Chemistry	4	4	15	25	60	100
PC-605	Foundation Course in Physical Chemistry	4	4	15	25	60	100
PC-607	Introduction to Bio-molecules	3	3	15	25	60	100
PC-651	Foundation Course Practical-I (Organic Chemistry)	4	8	40		60	100
PC-653	Foundation Course Practical-II (Physico-Inorganic Chemistry)	4	8	40		60	100
PC-655	Introduction to Computational Chemistry	1	2	40		60	100
<b>Total</b>		<b>24</b>	<b>33</b>				<b>700</b>

### Second Semester

Course Code	Nomenclature of the Paper	Credits	Teaching hours per week	Maximum Marks			Total
				Continuous Evaluation	Mid-Term Examination	End-Semester Examination	
PC-602	Conformational Analysis and Asymmetric Synthesis	4	4	15	25	60	100
PC-604	Synthetic Methods in Medicinal Chemistry (Organic Synthesis)	4	4	15	25	60	100
PC-606	Spectroscopic Studies	4	4	15	25	60	100
PC-608	Enzymes	2	2	15	25	60	100
PC-610	Green Chemistry	2	2	15	25	60	100
PC-612	History and Philosophy of Science (NUES)	1	1	15	25	60	100
PC-652	Medicinal Chemistry (Practical)	4	8	40		60	100
PC-654	Enzymology (Practical)	4	8	40		60	100
<b>Total</b>		<b>25</b>	<b>33</b>				<b>800</b>

*Deepa Arsal*  
*ix*  
*Dr. P. D. D. D.*



## CENTRE FOR EXCELLENCE IN PHARMACEUTICAL SCIENCES



### Third Semester

Course Code	Nomenclature of the Paper	Credits	Teaching hours per week	Maximum Marks		End-Semester Examination	Total
				Continuous Evaluation	Mid-Semester Examination		
PC-701	Advanced Organic Chemistry	4	4	15	25	60	100
PC-703	Bioenergetics and Metabolism	4	4	15	25	60	100
PC-705 (A1)	Separation Science	2	2	15	25	60	100
PC-705 (A2)	Molecular Spectroscopy						
PC-707	Introduction to Microbiology	3	3	15	25	60	100
PC-709	Concepts in Drug Design	2	2	15	25	60	100
PC-711	Developing an Entrepreneurial Mindset	2	2	15	25	60	100
PC-751	Computational Drug Design (Practical)	2	4	40		60	100
PC-753	Microbiology (Practical)	2	4	40		60	100
PC799#	Project/ Dissertation	4	8				
<b>Total</b>		<b>25</b>	<b>33</b>				<b>800</b>

#To be evaluated at the end of fourth semester

### Fourth Semester

Course Code	Nomenclature of the Paper	Credits	Teaching hours per week	Maximum Marks		End-Semester Examination	Total
				Continuous Evaluation	Mid-Semester Examination		
PC-702	Drug Synthesis and Mechanism of Action	4	4	15	25	60	100
PC-704	Molecular Pharmacology	3	3	15	25	60	100
PC-706	Medicinal Chemistry	4	4	15	25	60	100
PC-708 (A1)	Formulation Chemistry	2	2	15	25	60	100
PC-708 (A2)	Heat and Mass Transfer						
PC-710 (A1)	Bio-Statistics	2	2	15	25	60	100
PC-710 (A2)	Bio-Ethics						
PC-710 (A3)	Intellectual Property Rights (IPR)						
PC-712	Systemic Pharmacology	2	2	15	25	60	100
PC-800#	Project/ Dissertation	8	16				100
<b>Total</b>		<b>25</b>	<b>33</b>				<b>700</b>



 Deepa Deswal x  
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## CENTRE FOR EXCELLENCE IN PHARMACEUTICAL SCIENCES

### Total Marks of all Four Semesters

SEMESTER	CREDIT	MARKS
I	24	700
II	25	800
III	25	800
IV	25	700
<b>GRAND TOTAL</b>	<b>99</b>	<b>3000</b>

Internal Assessment in theory papers will be made on the basis of one test and continuous evaluation parameters as decided by the University from time to time, while in Laboratory papers it will be decided from continuous assessment in internal viva-voce examination of all the experiments performed. Current guidelines for determining Internal Assessment in theory papers are given as 'Annexure-A'.

Each student will submit a project report at the end of fourth semester duration on the topic to be allotted by the Centre through a constituted committee in 3<sup>rd</sup> Semester of the M. Sc. Course as per the prescribed schedule. The marks will be awarded by the external examiner and committee on the basis of performance presentation submitted by the student.

Total credits to be earned by the student is 95, leaving behind NUES.

*Deepa Desmal*  
*Dehgal*  
*Shuchi*  
*Paul*  
*Q*



## CENTRE FOR EXCELLENCE IN PHARMACEUTICAL SCIENCES

### Annexure-A

#### Scheme for awarding internal assessment: continuous mode

Criteria	Theory (4 Credits/2 Credits)
	Maximum Marks
Continuous Evaluation	15
Mid-Term	25
<b>Total</b>	<b>40</b>
Practical	Practical (4 Credits/2 Credits)
	Maximum Marks
Based on Practical Records, Regular viva voce, etc.	40
<b>Total</b>	<b>40</b>

(Objective Learning involves Multiple Choice Test, Matching Test, True / False Test Correct / Incorrect Test, Recall Test, Best Answer Test, Completion Test etc.)

Deepa Desmal  
Behera

Trilok

Ravi



## CENTRE FOR EXCELLENCE IN PHARMACEUTICAL SCIENCES

### Grading System

After adding the teaching continuous evaluation marks to the term end examinations marks, the marks secured by a student from maximum 100 shall be converted into a letter grade. The grade points are the numerical equivalent of letter grade assigned to a student in the points scale as given below:

Percentage of marks obtained	Grade	Grade Point
90-100	O	10
75-89	A+	9
65-74	A	8
55-64	B+	7
50-54	B	6
45-49	C	5
40-44	P	4
Less than 40 or absent	F	0

Grade P (grade point 4) shall be the course passing grade unless specified otherwise by the Syllabi and Scheme of Teaching and Examination for the programme. For grade(s) below the passing grade as defined in the Syllabi and Scheme of Teaching and Examination, the associated grade points shall be zero. Both acquired marks and grades shall be reflected on the term and marksheets.

### Calculation of Semester Grade Point Average (SGPA) and Cumulative Grade Point Average (CGPA)

1. Performance in a semester will be expressed as Semester Grade Point Average (SGPA) and shall be rounded to two decimal digits.
2. Cumulative performance of all the semesters together will reflect performance in the whole programme and it will be known as Cumulative Grade Point Average (CGPA), and shall be rounded to two decimal digits.
3. The formula for calculation for SGPA and CGPA is given below:

$$SGPA = \frac{\sum_i C_i G_i}{\sum_i C_i}$$

$$CGPA = \frac{\sum_n \sum_i C_{ni} G_{ni}}{\sum_n \sum_i C_{ni}}$$

*Panel*

*AL*

*Deepa Bernal*

*Ruchi*

*Aschgal*

Where;

Ci – number of credits for the  $i^{\text{th}}$  course.

Gi – grade point obtained in the  $i^{\text{th}}$  course.

Cni – number of credits of the  $i^{\text{th}}$  course of the  $n^{\text{th}}$  semester.

Mni – marks of the  $i^{\text{th}}$  course of the  $n^{\text{th}}$  semester.

Gni – grade points of the  $i^{\text{th}}$  course of the  $n^{\text{th}}$  semester.

4. The successful candidates as per clause 11.6 and having an overall CGPA higher than or equal to the minimum CGPA specified in the Syllabi and Scheme of Teaching and Examination for the award of the degree, shall be awarded the degree and shall be placed in Divisions as below:

- **CGPA of 4.00 – 4.99** shall be placed in the Third Division.
- **CGPA of 5.00 – 6.49** shall be placed in the Second Division.
- **CGPA of 6.50 or above** shall be placed in the First Division.
- **CGPA of 10** shall be placed in the Exemplary Performance. Exemplary Performance shall be awarded, if and only if, every course of the programme offered to the student is passed in the first chance of appearing in the paper that is offered to the student. A student with an academic break shall not be awarded the exemplary performance.
- The  $\text{CGPA} \times 10$  shall be deemed equivalent to percentage of marks obtained by the student for the purpose of equivalence to percentage of marks.

*Deepa Dismal*  
*Seehgal*  
*Kuchni*  
*AC*



## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### FOUNDATION COURSE IN INORGANIC CHEMISTRY

Course Code:  
PC-601(4 0 0)

Foundation Course in Inorganic Chemistry  
Compulsory Foundation Course

Maximum Marks: 60 + 40 (CE)

Credit: 4

**Instruction to Paper Setters:**

**Attempt five questions**

**Time: 3 hours**

**Maximum Marks: 60**

Question Paper shall contain **Five Sections**

- The student has to attempt **five questions** from five sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** to **V** shall have two questions in each section, and the student needs to attempt only one question from each section. (Section II to V shall reflect Unit I to IV of the syllabus respectively).

#### Course Objective:

1. On successful completion of this course, a student should be able to understand and appreciate basic concepts of structure and bonding in organometallic chemistry in general and also should be able predict stability of organometallic compounds.
2. It would equip students to understand the various mechanisms operative in inorganic complexes during substitution and in electron transfer reactions.
3. Further, the utility towards synthesis of newer compounds will be studied. Concept of Metal ligand equilibrium in solution is introduced.

#### Course/Learning Outcomes:

- Fundamental understanding for organometallic structure and bonding and inorganic synthetic chemistry through substitution reactions is learnt.
- Mechanistic aspect of transition metal chemistry including substitution reaction, electron transfer reaction and ligand reactions and theory of Spectroscopic Transitions in Inorganic Complexes is incorporated along with concept of nano materials.
- Basic concepts involved in the use of these compounds as catalysts is learnt.

#### **Unit-I**

##### **Organotransition Metal Chemistry**

General introduction, Structure and bonding, Survey of organometallic complexes according to ligands.  $\pi$  bonded organometallic compounds including carbonyls, nitrosyls, tertiary phosphines, hydrides, alkene, alkyne, cyclobutadiene, cyclopentadiene, arene compounds and their M.O. diagrams. Metal-carbon multiple bonds. Fluxional organometallic compounds including  $\pi$ -allyl complexes and their characterization. Metallocycles, unsaturated nitrogen ligands including dinitrogen complexes, metal-metal bonds, cluster compounds of  $d$ -block elements.

#### **Unit-II**

##### **Metal-Ligand Bonding**

Limitation of crystal field theory, crystal field effects, John Teller distortion, nephelauxetic series, spin-orbital coupling molecular orbital theory of octahedral, tetrahedral and square planar complexes (with and without  $\pi$  - bonding). Structure and bonding in complexes containing  $\pi$ -acceptor ligands.

##### **Theory of Spectroscopic Transitions in Inorganic Complexes**

Deepa Siswal

Term symbols, Russel-Saunders states, Crystal field theory and splitting in  $O_h$ ,  $T_d$ ,  $D_{4h}$  and  $C_{4v}$  systems, Orgel and Tanabe-Sugano diagrams, determination of  $Dq$  and Racah parameters, oxidation states and electronic absorption spectra of complex ions. Spectrochemical series and effects of covalency, nephelauxetic series, magnetic properties of transition metal complexes and lanthanides.

### Unit-III

#### Metal-Ligand Equilibria in Solution

Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry.

#### Inorganic Reaction Mechanisms

Inert and labile complexes, mechanisms of substitution reactions of tetrahedral, square planar (theories of trans effect w.r.t. Pt (II) complexes), trigonalbipyramidal, square pyramidal and octahedral complexes. Potential energy diagrams, transition states and intermediates, isotope effects, Berry's pseudo rotation mechanism, factors affecting the reactivity of square planar complexes, Swain-Scott equation, Trans effect and its application to synthesis of complexes.

### Unit-IV

#### Molecular Rearrangement Processes

Electron transfer reactions (outer and inner sphere), HOMO and LUMO of oxidant and reluctant, chemical activation. Precursor complex formation and rearrangement, nature of bridge ligands, fission of successor complexes, Two-electron transfers, Synthesis of coordination compounds using electron transfer reactions, mixed valence complexes and internal electron transfer.

#### Nanomaterials

Preparation of nanomaterials and their characteristic differences over bulk materials. Principles of Electron Microscopy, Dynamic Light Scattering, Atomic Force Microscopy and Characterization of Nanomaterials.

#### Suggested Reading:

1. Shriver D.F., Atkins P.W. & Langford C.H., *Inorganic Chemistry*, 5<sup>th</sup> Ed., Oxford Univ. Press (2010).
2. Gupta, B.D, Elias, A J; *Basic Organometallic Chemistry. Concepts, syntheses and applications*, 2<sup>nd</sup> Ed, Universities Press (2013).
3. Mabbs F.E. & Machin D.J., *Magnetism and Transition Metal Complexes*, Chapman and Hall, U.K. (2008) Digitized (2011).
4. Rossotti F.J.C. & Rossotti H., *The Determination of Stability Constants*, MacGraw Hill, London (1961).
5. Tobe M. & Wadlington F.C. (Ed.), *Inorganic Reaction Mechanism*, Thomas Nelson, London (1973).
6. Huhey J.E., Keiter R.L., Medhi O.K., *Inorganic Chemistry, Principles of Structure and Reactivity*, 4<sup>th</sup> Ed., Pearson Education (2008).
7. Cotton F.A. and Wilkinson G., *Advanced Inorganic Chemistry*, 11<sup>th</sup> Ed., Wiley & Sons, New York (1998).
8. Gilber Thomas, Kriss R.V. N. Foster & Davies G. Chemistry., 4<sup>th</sup> Ed., W.W. Norton & Co. Inc(2014).
9. Housecraft C.E. & Sharpe A.G. *Inorganic Chemistry*, 1<sup>st</sup> Ed., Pearson Prentice Hall, (2005).

#### References:

1. Hartwig J.F. *Organo-transition metal chemistry: From bonding to catalysis*, 1<sup>st</sup> Ed, University science books (2010).
2. Crabtree R. H., *The organometallic chemistry of the transition metals*, 6<sup>th</sup> Ed, Wiley (2014).
3. Eldik Rudi Van(Ed), *Advances in Inorganic Chemistry*, Volume 62-65 and other related Volumes Elsevier Pub(2012-2015).
4. Karlin Kenneth D.(Ed.) *Progress in Inorganic Chemistry Series*, Wiley Interscience (2014).
5. Wilkinson G., Gillars R.D. & A. McCleverty J.A.; *Comprehensive Coordination Chemistry*, Pergamon (1987, 2003).

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### FOUNDATION COURSE IN ORGANIC CHEMISTRY

Course Code:  
PC-603 (4 0 0)

Foundation Course in Organic Chemistry  
Compulsory Foundation Course

Maximum Marks: 60 + 40 (CE)

Credit: 4

**Instruction to Paper Setters:**  
**Attempt five questions**

**Time: 3 hours**  
**Maximum Marks: 60**

Question Paper shall contain **Five Sections**

- The student has to attempt **five questions** from five sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** to **V** shall have two questions in each section, and the student needs to attempt only one question from each section. (Section II to V shall reflect Unit I to IV of the syllabus respectively).

#### Course Objective:

1. On successful completion of this module, the learner will be able to identify and explain the reaction mechanisms in organic chemistry. An examination of methods used to probe the mechanism of organic reactions and chemistry of some important reactive intermediates.
2. Topics include Nucleophilic, electrophilic and elimination reactions; formation, reactivity and stability of free radicals, and the structure, bonding and rearrangement reactions.

#### Course/Learning Outcomes:

Students will gain an understanding of:

- Reaction intermediates, nucleophiles, electrophiles, electronegativity, and thermodynamic controlled reactions.
- The prediction of reaction mechanisms for organic reactions and chemistry of some important reaction intermediate.
- How to use their understanding of organic mechanisms to predict the outcome of reactions
- Topic includes rearrangements, carbocation, carbanions, carbenes, radicals and acyclic strained and strained molecule.

#### **Unit-I**

##### **Reaction Mechanism: Structure and Reactivity**

Reaction intermediates: Generation, structure, stability and reactivity of carbocations (classical and non-classical), ion-pairs, reactivity of bridgehead carbocations, carbanions, ambient ions, free radicals, cage effects, carbenes, and nitrenes.

##### **Reaction Mechanism**

Type of reaction and mechanism, Thermodynamic and Kinetic controlled reactions, Baldwin rule for ring closure, Potential energy diagrams and transition states, The Hammett equation, Taft equation, Hammond's postulate and Curtin-Hammett principle.

#### **Unit-II**

##### **Mechanism of Nucleophilic Substitution Reaction**

The  $S_N^2$ ,  $S_N^1$ ,  $S_N^i$ ,  $S_N^{2'}$ ,  $S_N^{1'}$  and  $S_N^i$  types of reaction mechanism with stereochemical aspects. Nucleophilicity and solvent effects, competition between nucleophilicity and basicity, ambident nucleophiles, hard and soft nucleophiles and electrophiles, leaving group effects, steric and other substituent effects on substitution and ionization rates. Mechanism of Nucleophilic substitution in aromatic systems via

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diazonium ions, by addition-elimination and elimination-addition mechanism (involving arynes);  $S_{RN}1$  mechanism; von Richter rearrangement and Stevens rearrangements.

### Unit-III

#### Aromatic Electrophilic Substitution

Theoretical treatment of aromatic substitution reactions, structure-reactivity relationship in mono substituted benzene ring, orientation in other ring system, energy profile diagram, Vilsmeier-Haack reaction, Reimer-Tiemann reaction, Bischler-Napieralski reaction, Pechmann reaction, Houben-Hoesch reaction, Fries rearrangement.

#### Aliphatic Electrophilic Substitution:

The  $S_N1$ ,  $S_N2$  and  $S_Ni$  mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and medium on the reactivity.

#### Mechanism of Elimination Reactions:

The  $E1$ ,  $E1cB$  and  $E2$  mechanism with stereochemical aspects. Saytzeff and Hoffman rules. Effect of Base, leaving group and medium on the mechanism. Mechanisms and orientation in pyrolytic eliminations, Dehydration of Alcohols.

### Unit-IV

#### Rearrangements

Anchimeric assistance, neighbouring group participation by non-bonding electrons, sigma and n-bonds, classical and non-classical carbocation, carbocations rearrangements, migratory aptitudes, Wagner Meerwein rearrangement, pinacol-pinacolone rearrangement, Demjanov rearrangement, Tiffeneau-Demjanov ring expansion, aldehyde-ketone rearrangement, dienone-phenol rearrangement and transannular rearrangements.

#### Suggested Reading:

1. Carey, F.A. & Sundberg, R.J. *Advanced Organic Chemistry*, 7<sup>th</sup> Ed., Parts A & B, Plenum: U.S. (2004).
2. March, J. *Advanced Organic Chemistry*, 6<sup>th</sup> Ed., John Wiley & Sons (2006).
3. Ingold C.K., *Structure and Mechanism in Organic Chemistry*, Cornell University Press (2000)
4. Peter Sykes, *A Guidebook to Mechanism in Organic Chemistry*, 6<sup>th</sup> Ed., Pearson Education (1986).
5. Clayden Jonathan, Greeves Nick and Warren Stuart, *Organic Chemistry*, 2<sup>nd</sup> Ed., Oxford Press (2012).

#### References:

1. Vollhardt P. and Schore N., *Organic Chemistry Structure and Function*, 5<sup>th</sup> Ed., (2007).
2. Solomon T.W.G. and Fryhle C.B., *Organic Chemistry*, 10<sup>th</sup> Ed., (2009).

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### FOUNDATION COURSE IN PHYSICAL CHEMISTRY

Course Code:  
PC-605 (4 0 0)

Foundation Course in Physical Chemistry  
Compulsory Foundation Course

Maximum Marks: 60 + 40 (CE)

Credit: 4

#### **Instruction to Paper Setters:**

Attempt five questions

Time: 3 hours

Maximum Marks: 60

Question Paper shall contain **Five Sections**

- The student has to attempt **five questions** from five sections.
- All sections are of 12 marks each.
- Section I is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section II to V shall have two questions in each section, and the student needs to attempt only one question from each section. (Section II to V shall reflect Unit I to IV of the syllabus respectively).

#### **Course Objective:**

1. To impart fundamental knowledge about the basic concepts of both classical and quantum statistical mechanics. This course covers statistical mechanics for chemical systems.
2. To understand the link between macroscopic thermodynamics and microscopic quantum mechanics through different statistical methods.
3. To highlight applications of Boltzmann distribution in the fundamental concepts of electrochemistry and kinetics. Also covered are ensembles, partition functions, thermodynamic functions, applications to various systems.

#### **Course/Learning Outcomes:**

- On successful completion of this course, a student should be able to appreciate microscopic connection between classical mechanics and thermodynamics and have a background in basic thermodynamics, statistical mechanics at the level of a standard physical chemist.
- The student will learn the basic principles of statistical mechanics, which correlates the microscopic properties of systems with the macroscopic observables.
- The students would also learn the applications of the Boltzmann distribution and partition functions in electrochemistry, theories of chemical kinetics surface chemistry and catalysis

#### **Unit-I**

##### **Chemical Kinetics**

Collision theory of reaction rates, the steric requirement, Arrhenius equation and activated complex theory (ACT), comparison of collision and activation complex theory, Potential energy surfaces (Only basic idea), thermodynamic formulation of activated complex theory, chain reactions (hydrogen-halogen reaction), unimolecular reactions, steady state approximation, Lindemann-Hinshelwood mechanism of unimolecular reactions, kinetics of solutions.

##### **Electrochemistry**

Debye-Huckel theory of ion-ion interaction and activity coefficient, applicability and limitations of Debye-Huckel limiting law, its modification for finite-sized ions, effect of ion-solvent interaction on activity coefficient. Physical significance of activity coefficients, mean activity coefficient of an electrolyte. Debye-Huckel-Onsager (D-H-O) theory of electrolytic conductance, Debye-Falkenhagen effect, Wein effect. D-H-O equation – its applicability and limitations, Pair-wise association of ions (Bjerrum treatment), Modification of D-H-O theory to account for ion-pair formation.

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## Unit-II

### Surface Chemistry and Catalysis

Gibbs adsorption equation, Langmuir Adsorption isotherm and its kinetic derivation for non-dissociative and dissociative adsorption, BET adsorption isotherm, its kinetic derivation and applications.

Heterogeneous catalysis, homogenous catalysis, kinetic of enzyme catalysis, evaluation of Michaelis-Menten constant and study the effect of substrate concentration on it. Study of surfaces by STM, SEM. Surface heterogeneity, surface catalyzed unimolecular and bimolecular reactions, temporary and permanent catalytic poisons, activation energy for surface reactions. Comparison of homogeneous and heterogeneous reaction rates.

## Unit-III

### Quantum Mechanics

The postulates of quantum mechanics, Linear and Hermitian operators. Commutation of operators and Uncertainty Principle. Schrodinger equation, eigen function and eigen values, free particle, Schrödinger equation for a particle in a box, the degeneracy, particle in a box with a finite barrier, Schrodinger equation for simple harmonic oscillator and its solution, zero point energy, Tunneling Problem: Tunneling through a rectangular barrier.

Energy levels and wave-function of Rigid rotator. Hydrogen atom: complete solution (separation of variables in spherical polar coordinates and its solution). Radial distributions functions, Angular momentum and its directional quantization, Angular momentum operators, commutation relation, shape of atomic orbitals upto d-level and their discussion.

## Unit-IV

### Statistical Mechanics and Thermodynamics

Fundamentals: Concept of distribution. Thermodynamic probability and most probable distribution. Canonical and other ensembles. Statistical mechanics for systems of independent particles and its importance in chemistry.

Types of statistics: Maxwell, Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Idea of microstates and macrostates. Thermodynamic probability ( $W$ ) for the three types of statistics. Derivation of distribution laws (most probable distribution) for the three types of statistics. Lagrange's undetermined multipliers. Stirling's approximation, Molecular partition function and its importance. Assembly partition function.

### Applications to Ideal Gases

The molecular partition function and its factorization. Evaluation of translational, rotational and vibrational partition functions for monatomic, diatomic and polyatomic gases. The electronic and nuclear partition functions. Calculation of thermodynamic properties of ideal gases in terms of partition function. Statistical definition of entropy. Ortho- and para-hydrogen, statistical weights of ortho and para states, symmetry number. Calculation of equilibrium constants of gaseous solutions in terms of partition function, perfect gas mixtures.

Einstein theory and Debye theory of heat capacities of monatomic solids.

Third law of thermodynamics, Residual entropy.

### Suggested Reading:

1. McQuarrie, D.A. *Statistical Mechanics* Viva Books Pvt. Ltd.: New Delhi (2003).
2. Atkins, P.W. & Paula, J. *De Atkin's Physical Chemistry*, 10<sup>th</sup> Ed., Oxford University Press (2013).
3. Nash, L.K. *Elements of Statistical Thermodynamics* 2<sup>nd</sup> Ed., Addison Wesley (2006) Reprint.
4. Laidler, K.J. *Chemical Kinetics* 3<sup>rd</sup> Ed., Benjamin Cummings (1987).
5. Hill, T.L., *Statistical Mechanics: Principle & Selected Applications*, Dower Publication, New York (1987).
6. Ball D.W., *Physical Chemistry*, Thomson Press, India (2011).
7. Castellan G.W., *Physical Chemistry*, 4<sup>th</sup> Ed. Narosa (2004).
8. Mortimer R.G., *Physical Chemistry*, 3<sup>rd</sup> Ed., Elsevier, Noida (2008).
9. Pilar, F.L. *Elementary Quantum Chemistry*, 2<sup>nd</sup> Ed., Dover Publication Inc.: N.Y. (2001).
10. Chandra A.K. *Introduction to Quantum Chemistry*, 3<sup>rd</sup> Ed., Tata McGraw Hill, (1989).
11. Glasstone Samuel, *An Introduction to Electrochemistry*, Reprint (2007).

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**References:**

1. Glasstone Samuel S., *Physical Chemistry*, Affiliated East-West.
2. Levine I.N., *Physical Chemistry*, 6<sup>th</sup> Ed.
3. Glasstone S., *Thermodynamics for Chemists*, Affiliated East-West Press, (2007).
4. Bockris S. and Reddy A.K.N., *Modern Electrochemistry*, Vol. 1 and 2, Butterworth London, (2006).

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### INTRODUCTION TO BIO-MOLECULES

Course Code:  
PC-607 (3 0 0)

Maximum Marks: 60 + 40 (CE)

Introduction to Bio-Molecules

Credit: 3

Skill Enhancement Course

#### **Instruction to Paper Setters:**

**Time: 3 hours**

**Attempt five questions**

**Maximum Marks: 60**

Question Paper shall contain **Five Sections**

- The student has to attempt **five questions** from five sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II to V** shall have two questions in each section, and the student needs to attempt only one question from each section. (Section II to V shall reflect Unit I to IV of the syllabus respectively).

#### **Course Objective:**

1. Students will be able to understand the central dogma of molecular biology
2. This course provides basic knowledge of metabolic process in all living organism.
3. The students will understand various pathways like ATP, role of various enzymes, role of amino acids, and proteins and also explain DNA structure, transfer of genetic information from one generation to another generation, disorders etc.

#### **Course/Learning Outcomes:**

The students will acquire knowledge of:

- Metabolic process in all living organism.
- Various pathways like ATP, role of various enzymes, role of amino acids, and proteins.
- DNA structure, transfer of genetic information from one generation to another generation.
- Understanding the complexity of biological reactions in a living organism.
- Role of vitamins, advantage and disadvantages in a living organism.

#### **Unit-I**

##### **Carbohydrates**

Introduction to Metabolic Processes: Catabolism and anabolism, ATP- currency of biological energy, energy rich and energy poor phosphates.

Classification of carbohydrates, basic chemical structure, general reactions and properties, biological significance, sugar derivatives, deoxy sugars, amino sugars and sugar acids. Furanose and Pyranose forms of glucose and fructose, Haworth projection formula for glucose; chair and boat forms of glucose, formation of Disaccharides, concept of reducing and non-reducing sugars, occurrence and Haworth projection of maltose, lactose and sucrose. Polysaccharides-homo and hetero-polysaccharides, storage polysaccharides (starch and glycogen) and structural polysaccharides (cellulose, peptidoglycan and chitin).

#### **Unit-II**

##### **Lipids**

Classification, structure and function of lipids. Building blocks of lipids – fatty acids, glycerol, ceramide. Storage lipids – triacyl glycerol and waxes. Structural lipids in membranes – glycerophospholipids, galactolipids and sulpholipids, sphingolipids and sterols, structure, distribution and role of membrane lipids. Introduction of lipid micelles, monolayer and bilayer, liposomes.

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## Vitamins

Structure and active forms of water soluble and fatsoluble vitamins, deficiency diseases and symptoms, hypervitaminosis.

## Unit-III

### Amino Acids

Structure and classification, physical, chemical and optical properties of amino acids.

### Protein:

Organisation of protein structure into primary, secondary, tertiary and quaternary structures. N-terminal and C-terminal amino acid analysis. Sequencing techniques –Edman degradation. Disulfide bonds and their location. Solid phase peptide synthesis. Nature of stabilizing bonds – covalent and non covalent. Importance of primary structure in folding. The peptide bond – bond lengths and configuration. Dihedral angles psi and phi. Helices, sheets and turns. Ramachandran map. Structures of myoglobin and hemoglobin.

## Unit IV

### Nucleic Acids

Chemical and enzymatic hydrolysis, structure and functions of DNA, RNA (m-RNA, t-RNA, r-RNA), an overview of gene expression (replication, transcription and translation).

### Suggested Reading:

1. Lehninger C., David L. Nelson and Michael M. Cox, *Principles of Biochemistry*, 6<sup>th</sup> Ed., (2013).
2. Stryer L., Freeman W.H., *Biochemistry*, 5<sup>th</sup> Ed., San Francisco, (2014).
3. Wood W.B. and Wilson J. H., Benbow R.M., and Hood L.E., *Problem Approaches in Biochemistry*, 1<sup>st</sup> Ed., Wiley, (1974).
4. Krebs Jocelyn E., Goldstein Aachorage Elliott S. and Kilpatrick Stephen T., Jones & Bartlett, *Lewin's Genes XII*, 2018.

### References:

1. Stryer, L. *Biochemistry* 4th Ed., W. H. Freeman & Co. (1995).
2. Zubay, S. *Biochemistry* Addison-Wesley (1983).
3. Litwak, G. *Vitamins and Hormones*, Academic Press, (2005).

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### FOUNDATION COURSE PRACTICAL-I (ORGANIC CHEMISTRY)

Course Code:

PC-651 (0 0 8)

Maximum Marks: 60 + 40 (CE)

Foundation Course Practical-I(Organic Chemistry)

Credit: 4

Compulsory Foundation Course

#### Course Objective:

1. Aimed at learning the techniques of separating organic mixtures as well as systematic identification of organic compounds based on their physical and chemical spectral properties.
2. To acquire knowledge of laboratory techniques for organic synthesis and characterization.

#### Course/Learning Outcome:

The students will acquire knowledge of:

- Safe laboratory practices by handling laboratory glassware, equipment, and chemical reagents
- Starting materials, functional groups, mechanism, and typical reaction conditions.
- Purification, Crystallization, and different Distillation processes.
- Synthetic procedures: aqueous workup, distillation, reflux, separation, isolation, and crystallization and Characterization

**Purification of organic compounds involving fractional crystallization, fractional distillation, steam distillation, sublimation and extraction.**

#### **Systematic identification of pure organic compounds**

Separation and identification of simple binary mixtures having acidic, basic and neutral components.

#### **Synthesis of Organic Molecules using following reactions (any five\*)**

1. Fischer Indole Synthesis
2. Baker-Venkatraman Reaction
3. Fries Reaction
4. Sandmeyer Reaction
5. Benzillic Acid Rearrangement
6. Photochemical Reaction
7. Pechman Synthesis
8. Friedel-Crafts Reaction
9. Beckmann Rearrangement
10.  $\text{NaBH}_4$  Reduction
11. Bromination and Bromine addition
12. Diazotisation Reactions

**Note:** Any experiment may be introduced/deleted in the practical class based on the availability/non-availability of the instruments/chemicals.

**\*Any new preparation may also be included.**

**Experiment  
Lab record & Viva-voce**

**Marks: 30  
Marks: 5+15**

#### **Suggested Reading:**

1. Saunders & Mann, *Practical Organic Chemistry*.
2. Shriner Ralph L, Hermann Christine K.F., Morrill Terence C. and Curtin David Y., *The Systematic Identification of Organic Compounds*.
3. Furhen B.S. et. Al., *Vogel's Text Book of Practical Organic Chemistry*, Longman-Group Ltd.

4. Vogel Arthur I., *Elementary Practical Organic Chemistry* EX CBS Publishers and Distributors.
5. Louis, *Experiments in Organic Chemistry*, D.C. Heath and Company Boston (1955).

**References:**

1. Furniss B.S., Hannaford A.J., Smith P.W.J. and Tatchell A.R., *Vogel's Text Book of Practical Organic Chemistry*, 5<sup>th</sup> Ed., Addison Wesley Longman (1997).
2. Harwood Laurence M., Moody Christopher J., Percy Jonathan M., *Experimental Organic Chemistry: Standard and Microscale*, 2<sup>nd</sup> Ed., Wiley-Blackwell Sevenlife, (1998).

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### **FOUNDATION COURSE PRACTICAL-II (PHYSICO INORGANIC CHEMISTRY)**

**Course Code:**

**PC-653 (0 0 8)**

**Maximum Marks: 60 + 40 (CE)**

**Foundation Course Practical-II (Physico-Inorganic Chemistry) Credit: 4**

**Compulsory Foundation Course**

#### **Course Objective:**

1. The course aims to make familiar with equipment and standard laboratory techniques for carrying out reaction and purification of products along with concept of green chemistry.
2. The study tracks practical skills in refractometry, chemical kinetics, polarimetry and potentiometry. The course aims to make aware of risk and hazards.

#### **Course/Learning Outcome:**

The students:

- Will acquire hands on experience on synthesizing various inorganic compounds by employing a variety of synthetic strategies and their characterization will be aimed.
- Will equip on the analytical applications and various ways of analyzing data derived from different experiments.
- Would make to know the process of selecting and adopting the synthetic route to a known compound using searching electronic database and primarily literature.

#### **Chemical Kinetics**

1. Determine the specific rate constant for the acid catalyzed hydrolysis of methyl acetate by the *Initial Rate Method*. Study the reaction at two different temperatures and calculate the thermodynamic parameters.

#### **Refractometry**

1. Determine the refractive index of simple organic liquids like methyl acetate, ethyl acetate, methanol, ethanol, n-hexane, chloroform.
2. Determine the refractivity and molar refractivity of some organic liquids like methyl acetate, ethyl acetate, methanol, ethanol, n-hexane, chloroform.

#### **Polarimetry**

1. Study the variation of angle of optical rotation with the concentration of any optically active substance (sucrose or glucose) and thereafter determine the unknown concentration of the same substance in given solution.
2. Determine the specific and molecular rotation of sucrose or glucose at number of concentrations.

#### **Potentiometry: (Any Two)**

1. Titrate hydrochloric acid and sodium hydroxide potentiometrically.
2. Determine the dissociation constant of acetic acid potentiometrically.
3. Titrate a mixture of:
  - (a) Strong and weak acids (Hydrochloric acid and acetic acids)
  - (b) Weak acid (acetic acid) and dibasic acid (oxalic acid)
  - (c) Strong acid (hydrochloric acid) and dibasic acid (oxalic acid) versus sodium hydroxide.
  - (d) Titrate a solution of Mohr's salt against potassium permanganate potentiometrically.

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### Cyclic Voltammetry

1. Reset the CV of aqueous solution of sulphuric acid (0.5 M) at Pt electrode as working electrode and counter electrode.
  - (a) Interpret and explain various peaks and regions of the CV and their significance.
  - (b) Determine the area and roughness factor of the electrode by H-adsorption and H-desorption.
  - (c) Determine the area and roughness factor of the electrode by Pt oxide region.
2. Determine the extent of catalytic activity of the Pt electrode by H<sub>2</sub> evolution reaction (HER) and O<sub>2</sub> evolution reaction (OER).

### Impedance

1. Verify Warburg equation using electrochemical impedance spectroscopy. Perform experiment with various bias potentials around CV peak potential.
2. Determine the exchange current density,  $\alpha$  (symmetry factor) and double layer capacity of a redox reaction using platinum electrode (aqueous solution of 10 mM (Fe(NH<sub>4</sub>)<sub>2</sub>(SO<sub>4</sub>)<sub>2</sub> + Fe(NH<sub>4</sub>)<sub>2</sub>(SO<sub>4</sub>)<sub>2</sub>)) in 1 M HClO<sub>4</sub>.

### Nanoscience (Any Two)

1. Determine the rate constant of the redox reaction between hexacyanoferrate and thiosulphate ions in the presence and absence of gold nanoparticles.
2. Determine the temperature coefficient, activation energy and other thermodynamic parameters of the reaction.
3. Prepare gold nanostructures by reducing auric chloride with tea extract in presence of CTAB as capping agent, and characterize spectrophotometrically.
4. Prepare CdS nanoparticles and record their UV/Vis spectra.
5. Prepare CdSe quantum dots and record their absorption and emission spectra.

### Preparations

Preparation of selected inorganic compounds and their spectroscopic studies (any three):

1. Hg[Co(SCN)<sub>4</sub>]
2. Prussian Blue and Turnbull's Blue
3. Mn(acac)<sub>3</sub>
4. [Ni(NH<sub>3</sub>)<sub>6</sub>]Cl<sub>2</sub>
5. Cis and trans [Co(en)<sub>2</sub>Cl<sub>2</sub>]
6. Bromination of Cr (III) acetylacetonatoCr(acac)<sub>3</sub>. [J. Chem. Edu. 1986, 63].
7. Separation of optical isomers of cis [Co(en)<sub>2</sub>Cl<sub>2</sub>]Cl: J. Chem. Soc. 1960, 4369.
8. Preparation of copper glycine complex-cis and trans bis (glycinatoCu(II))
9. Tris (acetylacetonato) cobaltate (III)
10. Tris (Thiourea) Copper (I) Sulphate. (Estimation of Cu-Iodometrically). Any other compound prepared in the lab.

### Complexometric Titrations (any two)

1. Determine the strength of Zn<sup>2+</sup> and Mg<sup>2+</sup> in the given solution mixture by titrating it against EDTA using Erichrome black T as the indicator.
2. Determine the strength of Ca<sup>2+</sup> & Mg<sup>2+</sup> (as CO<sub>3</sub><sup>2-</sup>) in the given solution mixture by titrating it against EDTA using Erichrome black T & Calcol as the indicators.
3. Estimation of Sn<sup>2+</sup> as (ZnO) by titrating it against EDTA using Xylol-orange as the indicator.
4. Estimation of Zn<sup>2+</sup> and Ba<sup>2+</sup> mixture by back titration.
5. Determine the strength of CuSO<sub>4</sub>, 5H<sub>2</sub>O solution by titrating it against Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> iodometrically.

**Note:** Any experiment may be introduced/deleted in the practical class based on the availability/non-availability of the instruments/chemicals.

Experiment  
Lab record & Viva-voce

Marks: 30  
Marks: 5+15

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**Suggested Reading:**

1. James A.M. and Prichard F.E., *Practical Physical Chemistry*, Longman.
2. Levitt B.P. *Frindeleys Practical Physical Chemistry*, Longman.
3. Palit S.R. and De S.K., *Practical Physical Chemistry*, Science.
4. Shomaker D.P., *Experiments in Practical Physical Chemistry*, 8<sup>th</sup> Ed., (1967) Rep. (2012).
5. Jolly W.B., *Synthesis and Characterization of Inorganic Compounds*, Prentice Hall, Englewood, (1970).
6. Bell C.F., *Synthesis and Physical Studies of Inorganic Compounds*, 1<sup>st</sup> Ed., Pergamon Press, (1972).
7. Palmer W.G., *Inorganic Preparations*, Cambridge, (1970).

**References:**

1. Mendham J., Denney R.C., Barnes J.D. and Thomas M.J.K., *Vogel's Text Book of Quantitative Chemical Analysis*, 6<sup>th</sup> Ed., Third Indian Reprint, Pearson Education Pvt. Ltd., New Delhi (2003).

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### INTRODUCTION TO COMPUTATIONAL CHEMISTRY

Course Code:  
PC-655 (0 0 2)

Introduction to Computational Chemistry  
Non University Examination Scheme

Maximum Marks: 60 + 40 (CE)

Credit: 1

#### Course Objective:

1. The emphasis would be placed on using small Microsoft Office software which will help students in making reports and presentations, along with data analysis.
2. Students will be able to use softwares that will help those making chemical structures, understand topology and different file formats.
3. To make students familiar with various types of Biological databases, data retrieval and statistical analysis that can be performed to check data quality.
4. To make students understand the basic concepts in python and biopython which will help them in various Bioinformatics applications.

#### Course Learning Outcomes:

- Use of software and introduction of computational chemistry as a tool and scope.
- Use of various chemical and biological databases, retrieval and analysis of data.
- Introductory Python and Biopython programming language, be able to write small programs for biological sequence data retrieval and analysis.

#### **Unit-I**

**Introductory Concepts of Desktop Applications:** Introduction to MS Office for report generation and presentation, incorporation of graphs, tables, pictures into document. Spreadsheet and mathematical packages for data analysis. Introduction to chemical structure drawing softwares: ChemOffice, Chemdraw, Chemschetch, standard structure format and extension: smiles format and CDX file format, Experimental data visualization and interpretation by ACD ChemDraw, ACD 1D NMR processor.

#### **Unit-II**

**Introduction to computational chemistry:** Scope and Applications, Molecular Mechanics / Force Field Methods, Molecular dynamics, Postulates of Quantum Mechanics, The Born-Oppenheimer approximation, potential energy surfaces, local and global minima, introduction to Hartree-Fock molecular orbital theory, introduction to basis sets, Density-functional theory, Geometry optimization, Biological databases: protein and nucleotide sequence databases; PDB, PIR, UniProt, EMBL, GenBank, Introduction to sequence Analysis: usage of BLAST; FASTA file format, Statistics of sequence analysis

#### **Unit-III**

**Introduction to Python and Biopython:** Introduction to Python, Installation and Syntax, Python Numbers, data types, Boolean and operators, Looping, if else conditions and statements, Introduction to biopython, Usage example: simple FASTA and GenBank parsing example, Sequence slicing, concatenating and transcription

#### **Suggested Readings:**

1. Attwood, *Introduction to Bioinformatics*, Pearson Education Singapore Pte Ltd, 2007. (ISBN: 978-81-775-8641-1)
2. HoomanRashidi, Lukas K. Buehler, *Bioinformatics Basics: Applications in Biological Science and Medicine*, CRC Press/Taylor & Francis Group, 2005. (ISBN: 978-08-493-2375-1)

3. Lesk, A.M., *Introduction to Bioinformatics*, Oxford University Press, UK, Fourth edition, 2014.
4. Gretchen Kenney, *Bioinformatics: Principles and Analysis*, Syrawood Publishing House USA, 2016.
5. Jeffrey Augen, *Bioinformatics in the Post-Genomic Era: Genome, Transcriptome, Proteome, and Information-Based Medicine*, Addison-Wesley, 2004. (ISBN: 978-03-211-7386-7)
6. Stephen A. Krawetz, David D. Womble, *Introduction to Bioinformatics: A Theoretical and Practical Approach*, Humana Press, 2003. (ISBN: 978-15-882-9241-4)
7. <https://www.python.org/about/gettingstarted/>
8. <http://biopython.org/DIST/docs/tutorial/Tutorial.html#sec2>

#### References:

1. OrpitaBosu and Simminder Kaur Thukral, *Bioinformatics: Databases, Tools & Algorithms*, Oxford Higher Education.
2. Singhal and Singhal, *A Text Book of Bio-informatics*, PragatiPrakashan.
3. Warren J., Gregory E. and Grant R, *Statistical methods in Bioinformatics*, First edition, Springer-Verlag, Berlin, 2004.

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### CONFORMATIONAL ANALYSIS AND ASYMMETRIC SYNTHESIS

Course Code:

PC-602 (4 0 0)

Conformational Analysis and Asymmetric Synthesis

Core Course

Maximum Marks: 60 + 40 (CE)

Credit: 4

**Instruction to Paper Setters:**

**Attempt five questions**

**Time: 3 hours**

**Maximum Marks: 60**

Question Paper shall contain **Five Sections**

- The student has to attempt **five questions** from five sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** to **V** shall have two questions in each section, and the student needs to attempt only one question from each section. (Section II to V shall reflect Unit I to IV of the syllabus respectively).

#### Course Objective:

1. The course aims to understand the biological significance of chirality and need for asymmetric synthesis general strategy of asymmetric synthesis mechanism of illustrated examples.
2. It also aims to translate the asymmetric reactions covered for use in the retro synthesis approach.
3. To know about conformational analysis and stereochemistry of ring systems. To learn about stereochemistry of fused and bridged rings, O.R.D. and C.D.

#### Learning Course/Learning Outcomes:

The students will acquire knowledge of:

- Conformational analysis of cycloalkanes, reactivity, chirality, interconversion, resolution and asymmetric synthesis.
- Develop a fundamental understanding of the concepts of stereoisomerism, optical activity and chirality.
- Learn the principal methods that are used to prepare enantiomerically pure products from achiral starting materials.

#### **Unit-I**

##### **Conformational Analysis (Cyclic Systems)**

Study of conformations of cyclohexane, mono, di and polysubstituted cyclohexanes, cyclohexene, cyclohexanone (2-alkyl and 3-alkyl ketone effect), 2-halocyclohexanones, cyclopentane, cyclobutane, cycloheptane and cyclooctane. Stereochemistry of decalins. Conformational effects on the stability and reactivity of diastereomers in cyclic molecules – steric and stereo electronic factors – examples factors governing the reactivity of axial and equatorial substituents in cyclohexanes. Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.

#### **Unit-II**

##### **Topicity, Prostereoisomerism**

Introduction and terminology. Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces – symmetry, substitution and addition criteria. Prochirality nomenclature: Pro-R, Pro-S, Re and Si faces.

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### Unit-III

#### Asymmetric Induction

Stereoselective reactions: Substrate stereoselectivity, product stereoselectivity, enantioselectivity and diastereoselectivity. Symmetry and transition state criteria, kinetic and thermodynamic control. Methods for inducing enantio and diastereoselectivity. % Enantiomeric excess, enantiomeric ratio, optical purity, % diastereomeric excess and diastereomeric ratio. Chiral derivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.

Cram's and Prelog's; Dynamic stereochemistry (acyclic and cyclic), Qualitative correlation between conformation and reactivity, Curran-Hammett Principle.

### Unit-IV

#### Organic Stereochemistry

Methodologies in Asymmetric Synthesis, Strategies in Asymmetric Synthesis: 1. Chiral substrate controlled, 2. Chiral auxiliary controlled, 3. Chiral reagent controlled 4. Chiral catalyst controlled.

1. **Chiral Substrate Controlled Asymmetric Synthesis**

Nucleophilic additions to chiral carbonyl compounds. 1, 2-Asymmetric induction, Cram's rule and Felkin-Anh model.

2. **Chiral Auxiliary Controlled Asymmetric Synthesis**

$\alpha$ -Alkylation of chiral enolates, azaenolates, imines and hydrazones. 1, 4-Asymmetric induction and Prelog's rule. Use of chiral auxiliaries in Diels-Alder reaction.

3. **Chiral Reagent Controlled Asymmetric Synthesis**

Asymmetric reductions using BINAL-H. Asymmetric hydroboration using  $\text{IPC}_2\text{BH}$  and  $\text{IPCBH}_2$ .

4. **Chiral Catalyst Controlled Asymmetric Synthesis**

Sharpless and Jacobsen asymmetric epoxidations. Sharpless asymmetric dihydroxylation. Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalysts. Enzyme mediated enantioselective synthesis.

5. **Asymmetric Aldol Reaction**

Diastereoselective aldol reaction (chiral enolate & achiral aldehydes and achiral enolate & chiral aldehydes) its explanation by Zimmerman-Traxel model.

#### Molecular dissymmetry and chiroptical properties:

Linear and circularly polarized lights, circular birefringence and circular dichroism, ORD and CD of ORD and CD curves, cotton effect. The axial haloketone rule, octant diagrams, helio structural and stereochemical problems.

#### Suggested Reading:

1. Lehniger C., David L. Nelson and Michael M. Cox, *Principles of Biochemistry*, 6<sup>th</sup> Ed., (2013).
2. Stryer L., Freeman W.H., *Biochemistry*, 5<sup>th</sup> Ed., San Francisco, (2014).
3. Wood W.B. and Wilson J. H., Benbow R.M., and Hood L.E., *Problem Approaches in Biochemistry*, 1<sup>st</sup> Ed., Wiley, (1974).
4. Nasipuri D., *Stereochemistry of Organic Compounds – Principles & Applications*, 2<sup>nd</sup> Ed., New Age Publication, (2005).
5. Eliel Ernest L. & Wilen Samuel H., *Stereochemistry of Organic Compounds*, 1<sup>st</sup> Ed., Wiley, (1994).
6. Kalsi P.S., *Stereochemistry: Conformation & Mechanism*, 6<sup>th</sup> Ed., New Age Pub., (2009).
7. Bassendale Alan, *The Third Dimension in Organic Chemistry*, 3<sup>rd</sup> Ed., John Wiley & Sons, (1984).
8. Stephenson G.R., Nogradi, *Asymmetric Synthesis*, 3<sup>rd</sup> Ed., John Wiley and Sons, (1984).
9. Izumi Y. & Akira Tai, *Stereo Differentiating Reactions*, 3<sup>rd</sup> Ed., Academic Press, (1977).
10. Smith M. B., *Organic Synthesis*, 3<sup>rd</sup> Ed., (1978).

#### References:

1. Morrison J.D. and Moscher H.S., *Asymmetric Organic Reactions*, Vol. 3, Academic Press, (1984).
2. Hawley Robert E. & Aube Jeffrey, *Principles in Asymmetric Synthesis*, 2<sup>nd</sup> Ed., Elsevier, (2012).

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Parul Behera



## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### SYNTHETIC METHODS IN MEDICINAL CHEMISTRY (ORGANIC SYNTHESIS)

Course Code:

PC-604 (4 0 0)

Maximum Marks: 60 + 40 (CE)

Synthetic Methods in Medicinal Chemistry (Organic Synthesis) Credit: 4  
Core Course

#### Instruction to Paper Setters:

Attempt five questions

Time: 3 hours

Maximum Marks: 60

Question Paper shall contain **Five Sections**

- The student has to attempt **five questions** from five sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** to **V** shall have two questions in each section, and the student needs to attempt only one question from each section. (Section **II** to **V** shall reflect Unit **I** to **IV** of the syllabus respectively).

#### Course Objective:

1. After a successful completion of this course one would demonstrate understanding of the key elements of developing practical methods for the synthesis of pure organic compounds with a special emphasis on the design of economically feasible chiral processes.

#### Course/Learning Outcomes:

The students will acquire knowledge of:

- Mechanistic pathway of organic reactions.
- Retrosynthetic approach to planning organic synthesis.
- Conversion of different functional group via rearrangement reaction.
- And become adept at identifying strengths and weaknesses of particular methods and determine which will be optimal for a particular synthetic operation

#### Unit-I

##### Retrosynthetic Analysis

Basic principles and terminology of retrosynthesis (Disconnection, synthons, functional group interconversions (FGI), synthetic equivalents), synthesis of aromatic compounds, one group C-X and two group C-X, one group C-C and two group C-C disconnections, amine and alkene synthesis, functional group transposition, important strategies of retrosynthesis, important functional group interconversions, regioselectivity and regiospecificity. Use of chiral auxiliaries in synthesis.

#### Unit-II

##### Oxidations & Reductions

- a) Application of DDQ, SeO<sub>2</sub>, PCC, PDC, Swern oxidation, Periodic acid.
- b) Application of Homogenous (Wilkinson's catalytic hydrogenation) and heterogeneous catalytic reduction, boron reagents, Birch reduction, LiAlH<sub>4</sub>, NaBH<sub>4</sub> and their modifications, BH<sub>3</sub>, DIBAL.

#### Unit-III

##### Organometallic Reagents

- a) Preparation and application of the following in organic synthesis:

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- (i) Grignard
- (ii) Organo lithium
- (iii) Organo copper reagents
- b) Organoboranes in C-C bond formation
- c) Organo silicon reagents: reactions involving  $\beta$ -carbocations and  $\alpha$ -carbanions, utility of trimethylsilyl halides, cyanides and triflates.
- d) Organophosphorus: Wittig reaction, Mitsunobu reaction + Tebbe + Sulphur ylides

#### Carbonyl methylenation

- a) Phosphorous ylide mediated olefination:
  - (i) Wittig reaction
  - (ii) Horner-Wordsworth-Emmons reaction
- b) Titanium-Carbene mediated olefination:
  - (i) Tebbe reagent
  - (ii) Petasis reagent
  - (iii) Olefination by Nysted reagent

#### Unit-IV

##### New Synthetic Reactions

1. **Metal mediated C-C and C-X coupling reactions**  
Suzuki, Heck, Stille, Sonogashira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions.
2. **C=C formation reactions**  
Shapiro, Bamford-Stevens, McMurrey reactions, Julia-Lythgoe olefination and Peterson's stereoselective olefination.
3. **Multicomponent reactions**  
Ugi, Passerini, Biginelli, Hantzsch and Mannich reactions.
4. **Ring formation reactions**  
Pausan-Khand reaction, Bergman cyclisation, Nazarov cyclisation.
5. **Click Chemistry**  
Criteria for Click reaction, Sharpless azide cycloadditions.
6. **Metathesis**  
Grubbs' 1<sup>st</sup> and 2<sup>nd</sup> generation catalyst, Olefin cross coupling metathesis (OCM), ring closing metathesis (RCM), ring opening metathesis (ROM), applications.

##### Suggested Reading:

1. Carruthers W., *Some Modern Methods of Organic Synthesis*, 1<sup>st</sup> Ed., Reprint, Cambridge University Press, (1986).
2. Smith B. Michael, *Organic Synthesis*, 3<sup>rd</sup> Ed., Elsevier, (2011).

##### References:

1. Meckie R.K., Smith D.M. & Atken R.A., *Guidebook to Organic Synthesis*, 3<sup>rd</sup> Ed., Longman Publishing Co., (1990).
2. Fieser & Fieser, *Reagents for Organic Synthesis*, Vol. 1-26, Wiley, (2011).
3. Reich and Rigby, *Handbooks of Reagents for Organic Synthesis*, Set of Volume, (2007).
4. Warren S., *Designing Organic Synthesis*, Wiley, (1978).
5. Carruthers W., *Some Modern Methods of Organic Synthesis*, 4<sup>th</sup> Ed., Cambridge University Press, (2004).
6. House H.O. & Benjamin W.A., *Modern Synthetic Reactions* 2<sup>nd</sup> Ed., (1965).

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Dr. Chandra

Dr. Arun

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### SPECTROSCOPIC STUDIES

Course Code:  
PC-606 (4 0 0)

Spectroscopic Studies  
Skill Enhancement Course

Maximum Marks: 60 + 40 (CE)  
Credit: 4

Instruction to Paper Setters:  
Attempt five questions

Time: 3 hours  
Maximum Marks: 60

Question Paper shall contain **Five Sections**

- The student has to attempt **five questions** from five sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** to **V** shall have two questions in each section, and the student needs to attempt only one question from each section. (Section II to V shall reflect Unit I to IV of the syllabus respectively).

#### Course Objective:

1. The course covers structural elucidation by joint applications of spectroscopic techniques.
2. Emphasis would be on the qualitative analysis of molecules, biological active compounds using NMR, MS, UV, and IR.
3. The students will solve structural problems based on UV-Vis, IR,  $^1\text{H}$ NMR,  $^{13}\text{C}$ NMR and Mass Spectral data. Some emphasis will be given on quantitative aspects of these techniques.

#### Course/Learning Outcomes:

The students will be able to:

- Describe the basic instrumental principles involved in the operation of mass spectrometers, infrared spectrometers, and nuclear magnetic resonance spectrometers. This includes methods of sample handling and preparation, signal generation and detection, and data analysis for each method.
- Describe the physical and chemical principles that occur at the molecular level during a MS, IR, or NMR experiment.
- Evaluate the utility of UV/Vis spectroscopy as a qualitative and quantitative method.
- Identification of functional group based on IR spectra
- Analyze MS, IR, and/or NMR spectral data (either alone or in combination) to elucidate the structure of an organic molecule. This includes being able to make correlations of spectral features to specific portions of a molecule's structure. Students should be in a position to use spectroscopic methods for qualitative and quantitative analysis.

#### Unit-I

##### Symmetry and Group Theory in Chemistry

Definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Symmetry elements and symmetry operation, symmetry point group, Schönflies symbols, representation of groups by matrices (representation for the  $C_n$ ,  $C_{nv}$ ,  $C_{nh}$ ,  $D_{nh}$  etc. groups to be worked out explicitly). Character of a representation, reducible and irreducible representations, the great orthogonality theorem (without proof). Molecular asymmetry, dissymmetry and optical activity.

#### Unit-II

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### Ultraviolet and Visible Spectroscopy

Various electronic transitions (185-800nm), Beer-Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls.

### Infrared Spectroscopy

Instrumentation and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance. FTIR, IR of gaseous, solids and polymeric materials.

### Unit-III

#### Nuclear Magnetic Resonance Spectroscopy

General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, measurement of chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), complex spin-spin interaction between two, three, four and five nuclei (first order spectra), spin system-Pople notation, virtual coupling, Stereochemistry, concept of topicity, effect of enantiomeric and diastereomeric protons, hindered rotation, Karplus curve – variation of coupling constant with dihedral angle. Fourier transform technique, Hetero nuclei NMR-F, P.

#### Carbon-13 NMR Spectroscopy

Resolution and multiplicity of  $^{13}\text{C}$  NMR,  $^1\text{H}$ -decoupling, noise decoupling, broad band decoupling; Deuterium, fluorine and phosphorus coupling; NOE signal enhancement, off-resonance, Structural applications of CMR. DEPT and INEPT experiments; Introduction to 2D-NMR; COSY, HMQC and HETEROR spectra.

### Unit-IV

#### Mass Spectrometry

Theory, instrumentation, and modifications; Unit mass and molecular ions; Important terms – singly, doubly/multiple charged ions, metastable peak, base peak, isotopic mass peaks, relative intensity, FTMS, etc.; Recognition of M ion peak; Ionization methods (EI, CI and FAB), General fragmentation rules: Fragmentation of various classes of organic molecules, including compounds containing oxygen, sulphur, nitrogen and halogens;  $\alpha$ -,  $\beta$ -, allylic and benzylic cleavage; McLafferty rearrangement; ESI, APCI and MALDI, etc.

**Combined problems on UV, IR, NMR and MASS.**

#### Suggested Reading:

1. Kemp. W. *Organic Spectroscopy* 3<sup>rd</sup> Ed., W.H. Freeman & Co. (1991).
2. Silverstein, R.M., Webster Francis X., Kiemle David J., Bryce David L., *Spectroscopic Identification of Organic Compounds*, 8<sup>th</sup> Ed., John Wiley & Sons (2014).
3. Pavia Donald L., Lampman Gary M. and Kriz George S., *Introduction to Spectroscopy*, 5<sup>th</sup> Ed., Saunders Golden Sunburst Series. Harcourt Brace College Publishers, New York, (2015).
4. Dyer J.R., *Application of Absorption Spectroscopy of Organic Compounds*, Prentice Hall, (1965).
5. Williams D.H. and Fleming I., *Spectroscopic Methods in Organic Chemistry*, 6<sup>th</sup> Ed., Tata McGraw-Hill (2007).
6. Das K.G. & James E.P., *Organic Mass Spectrometry*, Oxford & IBH Publishing Co. (1976).
7. Kemp William, *NMR in Chemistry – A Multinuclear Introduction*, Macmillan, (1988).
8. Atta-ur-Rahman, *Nuclear Magnetic Resonance Basic Principles*, 1<sup>st</sup> Ed., Springer, (1986).

#### References:

1. Derome Andrew B., *Modern NMR Techniques for Chemistry Research*, Elsevier.
2. Levy G.C. and Nelson O.L., *Carbon-13 NMR for Organic Chemists*, 2<sup>nd</sup> Ed., Plenum Press.

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3. Bovey F. and Jelinski L., *Nuclear Magnetic Resonance Spectroscopy*, Academic Press.
4. Gross, *Mass Spectrometry: A Textbook*.

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### ENZYMES

Course Code:

(CE)PC-608 (2 0 0)

Maximum Marks: 60 + 40

Enzymes

Credit: 2

Ability Enhancement Compulsory Course

**Instruction to Paper Setters:**

**Time: 3 hours**

**Attempt five questions**

**Maximum Marks: 60**

Question Paper shall contain **Three Sections**

- The student has to attempt **five questions** from three sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** and **III** shall have three questions in each section, and the student needs to attempt two questions from each section. (Section II and III shall reflect Unit I and II of the syllabus respectively).

### Course Objective:

1. This course provides theory and knowledge relevant to enzymology principles including fundamental properties of enzymes, enzyme catalytic mechanisms and enzyme kinetics.

### Course/Learning Outcomes:

The students will be able to:

- Describe the structure and the function of an enzyme.
- Identify and explain the factors that affect the enzyme activity.
- Derive a rate law for general enzyme catalysed reaction.

### **Unit-I**

#### **Introduction to enzymes**

Nature of enzymes – protein and non-protein (ribozyme), Cofactor and prosthetic group, apoenzyme, holoenzyme. Factors affecting the rate of chemical reactions, collision theory, activation energy and transition state theory, catalysis, reaction rates and thermodynamics of reaction. Catalytic power and specificity of enzymes (concept of active site), Fischer's lock and key hypothesis, Koshland's induced fit hypothesis.

#### **Enzyme Kinetics**

Relationship between initial velocity and substrate concentration, steady state kinetics, equilibrium constant – monosubstrate reactions. Michaelis-Menten equation, Lineweaver-Burk plot, Eadie-Hofstee and Hanes plot,  $K_m$  and  $V_{max}$ ,  $K_{cat}$  and turnover number. Effect of pH, temperature and metal ions on the activity of enzymes.

#### **Enzyme inhibition**

Reversible inhibition (competitive, uncompetitive, non-competitive, mixed and substrate). Mechanism based inhibitors – antibiotics as inhibitors.

### **Unit-II**

#### **Mechanism of Action of Enzymes**

General features – proximity and orientation, strain and distortion, acid base and covalent catalysis (chymotrypsin, lysozyme). Metal activated enzymes and metalloenzymes, transition state analogues.

### Regulation of enzyme Activity

Control of activities of single enzymes (end product inhibition) and metabolic pathways, feedback inhibition (aspartate transcarbamoylase), reversible covalent modification phosphorylation (glycogen phosphorylase). Protoclytic cleavage - zymogen. Multienzymes complex as regulatory enzymes. Occurrence and isolation, phylogenetic distribution and properties (pyruvate dehydrogenase, fatty acyl synthase) Isoenzymes - properties and physiological significance (lactate dehydrogenase).

### Enzyme Immobilization

Methods of immobilization, advantage and applications of immobilization.

#### Suggested Reading:

1. Balasubramanian D., *Concepts in Biotechnology*, University Press, (1996).
2. Moran Laurence A., Horton Robert A. Gray Strimeom and Marc Perry, *Principals of Biochemistry*, Prentice Hall, (2011).
3. Dugas Herman and Penney Christopher, *Bioorganic Chemistry - A Chemical Approach to Enzyme Action*, 3<sup>rd</sup> Ed., Springer, (1986).

#### References:

1. Drauz, Karlheinz, *Enzyme Catalysis in Organic Synthesis*, a comprehensive handbook. Vol. I and II, John Wiley & Sons, (2012).
2. D-Fessner W., *Biocatalysis from Discovery to Application*, 1<sup>st</sup> Ed., Springer (1999).

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### GREEN CHEMISTRY

Course Code:  
PC-610 (2 0 0)

Green Chemistry  
Skill Enhancement Course

Maximum Marks: 60 + 40 (CE)  
Credit: 2

**Instruction to Paper Setters:**  
**Attempt five questions**

**Time: 3 hours**  
**Maximum Marks: 60**

Question Paper shall contain **Three Sections**

- The student has to attempt **five questions** from three sections.
- All sections are of 12 marks each.
- Section I is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section II and III shall have three questions in each section, and the student needs to attempt two questions from each section. (Section II and III shall reflect Unit I and II of the syllabus respectively).

### Course Objective:

1. Green Chemistry is the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances.

### Course/Learning Outcomes:

The students will be able to:

- A functional understanding of the field of green chemistry.
- A working understanding of the 12 principles of green chemistry.
- An understanding of several real world examples where organizations used green chemistry to improve the sustainability performance of their products.

### **Unit-I**

#### **Green Chemistry**

History of emergence of Green Chemistry through some industrial disasters, environmental movements for public awareness and some important environmental laws, Definition of Green Chemistry, Need for Green Chemistry, goals of Green Chemistry, Green Chemistry advances towards a sustainable future, Green Chemistry v/s Environmental Chemistry, Green Chemistry and its interdisciplinary nature, Twelve Principles of Green Chemistry and their illustrations with examples. Green starting materials, Green reagents, Green solvents and reaction conditions, Green catalysis (Introduction to Industrial Enzymes).

Green synthesis: Microwave assisted Synthesis, Ultrasound assisted reactions. Synthesis of adipic acid and BHC, synthesis of Ibuprofen involving principle of green chemistry.

Green energy and sustainability. Wealth from waste, Industrial case studies.

Pharmaceutical industries: The largest waste producer problems and solutions through Green Chemistry, benefits of greening industries, Emerging Green Technologies.

### **UNIT-II**

**Elucidation of metabolic pathways**

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Introduction-Metabolism: Catabolism and Anabolism, Difference between Biosynthesis and Biogenesis; Biomimetics. Methods for determination of biosynthetic mechanism- Radioisotopic labelling, enzymatic method, kinetics. Feeding experiments – use of radioisotopes measurement of incorporation – absolute incorporation, specific incorporation. Identification of the position of labels in labelled natural products by degradation, and spectral methods. Secondary metabolites derived from acetate: fatty acids

**Suggested Reading:**

1. Anastas, P.T. and Warner, J.K. Oxford Green Chemistry -Theory and Practical, University Press, (1998)
2. I.L Finar Vol II
3. Mann, J, Secondary Metabolism, 2<sup>nd</sup> Ed. Oxford Science Publication
4. Biosynthesis of Heterocycles: From Isolation to Gene Cluster, Ch:1 & Ch:2, 2015, John Wiley & Sons
5. Organic Synthesis by Michael B Smith, 4<sup>th</sup> Ed, Elsevier
6. Tetrahedron, 1958, 2, 1-57, The Total Synthesis of Reserpine.
7. Synthetic Communications, 2018, 48(10), 1128-1147, Synthetic Approaches Toward the Reserpine.
8. Goldberg, M.W, Sternbach, L. H., US Patent 2489238 (1949), Synthesis of Biotin.

**References:**

1. Drauz, Karlheinz, *Enzyme Catalysis in Organic Synthesis*, a comprehensive handbook. Vol. I and II, John Wiley & Sons, (2012).
2. D-Fessner W., *Biocatalysis from Discovery to Application*, 1<sup>st</sup> Ed., Springer (1999).

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### HISTORY AND PHILOSOPHY OF SCIENCE

Course Code:  
PC-612 (1 0 0)

Maximum Marks: 60 +40 (CE)

History and Philosophy of Science Credit: 1  
Non University Examination Scheme

Instruction to Paper Setters:  
Attempt five questions

Time: 3 hours  
Maximum Marks: 60

Question Paper shall contain **Three Sections**

- The student has to attempt **five questions** from three sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** and **III** shall have three questions in each section, and the student needs to attempt two questions from each section. (Section II and III shall reflect Unit I and II of the syllabus respectively).

**Course Objective:** To examine the inter-relationship between science and philosophy so as to emphasize on and explore the epistemological, discursive and metaphysical domain of science and technology.

#### Unit-I:

##### History of Science & Technology

Greek Age, Medieval Period, Renaissance, The Age of Reason, Modern Age and Contemporary Period.

##### Evolution of Scientific & Technological Thought

Brief historical introduction focusing on key thinkers and their ideas with special focus on Francis Bacon, David Hume, Immanuel Kant, Karl Popper and Thomas Kuhn.

#### Unit-II:

##### Understanding Philosophy of Science

The relationship between Science and Philosophy, Scientific Questions and Questions about Science, Modern Science as Philosophy, Science as Epistemology and Metaphysics.

##### The Scientific Method

Induction and Inductivism, Falsification, Revolutions and Rationality, Scientific realism, under determination, Explanation and Interference, Theory Change

#### Suggested Reading:-

1. *Understanding Philosophy of Science*, Ladyman, James, London/New York; Routledge, 2002.
2. *Philosophy of Science: A Contemporary Introduction*, Rosenberg, Alex London/New York; Routledge, 2001.

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### MEDICINAL CHEMISTRY PRACTICAL

Course Code:  
PC-652 (0 0 8)

Medicinal Chemistry Practical  
Core Course

Maximum Marks: 60 + 40 (CE)  
Credit: 4

#### Course Objective:

1. To study special techniques of importance in phytochemical research such as extraction procedures, open column chromatography, thin layer chromatography, preparative HPLC, GC, GCMS and LCMS.

#### Course/Learning Outcomes:

The students will be able to:

- Isolation and identification of natural products.
- Estimation of bio-molecules by chemical methods.
- Synthetic procedures: aqueous workup, distillation, reflux, separation, isolation, and crystallization.
- Characterization of compounds by using modern analytical techniques

#### Qualitative Analysis:

1. Isolation of natural products, by chemicals and chromatographic methods (TLC/Column/GC/HPLC) and characterization using spectroscopic techniques (any five):
  - (i) Isolation of caffeine from tea leaves
  - (ii) Isolation of piperine from black pepper
  - (iii) Isolation of  $\beta$ -carotene from carrots
  - (iv) Isolation of lycopene from tomatoes
  - (v) Isolation of cholesterol from bile stones
  - (vi) Isolation of limonene from lemon peel
  - (vii) Isolation of eugenol from cloves

#### Estimation of Natural Biomolecules (any nine):

1. Separation of amino acid mixture by Paper chromatography.
2. Estimation of amino acid by Ninhydrin method.
3. Estimation of protein by Biuret method.
4. Estimation of protein by Lowry et.al method.
5. Estimation of protein by Bradford method.
6. Specific reactions of Carbohydrate.
7. Estimation of sugar by Folin-wu method.
8. Estimation of sugar by Ferricyanide method.
9. Estimation of sugar by DNSA method.
10. Identification of carbohydrate mixture with suitable tests.
11. Isolation of amino acid cysteine from hair hydrolysate.
12. Estimation of Vitamin C from lemon fruits.
13. Determination on alpha amino nitrogen of amino acid.
14. Estimation of inorganic phosphorus by Fiske-Subbarow method.

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Note: Any experiment may be introduced/deleted in the practical class based on the availability/non-availability of the instruments/chemicals.

Experiment  
Lab record & Viva-voce

Marks: 30  
Marks: 5+15

**Suggested Reading:**

1. Vogel's, *Practical Organic Chemistry*, Longman Group, B.S. Furness et al., Ltd.
2. Fieser Louis F., *Experiments in Organic Chemistry*, O.C. Health and Company Boston (1955).
3. *Organic Synthesis*, Collective Vol. I
4. Pavy, *A Guide to Spectroscopy in Organic Chemistry*
5. Bansal R.K., *Laboratory Manual in Organic Chemistry*, Wiley Eastern Ltd., New Delhi (1980)
6. Sounder and Mann, *Practical Organic Chemistry*

**References:**

1. Plumm David T., *An Introduction to Practical Biochemistry*, Tata McGraw Hill Publishing Company Ltd., New Delhi.
2. Raphael I., *Natural Products: A Laboratory Guide*, 2<sup>nd</sup> Ed. New Delhi, Elsevier.

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### ENZYMOLGY

Course Code:  
PC-654 (0 0 8)

Maximum Marks: 60 + 40 (CE)

Enzymology  
Ability Enhancement Compulsory Course

Credit: 4

#### Course Objective:

1. The course aims to develop the key scientific skill required in scientific works. These includes practical research skill on experimental basis and to enable to acquire specialized knowledge.

#### Course/Learning Outcomes:

The students will be able to learn:

- A broad experimental approach, along with a theoretical introduction together with practical protocols, considering all aspects of enzymology.
- The fundamental experiments in enzymology and work on easily realizable protocols.

#### Experiments:

1. Detection of some common enzymes.
2. Extraction and Isolation of enzyme invertase/amylase/peroxidase/catalase.
3. Study of specific activity and progress curve.
4. To Assess effect of substrate conc. ( $V_{max}$  and  $K_m$ ) on enzyme activity.
5. To Assess effect of pH on enzyme activity.
6. To Assess effect of enzyme conc.
7. To Assess temperature stability of the enzyme.
8. To Assess effect of activator on enzyme activity.
9. To Assess effect of inhibitor on enzyme activity.
10. Effect of enzyme immobilization on its activity.
11. Statistical analysis of data.

**Note:** Any experiment may be introduced/deleted in the practical class based on the availability/non-availability of the instruments/chemicals.

**Experiment**

**Lab record & Viva-voce**

**Marks: 30**

**Marks: 5+15**

#### Suggested Reading:

1. Robyt J.R. and White B.J., *Biochemical Techniques Theory and Practice*.
2. Wilson K. and Walker J., *Practical Biochemistry: Principles and Techniques*.
3. Plummer David, *Practical Biochemistry*.
4. Sawhney S.K. and Singh R., *Introductory Practical Biochemistry*.

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### ADVANCED ORGANIC CHEMISTRY

Course Code:  
PC-701 (4 0 0)

Advanced Organic Chemistry  
Compulsory Foundation Course

Maximum Marks: 60 + 40 (CE)  
Credit: 4

Instruction to Paper Setters:  
Attempt five questions

Time: 3 hours  
Maximum Marks: 60

Question Paper shall contain **Five Sections**

- The student has to attempt **five questions** from five sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II to V** shall have two questions in each section, and the student needs to attempt only one question from each section. (Section II to V shall reflect Unit I to IV of the syllabus respectively).

#### Course Objective:

1. To provide knowledge of photochemistry, pericyclic reactions and heterocyclic chemistry.
2. To make understand the orbital interactions (Woodward Hoffmann rules) in concerted reactions.
3. A survey of chemical nature of heterocyclic moieties of medical substances with emphasis on methods of synthesis of medicinally important compounds containing heterocyclic ring.

#### Course/Learning Outcomes:

At the end of the course, the learners should be able to:

- Comprehend the structure-reactivity pattern of reactive intermediates involved in organic reactions.
- Comprehend the orbital interactions and orbital symmetry correlations of various pericyclic reactions.
- Write the mechanism of organic reactions involving reactive intermediates and concerted processes.
- Apply these reactions in organic synthesis.
- Predict the course of an organic photochemical reaction and identify the product with the type of functional group present on the molecule.
- Comprehend Nomenclature and reactivity and synthesis of different heterocyclic compounds and learn the synthesis different heterocyclic compounds

#### **Unit-I**

##### **Concerted reactions:**

Pericyclic Reaction: Classification, electrocyclic, sigmatropic, cycloaddition, chelotropic and ene reactions, Woodward Hoffmann rules, Frontier Molecular Orbital and Orbital symmetry correlation approaches, examples highlighting pericyclic reactions in organic synthesis such as Claisen, Cope, Diels-Alder, Sommelet-Hauser and Ene reactions (with stereochemical aspects), introductory dipolar cycloaddition.

##### **Unimolecular Pyrolytic Elimination Reactions:**

Chelotropic elimination, Decomposition of cyclic azo compounds,  $\beta$ -eliminations involving cyclic transition states such as sulfoxides, selenoxides, N-oxides, acetates, xanthates eliminations.

#### **Unit-II**

##### **Photochemistry**

Principles and concepts: An overview of Laws of photochemistry, Beer-Lambert law, electronic energy levels, singlet-triplet state, intensity and strength of electronic transition, selection rules for electronic transition, Jablonski diagram and photophysical processes, Franck-Condon principle. Excited state lifetime, steady state and time resolved emission, factors affecting excited state energy: solvent effect, TICT.

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Reactions: Photochemistry of alkene, cis-trans isomerization, photocycloaddition reactions of alkene, photochemical electrocyclic and sigmatropic reactions, di-pi-methane rearrangement, electron transfer mediated reactions of alkene. Photochemistry of carbonyl compounds, Norrish type I and type II reactions, enone and dienonecycloadditions. Photochemistry of aromatic systems, electron transfer and nucleophilic substitution reactions. Photochemistry of nitro, azo and diazocompounds. Photochemistry involving molecular oxygen, generation and reactions of singlet oxygen. Photo-fragmentation reactions (Barton, Hofmann-Löffler-Freytag). Photosynthesis, Phototherapy.

### Unit-III

#### Heterocyclic Chemistry

Introduction to Heterocycles: Nomenclature, spectral characteristics, reactivity and aromaticity. Synthesis and reactions of three and four membered heterocycles, e.g., aziridine, azirine, azetidine, oxiranes, thiarines, oxetenes and thietanes.

Five membered rings with two heteroatoms: pyrazole, esoxazoles, imidazoles, oxazoles, thiazoles, isothiazole.

### Unit-IV

#### Chemistry of Fused Heterocyclic Compounds

Benzofused five membered heterocycles with one heteroatom, e.g. indoles, benzofuran, benzothiophenes.

Chemistry of bicyclic compounds containing one or more heteroatoms.

Benzofused six membered rings with one, two and three heteroatoms: benzopyrans, quinolines, isoquinolines, quinoxalines, acridines, phenoxazines, phenothiazines, benzotriazines, pteridines.

Seven and large membered heterocycles: azepines, oxepines, thiepinones. Chemistry of porphyrins and spiroheterocycles.

#### Suggested Reading:

1. March, J. *Advanced Organic Chemistry* John Wiley & Sons (2006).
2. Carey, F. A. & Sundberg, R. J. *Advanced Organic Chemistry*, Parts A & B, Plenum: U.S. (2004).
3. Acheson Van R. M., *Introduction to the Chemistry of Heterocyclic Compounds*, 1<sup>st</sup> Ed., John Wiley & Sons (1977).
4. Mukherjee S. M., *Pericyclic Reactions*, 1<sup>st</sup> Ed., Macmillan, (1980).
5. Harspool W. M., *Aspects of Organic Photochemistry*, 1<sup>st</sup> Ed., Academic Press (1976).
6. Marchand A. P., & Lehr R. E., *Pericyclic Reactions*, 1<sup>st</sup> Ed., Academic Press (1977).
7. Turro N. J., Ramamurthy V., Scamman J. C., *Modern Molecular Photochemistry of Organic Molecules*, Angew Chemistry, Int. Ed., (2010).
8. Coyle D., *Introduction of Organic Photochemistry*, Wiley (1986).
9. Joule J. A. & Mills K., *Heterocyclic Chemistry*, 5<sup>th</sup> Ed., Wiley, (2010).
10. Paquette A., *Principles of Modern Heterocyclic Chemistry*, 1<sup>st</sup> Ed., Wiley, (1976), Digitized (2010).

#### Reference:

1. Katritzky A. R., *Handbook of Heterocyclic Chemistry*, 3<sup>rd</sup> Ed., Elsevier, (2010).
2. Gilchrist T. L., *Heterocyclic Chemistry*, 3<sup>rd</sup> Ed., Longman Scientific Technical, (1997).
3. Katritzky A. R. and Rees C. W., *Comprehensive Heterocyclic Chemistry*, Vol. 1 to 15, Elsevier.

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### BIOENERGETICS AND METABOLISM

Course Code:  
PC-703 (4 0 0)

Bioenergetics and Metabolism  
Skill Enhancement Course

Maximum Marks: 60 + 40 (CE)  
Credit: 4

**Instruction to Paper Setters:**  
**Attempt five questions**

**Time: 3 hours**  
**Maximum Marks: 60**

Question Paper shall contain **Five Sections**

- The student has to attempt **five questions** from five sections.
- All sections are of 12 marks each.
- Section I is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section II to V shall have two questions in each section, and the student needs to attempt only one question from each section. (Section II to V shall reflect Unit I to IV of the syllabus respectively).

#### Course Objective:

1. The objectives of this Course is to study and consolidate concepts in the areas of Metabolism and Bioenergetics, focusing on the main metabolic pathways in living cells, their regulation and energy requirement.
2. The focus will be on bringing the students up to date on new advances in these areas while stressing the fundamental principles and molecules involved.

#### Course/Learning Outcomes:

By the end of this course a learner would:

- Understands the concepts of metabolism and how metabolism is regulated at the level of the cell and the whole organism.
- Understands which organic compounds are used as 'fuel' or metabolic substrates and understand how cells and organisms use these fuels.
- Knows which metabolic pathways and reactions contribute to cellular metabolism.
- Understands the concepts of bioenergetics including determining and evaluating free energy and redox potential in relation to metabolism.
- Understands the central importance of ATP in energy currency.
- Knows the mechanisms involved in the generation of ATP. Understands how enzymes and cofactors function in bioenergetic reactions.
- Be familiar with the molecular complexes and pathways involved in photosynthesis and carbon fixation (PSI, PSII and Calvin cycle).
- Be familiar with the key steps in the main pathways of carbohydrate, fat, lipid and nitrogen metabolism (synthesis and breakdown), how they are regulated and their importance.
- Understands the switches in metabolic pathways during fasting and feeding.
- Be able to apply your knowledge of metabolism to your understanding of health and disease

#### **Unit-1**

##### **Basic Design of Metabolism**

Autotrophs, heterotrophs, metabolic pathways, catabolism, anabolism, ATP as energy currency, reducing power of the cell.

##### **Glycolysis**

Glycolysis – a universal pathway, reactions of glycolysis, fermentation, fates of pyruvate, feeder pathways for glycolysis, galactosemia.

##### **Gluconeogenesis and Pentose Phosphate Pathway**

Synthesis of glucose from non-carbohydrate sources, reciprocal regulation of glycolysis and gluconeogenesis, pentose phosphate pathway and its importance.

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## **Glycogen Metabolism**

Glycogenesis and glycogenolysis, regulation of glycogen metabolism, glycogen storage diseases.

## **Citric Acid Cycle**

Production of acetyl CoA, reactions of citric acid cycle, anaplerotic reactions, amphibolic role, regulation of citric acid cycle, glyoxalate pathway, coordinated regulation of glyoxalate and citric acid pathways.

## **Synthesis of Carbohydrates**

Calvin cycle, regulation of calvin cycle, regulated synthesis of starch and sucrose, photorespiration, C<sub>4</sub> and CAM pathways.

## **Unit-II**

### **Fatty Acid Oxidation**

Digestion, mobilization and transport of cholesterol and triacylglycerols, fatty acid transport to mitochondria,  $\beta$  oxidation of saturated, unsaturated, odd and even numbered and branched chain fatty acid, regulation of fatty acid oxidation, peroxisomal oxidation,  $\omega$  oxidation, ketone bodies metabolism, ketoacidosis.

### **Fatty Acid Synthesis**

Fatty acid synthase complex. Synthesis of saturated, unsaturated, odd and even chain fatty acids and regulation. Lipid storage diseases.

### **Starve-feed Cycle**

Well-fed state, early fasting state, fasting state, early re-fed state, energy requirements, reserves and caloric homeostasis, five phases of glucose homeostasis.

## **Unit-III**

### **Proteins and Nucleic Acids**

1. **Oxidative Degradation of Amino Acids:** Proteolysis, transamination, oxidative deamination, acetyl CoA, alpha ketoglutarate, acetoacetyl CoA, succinate, fumarate and oxaloacetate pathway. Decarboxylation, urea cycle, ammonia excretion.
2. **Biosynthesis of Amino Acids:** Amino acid biosynthesis, precursor functions of amino acid (Biosynthesis of glycine, serine, cysteine, methionine, threonine).
3. Inborn errors of amino acid metabolism.
4. Peptides, polyamines, porphyrins, gamma glutamyl cycle, glutathione biosynthesis, nonribosomal protein biosynthesis.
5. Disorders of amino acids metabolism. phenylketonuria, alkaptonuria, maple syrup urine disease, methylmalonic academia (MMA), homocystinuria and Hartnup's disease.

## **Unit-IV**

### **Biosynthesis of Purine and Pyrimidine Nucleotides**

De novo synthesis of purine and pyrimidine nucleotides, regulation and salvage pathways.

### **Deoxyribonucleotides and Synthesis of Nucleotide Triphosphate**

Biosynthesis of deoxyribonucleotides and its regulation, conversion to triphosphates, biosynthesis of coenzyme nucleotides.

### **Degradation of Purine and Pyrimidine Nucleotides**

Digestion of nucleic acids, degradation of purine and pyrimidine nucleotides. Inhibitors of nucleotide metabolism. Disorders of purine and pyrimidine metabolism – Lesch-Nyhan syndrome, Gout, SCID, adenosine deaminase deficiency.

### **Suggested Reading:**

1. Berg Jeremy M., Tymoczko John L. and Stryer Lubo, *Biochemistry*, 7<sup>th</sup> Ed., W.H. Freeman (2011).
2. Conn E.E. and Stumpf P.K., *Outlines of Biochemistry*, John Wiley, (1987).
3. Finar, I.L. & Finar, A.L. *Organic Chemistry* Vol. 2, Pearson (2002).
4. Finar, I.L. *Organic Chemistry* Vol. 1 Longman (1998).
5. Sinden, R.P. *DNA Structure and Function*, 1<sup>st</sup> Ed., Academic Press (1994).
6. Zubay G., *Biochemistry*, 4<sup>th</sup> Ed., Addison Wesley Publ. (1999).
7. Horton & others, *Principals of Biochemistry*, 5<sup>th</sup> Ed., Prentice Hall, (2011).

### **References:**

1. Murray Robert K., Graner Daryl K., Rodwell Victor W., *Harper's Biochemistry*, 29<sup>th</sup> Ed., Lange McGraw Hall (2012).
2. Lehniger A.L., David L. Nelson, Michael M. Cox, *Principles of Biochemistry*, 5<sup>th</sup> Ed., W.H. Freeman, (2008).

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### SEPARATION SCIENCE

Course Code:  
PC-705(A1) (2 0 0)\*

Maximum Marks: 60 + 40(CE)  
Credit: 2

Separation Science  
Discipline Centric Elective

**Instruction to Paper Setters:**  
**Attempt five questions**

**Time: 3 hours**

**Maximum Marks: 60**

Question Paper shall contain **Three Sections**

- The student has to attempt **five questions** from three sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** and **III** shall have three questions in each section, and the student needs to attempt two questions from each section. (Section II and III shall reflect Unit I and II of the syllabus respectively).

#### Course Objective:

1. The main objective of this course is to familiarize students with the fundamental principles of separation processes used in analytical chemistry such as various extraction techniques, gas and liquid chromatography, size and ion chromatography and electrophoresis.
2. By completion of the course, students are also expected to gain independent laboratory skills in certain separation techniques
3. The learner will have the ability to interpret data from analytical separation methods.

#### Course/Learning Outcomes:

On completion of the course, the student should be able to:

- Have understanding of different purification criteria at separation.
- Account for fundamental separation processes and their connection to molecular properties.
- Have awareness about the most common separation and detection methods.
- Account for application of different chromatographic methods regarding examination type, component analysis and concentration range.
- Be able to choose and apply appropriate separation and detection methods on the basis of a simpler problem.

#### **Unit-I:**

##### **Separation Techniques:**

Need for learning separation techniques, separation techniques in natural product research and drug discovery, extraction techniques.

##### **Chromatography:**

General principles, classification of chromatographic techniques, normal and reverse phase, bonded phase chromatography, stationary phases, activity of stationary phases, elutropic series and separation mechanisms.

##### **Column Chromatography and Short Column Chromatography:**

Column packing, sample loading, column development, detection.

##### **Flash Chromatography and Vacuum Liquid Chromatography:**

Objectives, optimization studies, selecting column and stationary phases, selecting suitable mobile phases, automated flash chromatography and reverse phase flash chromatography.

##### **High Performance Liquid Chromatography:**

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Principles, instrumentation, peak shapes, capacity factor, selectivity, plate number, plate height, resolution, band broadening, pumps, injector, detectors, columns, column problems, gradient HPLC, HPLC solvents, trouble shooting, sample preparation, method development.

#### **Planar Chromatography-TLC/HPTLC/OPLC**

Basic principles sample application, development of plates, visualization of plates, 2D, TLC, densitometry, over pressure layer chromatography.

#### **Counter Current Chromatography**

Basic principles, droplet countercurrent chromatography, centrifugal partition chromatography, choice of solvents for SP and MP.

#### **Gas Chromatography**

Principles, instrumentation, split-splitless injector, head space sampling, columns for GC, detectors, quantification.

#### **Gel Permeation Chromatography**

#### **Biochromatography**

Size exclusion chromatography, ion exchange chromatography, ion pair chromatography, affinity chromatography general principles, stationary phases and mobile phases.

#### **Hyphenated Techniques**

Introduction to GC-MS and LC-MS techniques and their applications in natural products.

### **Unit-II:**

#### **Separation and Characterization of Proteins**

Ammonium sulphate fractionation, solvent fractionation, dialysis and lyophilization. Ion-exchange chromatography, molecular sieve chromatography, hydrophobic interaction/reverse phase chromatography, affinity chromatography.

Determination of purity, molecular weight, extinction coefficient and sedimentation coefficient, IEF, SDS-PAGE and 2-D electrophoresis.

#### **Suggested Reading:**

1. Mermet J.M., Otto M., R. Kellner, *Analytical Chemistry*, Wiley-VCH (2004).
2. Dick J.G., *Analytical Chemistry*, 3<sup>rd</sup> Ed., R.E. Krieger Pub., (1978).
3. Willard H.H., Merritt L.L., Dean J.A., *Instrumental Methods of Analysis*, 7<sup>th</sup> Ed., Van Nostrand, (2004).
4. Christian G.D., O'Reilly J.E., *Instrumental Analysis*, 2<sup>nd</sup> Ed., Allyn & Bacon, (1986).
5. Wendlandt W.W., *Thermal Methods of Analysis*, 2<sup>nd</sup> Ed., Inter Science, (1964).
6. Hatakeyama T., Zenhai, *Thermal Analysis*, John Wiley & Sons, (1998).
7. Wiesendanger R., *Scanning Probe Microscopy and Spectroscopy*, Cambridge University Press, (1998) Reprint.

#### **References:**

1. Kennedy John H., *Analytical Chemistry Principles*, 2<sup>nd</sup> Ed., Sounders College Publishing, California (1990).
2. Harvey, *Modern Analytical Chemistry*, McGraw Hill. (2000).
3. Skoog, *Principles of Instrumental Analysis*, 6<sup>th</sup> Ed., (2014).
4. Settle F.A., *Handbook of Instrumental Techniques for Analytical Chemistry*, Prentice Hall PTR, (1997).

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- One course to be selected among 705A1/705A2
- The course would be offered with a minimum of 7 students

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### MOLECULAR SPECTROSCOPY

Course Code:

PC-705(A2) (2 0 0)

Maximum Marks: 60 + 40(CE)

Molecular Spectroscopy

Credit: 2

Discipline Centric Elective

**Instruction to Paper Setters:**

**Attempt five questions**

**Time: 3 hours**

**Maximum Marks: 60**

Question Paper shall contain **Three Sections**

- The student has to attempt **five questions** from three sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** and **III** shall have three questions in each section, and the student needs to attempt two questions from each section. (Section II and III shall reflect Unit I and II of the syllabus respectively).

#### Course Objective:

1. The course aims to teach the students the theoretical background and to make conversant with the quantum mechanical nature of atoms and molecules, building on basic materials.

#### Course/Learning Outcomes:

Upon successful completion of this course, the student will be able to:

- Explain the change in behavior of atoms in external applied electric and magnetic field.
- Explain rotational, vibrational, electronic and Raman spectra of molecules.
- Apply these concepts to understand the structure of molecules
- Able to apply knowledge to detailed understanding of electronic states of atoms, molecules, Franck-Condon Factors

#### **Unit-I**

##### **Unifying Principles**

Electromagnetic radiation, interaction of electromagnetic radiation with matter-absorption, emission, transmission, reflection, refraction, dispersion, polarization and scattering. Uncertainty relation and natural line width and line broadening, transition probabilities, results of the time dependent perturbation theory, transition moment, selection rule, intensity of spectral lines, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels.

##### **Microwave Spectroscopy**

The rotation of molecules, rotational spectra of rigid diatomic molecules, intensities of rotational spectral lines, isotopic effect, non-rigid rotator, spectra of polyatomic linear, molecules and symmetric top molecules.

##### **Infrared Spectroscopy**

The vibrating diatomic molecule, force constant, zero point energy, simple harmonic vibrator, anharmonicity, Morse potential, overtones, hot bands, diatomic vibrating rotators, P, Q, R branches, vibration of polyatomic molecules, normal mode of vibrations. Fourier transform spectroscopy.

##### **Raman Spectroscopy**

Classical and quantum theories, pure rotational raman spectra of linear molecules, vibrational raman spectra, mutual exclusion principle, polarization of the light and raman effect, depolarization of raman lines, technique.

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## Unit-II

### Electron Spin Resonance Spectroscopy

Basic principle of ESR, experimental technique, the g-value hyperfine structure, applications of ESR spectroscopy to the study of free radicals and fast reactions, spin densities and Mc Connell relationship.

### X-Ray

Production of X-rays, X-ray spectra, absorption edges, X-ray filters, reciprocal lattice concept and its importance, Definition of Reciprocal lattice vector (derivation excluded). Interplanar spacing using reciprocal lattice concept for cubic, tetragonal, orthorhombic and hexagonal crystal systems. Equivalence of Bragg's and Laue condition. Structure factor calculations for primitive, base-centered, body-centered and face centered unit cells. Relation of structure factor to electron density and intensities (derivation excluded). Data collection and data reduction, Phase problem-Patterson method and Heavy-atom method, refinement of structure by successive and difference fourier synthesis. Correctness of a structure (Discrepancy index).

### Electron Diffraction

Basics, measurement technique, Comparison with X-ray diffraction technique. Applications in structure determination.

### Neutron Diffraction

Basics, measurement technique, applications and comparison with X-ray diffraction technique.

### Suggested Reading:

1. Banwell C.N. *Fundamentals of Molecular Spectroscopy*, 4<sup>th</sup> Ed., Tata McGraw Hill. (2008).
2. Barrow, G.M. *Introduction to Molecular Spectroscopy* McGraw-Hill (1962).
3. Chang, R. *Basic Principles of Spectroscopy*, 2<sup>nd</sup> Ed., McGraw-Hill, New York, N.Y. (1973).
4. Warren, B.E. *X-Ray Diffraction* Dover Publications (1991).

### References:

1. Gullavy W.A., *Introduction to Molecular Structure and Spectroscopy*, 1<sup>st</sup> Ed., Allyn and Bacon (1977).

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- One course to be selected among 705A1/705A2
- The course would be offered with a minimum of 7 students

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### INTRODUCTION TO MICROBIOLOGY

Course Code:  
(CE)PC-707 (3 0 0)

Introduction to Microbiology  
Ability Enhancement Compulsory Course

Maximum Marks: 60 + 40

Credit: 3

Instruction to Paper Setters:  
Attempt five questions

Time: 3 hours

Maximum Marks: 60

Question Paper shall contain **Five Sections**

- The student has to attempt **five questions** from five sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** to **V** shall have two questions in each section, and the student needs to attempt only one question from each section. (Section II to V shall reflect Unit I to IV of the syllabus respectively).

#### Course Objective:

1. The primary objective of the course is to build a strong foundation in the area of bacterial cell structure, division, survival and propagation and to develop clear understanding of various aspects of microbial physiology and interactions along with diverse metabolic pathways existing in bacteria in relation to its survival and propagation.
2. The course will facilitate in understanding of molecular virology by examining common processes and principles in viruses to illustrate viral complexity, to understand viral reproduction.
3. Demonstrate scientific literacy in major concepts and processes relative to the major groups of fungi and fungal-like organisms.

#### Course/Learning Outcomes:

Upon successful completion of the course, the student:

- Will be able to describe the morphological features, cell arrangement and structural components of bacterial cell in detail;
- Will be able to differentiate between Gram-positive and Gram-negative bacteria.
- Will have gained knowledge about cell wall structure and extracellular appendages in different bacteria.
- Will have gathered detailed information regarding bacterial cell division and endospore formation.
- Can enlist the characteristics of archaea that differentiate it from eubacteria, and will have learnt key features of some model archaeal organisms.
- Can enlist the salient features of the genome organization.
- Understands different secretion systems existing in bacteria for toxins and biomolecules secretion, and their role in bacterial survival and pathogenesis.
- Develop an understanding of microbes, fungi and lichens and appreciate their adaptive strategies

#### **Unit-I**

##### **History of Development of Microbiology**

Development of microbiology as a discipline. Spontaneous generation vs. biogenesis. Contributions of Anton von Leeuwenhoek, Louis Pasteur, Robert Koch, Joseph Lister, Alexander Fleming. Germ theory of disease, Development of various microbiological techniques and golden era of microbiology. Establishment of fields of medical microbiology and immunology through the work of Paul Ehrlich, Elie Metchnikoff, Edward Jenner.

##### **Bacterial Cell Organization**

Cell size, shape and arrangement, glycocalyx, capsule, flagella, endoflagella, fimbriae and pili. Cell-wall: Composition and detailed structure of Gram-positive and Gram-negative cell walls, Archaeobacterial cell wall, Gram and acid fast staining mechanisms, lipopolysaccharide (LPS).

##### **Bacteriological Techniques**

Pure culture isolation: Streaking, serial dilution and plating methods; cultivation, maintenance and preservation/stocking of pure cultures; cultivation of anaerobic bacteria, and accessing non-culturable bacteria.

## Unit-II

### Growth and nutrition

Definitions of growth, Batch culture, Continuous culture, generation time and specific growth rate, Effect of temperature and pH on microbial growth, Effect of solute and water activity on growth, Effect of oxygen concentration on growth, Nutritional categories of microorganisms.

Nutritional requirements in bacteria and nutritional categories, Culture media: components of media, natural and synthetic media, chemically defined media, complex media, selective, differential, indicator, enriched and enrichment media.

Logarithmic representation of bacterial populations, phases of growth, calculation of generation time and specific growth rate.

## Unit-III

### Virus

Discovery of viruses, nature and definition of viruses, general properties, concept of viroids, virusoids, satellite viruses and Prions. Theories of viral origin. Structure of Viruses: Capsid symmetry, enveloped and non-enveloped viruses. Isolation, purification and cultivation of viruses. Viral taxonomy: Classification and nomenclature of different groups of viruses. Bacteriophages: Diversity, classification, one step multiplication curve, lytic and lysogenic phases (lambda phage).

### Fungi

Fungi General characteristics of fungi including habitat, distribution, nutritional requirements, fungal cell ultra-structure, thallus organization and aggregation, fungal wall structure and synthesis, asexual production, sexual reproduction, heterokaryosis, heterothallism and parasexual mechanism.

## Unit-IV

### Microbial Interactions

Microbial genetics-transformation, conjugation, transduction, protoplast fusion, genetic recombination.

Microbe interactions: Mutualism, synergism, commensalism, competition, amensalism, parasitism, predation.

Microbe-animal interaction: termite gut microflora, nematophagus fungi and symbiotic luminescent bacteria.

Normal microflora of the human body; Importance of normal microflora, normal microflora of skin, throat, gastrointestinal tract, urogenital tract.

Host pathogen interaction: Definitions – Infection, Invasion, Pathogen, Pathogenicity, Virulence, Toxigenicity, Carriers and their types, Opportunistic infections, Nosocomial infections. Transmission of infection.

Collection, transport and culturing of clinical samples, principles of different diagnostic tests (ELISA, Immunofluorescence).

### Suggested Reading:

1. Ananthanarayan & Paniker's, *Textbook of Microbiology*, 9<sup>th</sup> Ed., University Press, (2012).
2. Dawes G.W., *Microbial Physiology*, 2<sup>nd</sup> Ed., Oxford, (1992).
3. Gardner J.F. and Peel M.M., *Introduction to Sterilization and Disinfection*, 2<sup>nd</sup> Ed, (1986).
4. Murray P. R., *Manual of Clinical Microbiology*, 7<sup>th</sup> Ed., Amer Society for Microbiology, (1999).
5. Collier L and Oxford J. *Human Virology*, 4<sup>th</sup> Ed., London Oxford University Press, (2011).
6. Stanimir R.V., Ingraham J.L., Wheelis M.L., Painter P.R., *The Microbial World*, 5<sup>th</sup> Edition, Prentice-Hall, (1990).
7. Wileman A., *Principles of Biotechnology*, 2<sup>nd</sup> Edition, Surrey University Press.

### References:

1. Schwartz R.S., *Diversity of the Immune Response*, New Eng J Med 348:1017 (2003).
2. Talaro K.P., Chess B., *Foundation in Microbiology: Basic Principle*, 8<sup>th</sup> Ed., McGraw Hill Science, (2014).
3. Law Chamber, *Medical Microbiology-The Big Picture*, 1<sup>st</sup> Ed., McGraw Hill, (2008).

Deepa Sasmal

Archit. Parul Beergal.



## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### CONCEPTS IN DRUG DESIGN\*

Course Code:  
PC-709 (2 0 0)

Concepts in Drug Design\*  
Core Course

Maximum Marks: 60 + 40 (CE)  
Credit: 2

**Instruction to Paper Setters:**  
**Attempt five questions**

**Time: 3 hours**  
**Maximum Marks: 60**

Question Paper shall contain **Five Sections**

- The student has to attempt **five questions** from three sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** and **III** shall have three questions in each section, and the student needs to attempt two questions from each section. (Section II and III shall reflect Unit I and II of the syllabus respectively).

#### Course Objective:

1. Course aims to provide students with an understanding of the process of drug discovery and development from the identification of novel drug targets to the introduction of new drugs.
2. It covers the basic principles of how new drugs are discovered with emphasis on lead identification, lead optimization, classification and kinetics of molecules targeting enzymes and receptors, prodrug design and applications, as well as structure-based drug design methods.
3. Recent advances in the use of computational and combinatorial chemistry in drug design will also be presented.

#### Course/Learning Outcomes:

Upon successful completion of the course, the student:

- Would understand the various stages of drug discovery and target identification to final drug registration.
- Learn the concept of bioisosterism and drug resistance.
- Describe physicochemical Properties and the techniques involved in QSAR.
- Explain various structure based drug design methods (Molecular docking).
- Learn the concept of pharmacophore and modeling techniques target selection, lead discovery using computer-based methods and combinatorial chemistry/high-throughput screening

#### **Unit-I**

##### **Computational Molecular Modeling**

Molecular Mechanics (MM), Force Field, Energy minimization, Geometry optimization methods: Linear and non-linear methods of minimization, Confirmation search different methods: (Systematic Search, Random Search, Monte Carlo Methods, Tabu Search, Simulated Annealing, Matrix Method, Genetic Algorithmsetc) Advantages and limitations of different method.

##### **Structure Based Drug Design**

Introduction, Protein structure selection-preparation; Binding Site Analysis; Docking; Search algorithms; Scoring methods: Grid based docking, validation of the results; Comparison of different docking software; Rigid docking Vs Flexible docking methods; Induced fit docking; Covalent docking; Binding affinity calculations; Structure based Virtual screening workflow; De-novo Drug Design methods

*Prasad*

## Protein Structure Prediction and Biologics

Introduction: Homology modeling, Threading method; Template identification; Sequence alignment methods: Sequence based alignment, Fold based alignment; Model building; Protein-loop refinement; Protein model validation; Protein-protein Docking; Antibody modeling, Protein Engineering tools: Cysteine Scanning, Residue Scanning, protein aggregation analysis.

## Unit-II

### Quantitative Structure Activity Relationship (QSAR)

Introduction; Physicochemical properties; Electronic effects: Hammett equation; lipophilicity effects: Hansch equation; steric effects: Taft equation; Descriptors for QSAR: Physico chemical descriptors, Steric descriptors: 1D, 2D, 3D-QSAR; atom based QSAR, Field based QSAR; ADME Screening.

### Ligand Based Drug Design

Introduction; 3D-Pharmacophore; Hypothesis development; Validation of the pharmacophore; energy based pharmacophore; Shape based search methods for virtual screening.

### Molecular Dynamics

Introduction and theory; Ensembles: Canonical and micro-canonical ensemble, Free Energy perturbation method; Total free energy calculation,

### Suggested Reading:

1. Young David C., *Computational Drug Design: A Guide for Computational and Medicinal Chemist*, Wiley (2009).
2. Silverman R.B., *Organic Chemistry of Drug Design and Drug Action*, 3<sup>rd</sup> Edition, Academic Press, (2014).
3. Charifson P.S., *Practical Applications of Computer Aided Drug Design*, Marcel Dekker, (1997).
4. Cohen N.C., *Molecular Modeling in Drug Design*, Online.
5. Goodman J., *Chemical Applications of Molecular Modeling*, RSC, (2004).
6. Guner O.F., *Pharmacophore Perception, Development and use in Drug Design*, International University, (2000).
7. Lemke Thomas L. and William David A., *Berger's Medicinal Chemistry and Drug Design*, 6<sup>th</sup> Edition, Lippincott, (2008).
8. Purcell William P., *Strategies of Drug Design*, RSC, (2011).
9. Abraham Donald J. and Rotella D.P., *Foye's Medicinal Chemistry*, Vol. 1-8, 7<sup>th</sup> Edition, Wiley, (2010).
10. Korolkovas A. and Burckhalter J.H., *Essentials of Medicinal Chemistry*, John Wiley, (1976).
11. Veerapandion Pandi, *Structure Based Drug Design*, Monograph, Vol. II and III, Academic Press.

### References:

1. Leach A.R., *Molecular Modeling*.

Deepa Desmal

Dr. S. S. S. S.

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### Developing Entrepreneurial Mindset

Course Code:  
PC-711 (2 0 0)

Developing Entrepreneurial Mindset  
Non-University Examinational Subject

NUES\*  
Credit: 2

**Instruction to Paper Setters:**  
**Attempt five questions**

**Time: 3 hours**  
**Maximum Marks: 60**

Question Paper shall contain **Five Sections**

- The student has to attempt **five questions** from five sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** to **V** shall have two questions in each section, and the student needs to attempt only one question from each section. (Section II to V shall reflect Unit I to IV of the syllabus respectively).

#### **Course Objective:**

1. The course aims at developing entrepreneur attitude in the student by helping them to understand the steps involved in becoming entrepreneur and developing a mindset of entrepreneurship.

#### **Unit-I**

##### **Introduction to entrepreneurship:**

Who is an Entrepreneur? Advantage of becoming entrepreneur, Characteristics of entrepreneur, Competencies and skills possessed by entrepreneur, Myths about entrepreneur etc. Difference between entrepreneur and manager, between entrepreneur and entrepreneurship. Case studies on Indian entrepreneur.

#### **Unit-II**

##### **Steps involving in starting enterprise:**

Deciding the type of organization to start business, deciding the name of the enterprise, registration formalities, identification of opportunities, sources of finance, arranging finance and managing the enterprise.

#### **Unit-III**

##### **Definition of MSME & Institutional support:**

Definition as per MSMED Act 2016, revised guideline 2020, incentives available to MSME by Govt. of India, Institutional setups available at the center and state level supporting MSME. Case study on MSME enterprises in India.

#### **Unit-IV**

##### **Developing entrepreneurship attitude:**

Practical training on developing creativity and Innovation in the students, entrepreneur attitude using behavioral scales, entrepreneurship scorecard for the students. Improving public speaking and negotiation skills, doing a live project.

#### **Suggested Reading:**

1. NathSuryakant, *Entrepreneurship Development and Small Scale Industries*, Neha Publishers & Distributors, Delhi(2012).
2. Holt D.H., *Entrepreneurship New Venture Creation*, Pearson Education (2016).

Deepa Arun

Parul

3. Charantimath, *Entrepreneurship Development and Small Business Enterprise* Pearson Education (2013).
4. Scarborough N.M. and Cornwall H.R., *Essentials of Entrepreneurship and small Business Management*, 8/e, Pearson Education (2016).
5. TaingKalpana, *Entrepreneurship Theory and Practice*, Anmol Publication Pvt. Ltd., Delhi (2014).

\*NUES: Non University Examination System

Deepa Sural

Shruti

Pavul

Keerthi

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### COMPUTATIONAL DRUG DESIGN PRACTICAL

Course Code:  
PC-751 (0 0 4)

Computational Drug Design Practical  
Core Course

Maximum Marks: 60 + 40 (CE)

Credit: 2

#### Course Objective:

1. This practical introduces modern protein engineering techniques available to researchers to understand protein structure and function.
2. This is field that lies on the interface of chemistry, biology and engineering and involve use of computational, biochemical and self-based screening technologies to identify natural and synthetic compounds with pharmacological activity.
3. Study of structural activity relationship to understand mechanism of drug action.

#### Course/Learning Outcomes:

Upon successful completion of the course, the student would know:

- Computational molecular modeling tools which are used to aid in drug discovery and design and to incorporate these tools into drug discovery.
- To apply Molecular Modeling to Drug Discovery
- To Create Computational Molecules
- To View Protein-Ligand Interactions
- Ligand-Based Virtual Screening in Preparation for SAR
- Combining Modeling and Experimental Data for SAR Development and would carry Drug Discovery Case Study

#### Topics

1. Visualization of small / Macro-molecule structure, drawing of small molecules and optimization of small molecule (ligand Preparation).
2. Sequence Database: Swiss-Prot/Uniprot; Protein Database (PDB); Selection and optimization of the protein structure (Protein Preparation).
3. Docking: Protein grid generation, small molecule docking and analysis of docking results.
4. Flexible protein docking: Induced fit docking.
5. Covalent docking.
6. Homology modeling generation; Model refinement and validation of generated model.
7. De-novo structure based drug design: Combinatorial library design and identification of potential molecule by virtual screening workflow.
8. Pharmacophore generation and virtual screening of database.
9. 2D-QSAR, 3D-QSAR development for series of molecules by atom based QSAR and Field based QSAR techniques and ADME Toxicity predictions.
10. Energy based Pharmacophore (E-Pharmacophore) generation and Shape based virtual screening.
11. Antibody modeling, model validation, Antigen-Antibody docking or Protein-Protein Docking.
12. Residue-scanning and associated property predictions, Cysteine scanning, Reactive hot spots prediction and Affinity Maturation.
13. QM: Small molecule Geometry optimization, Single point energy calculation, spectral (UV/Visible, VCD, IR, NMR, Raman) and molecular property calculation (HOMO and LUMO, molecular orbitals, density, potential).
14. Molecular Dynamics Simulations and trajectory analysis.
15. Chemo informatics analysis of chemical database (Binary finger print analysis, Similarity search, Clustering, Scaffold decomposition)

Dr. S. S. Desai

Dr. S. S. Desai

Note: Any experiment may be introduced/deleted in the practical class based on the availability/non-availability of the instruments/chemicals.

Experiment  
Lab record & Viva-voce

Marks: 30

Marks: 5+15

References:

1. Internet, Documentation of Software.

Deepa Desmal

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### MICROBIOLOGY PRACTICAL

Course Code:  
PC-753 (0 0 4)

Microbiology Practical  
Skill Enhancement Course

Maximum Marks: 60 + 40 (CE)  
Credit: 2

#### Course Objective:

1. The major objective of the course is to impart hands-on training in basic microbiological, biochemical and immunological techniques.
2. Students will be trained in basic bacterial culturing and identification methods, as well as working in biosafety cabinet.
3. Student will become familiar in basic enzyme and immunological assays and be taught to present the results both, qualitatively and quantitatively.

#### Course /Learning Outcomes:

Upon successful completion of the course, the student:

- Is able to use different sterilization procedures and learn handling of micropipette.
- Is able to work in Biosafety Cabinet for culturing cells,
- Can use Fluorescence Microscopy for live cell imaging
- Is versed with identification and classification of given bacterial isolate by performing variety of cultural, biochemical and molecular tests.
- Can determine pI of amino acids by titration method
- Is able to determine concentration of sugar and protein in a given sample after drawing a standard curve. Is able to study glucose uptake by E.coli.
- Is able to perform TLC for separating a mixture of amino acids, lipids, and sugars.
- Is able to study ammonium uptake by E.coli.
- Is able to determine specific growth rate of E.coli in different media.
- Understands the techniques of enzyme assay to determine its specific activity, pH optima, pH stability, temperature optima and temperature stability and calculate inactivation constant ( $K_d$ ) and  $t_{1/2}$  of the enzyme reaction based on the temperature stability curve.
- Can determine  $K_m$ ,  $V_{max}$  and  $K_{cat}$  of a purified enzyme and determine its activation energy by plotting Arrhenius curve.

#### **Microbial Techniques**

1. Permanent Slides (Bacteria, Fungi)
2. Media preparation, pour plate and streak plate techniques.
3. Microscopic examination (motility, monochrome staining and gram staining).
4. **Sterilization:** Steam, Dry heat and filter.
5. Detection of amylase, caseinase, catalase activity.
6. Preservations of bacterial cultures.
7. Growth curve of *E. coli*.
8. Total viable count determination (pour plate and spread plate).
9. Ultraviolet irradiation and survival curve.
10. Isolation of auxotrophic mutants.
11. Plaque assay for phage.
12. Immobilization of yeast cells.
13. Microbial assay of vitamin and antibiotic.
14. Transformation
15. Lac operon by studying  $\beta$ -galactosidase.

**Note:** Any experiment may be introduced/deleted in the practical class based on the availability/non-availability of the instruments/chemicals.

*David*

**Experiment**  
**Lab record & Viva-voce**

**Marks: 30**  
**Marks: 5+15**

**Suggested Reading:**

1. Collins J., *Microbial Methods*.
2. Cruickshank, *Medical Microbiology*, Vol-II.

**References:**

1. Singer, *Laboratory Auditing for Quality and Regulatory Compliance*.

Deepa Siswal

Dr. P. S. Parul  
Dr. P. S. Parul  
Dr. P. S. Parul



## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### PROJECT/DISSERTATION

Course Code:  
PC-799 (0 0 8)

Project/Dissertation

Maximum Marks: -----  
Credit: 4

Dissertation work would comprise of research work carried out by each student during semester IV under the supervision of a particular faculty member. The student would carry out the review of literature on the topic of research and formulate the plan of work in consultation and in the supervision of the mentor. The student would then conduct the research experiments for the proposed work. Towards the end of semester IV, the student will compile the research work including review of literature, aims and objectives, methodology and results and discussion in the form of a dissertation in the supervision of the mentor. At the end of semester 4, students would make presentations in the presence of all faculty members and would be collectively judged by the faculty members. Marks will be assigned to each student collectively by the faculty based on his/her performance, work and continuous assessment throughout the year by the mentor.

# To be evaluated after IV semester

Deepa Deswal

Dr. Anurag K. Singh

Dr. Anurag K. Singh

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### DRUG SYNTHESIS AND MECHANISM OF ACTION

Course Code:  
(CE)PC-702 (4 0 0)

Maximum Marks: 60 + 40  
Drug Synthesis and Mechanism of Action  
Core Course

Credit: 4

**Instruction to Paper Setters:**  
**Attempt five questions**

**Time: 3 hours**  
**Maximum Marks: 60**

Question Paper shall contain **Five Sections**

- The student has to attempt **five questions** from five sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** to **V** shall have two questions in each section, and the student needs to attempt only one question from each section. (Section **II** to **V** shall reflect Unit **I** to **IV** of the syllabus respectively).

#### Course Objective:

1. The course aims to provide an advanced understanding of the core principles and topics of biochemistry and their experimental basis, to enable acquire a specialized knowledge on mode of action of drugs and their chemical synthesis.

#### Course / Learning Outcomes:

Upon successful completion of the course, the student would know:

- The principles governing drug actions in humans and acquire the specific knowledge related to the different classes of drugs, and important distinctions among members of each class, in relation to the organ systems they affect, and the diseases for which they are used therapeutically.
- The basis for continued development in drug discovery
- How to build a rational approach to the use of drugs in practice.
- To develop a foundation to effectively use the medical literature to evaluate new drugs in the context of evidence-based drug discovery

#### **Unit-I**

##### **Drug Acting on Metabolic Process, Cell Wall and Specific Enzymes**

Basic concepts of mechanism of drug action: Introduction to macromolecular targets, carbohydrates, proteins, lipids and nucleic acids as possible drug targets. Classification of drugs. Enzyme inhibition and its types.

- a) **Drug acting on metabolic process:** Antifolates – Discovery and mechanism of action of sulphonamides, Synthesis of sulfamethoxazole, sulfadoxine, sulfaguanidine and dapsone. Diaminopyrimidines – trimethoprim, bacterial resistance of sulfonamides and drug synergism.
- b) **Drugs acting on cell wall:** Structure of bacterial cell wall,  $\beta$ -Lactam antibiotics – mechanism of action of penicillins and cephalosporins. Synthesis of penicillin-G and cephalosporin-C, cephalexin and cycloserine. Resistance to penicillins, broad spectrum penicillins – cloxacillin, methicillin, ampicillin, amoxicillin and carbenicillin. B-Lactamase inhibitors – Structural formulae and mode of action of clavulanic acid and sulbactam.
- c) **Drugs acting on specific enzymes:**  $H^+/K^+$ -ATPase inhibitors – synthesis of Omeprazole and Carbonic anhydrase inhibitors – synthesis of Acetazolamide.

#### **Unit-II**

##### **Drugs Acting on Genetic Material and Immune System**

Drugs acting on genetic material: Introduction, classification and mechanism of action.

- a) DNA-intercalating agents – Anticancer and antimalarial agents. Structural formulae of Daunomycin, Adriamycin and Amsacrine. Synthesis of Amsacrine, Nitracrine, Quinacrine and Chloroquine.
- b) DNA – Binding and nicking agents: Antiprotozoal drugs. Synthesis of Metronidazole, Dimetridazole and Tinidazole.
- c) DNA – Alkylators: Synthesis of Cyclophosphamide and Bisulphan.

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### DRUG SYNTHESIS AND MECHANISM OF ACTION

Course Code:  
(CE)PC-702 (4 0 0)

Maximum Marks: 60 + 40

Drug Synthesis and Mechanism of Action  
Core Course

Credit: 4

**Instruction to Paper Setters:**  
**Attempt five questions**

**Time: 3 hours**  
**Maximum Marks: 60**

Question Paper shall contain **Five Sections**

- The student has to attempt **five questions** from five sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** to **V** shall have two questions in each section, and the student needs to attempt only one question from each section. (Section II to V shall reflect Unit I to IV of the syllabus respectively).

#### Course Objective:

1. The course aims to provide an advanced understanding of the core principles and topics of biochemistry and their experimental basis, to enable acquire a specialized knowledge on mode of action of drugs and their chemical synthesis.

#### Course / Learning Outcomes:

Upon successful completion of the course, the student would know:

- The principles governing drug actions in humans and acquire the specific knowledge related to the different classes of drugs, and important distinctions among members of each class, in relation to the organ systems they affect, and the diseases for which they are used therapeutically.
- The basis for continued development in drug discovery
- How to build a rational approach to the use of drugs in practice.
- To develop a foundation to effectively use the medical literature to evaluate new drugs in the context of evidence-based drug discovery

#### **Unit-I**

##### **Drug Acting on Metabolic Process, Cell Wall and Specific Enzymes**

Basic concepts of mechanism of drug action: Introduction to macromolecular targets, carbohydrates, proteins, lipids and nucleic acids as possible drug targets. Classification of drugs. Enzyme inhibition and its types.

- a) **Drug acting on metabolic process:** Antifolates – Discovery and mechanism of action of sulphonamides. Synthesis of sulfamethoxazole, sulfadoxine, sulfaguanidine and dapsone. Diaminopyrimidines – trimethoprim, bacterial resistance of sulfonamides and drug synergism.
- b) **Drugs acting on cell wall:** Structure of bacterial cell wall,  $\beta$ -Lactam antibiotics – mechanism of action of penicillins and cephalosporins. Synthesis of penicillin-G and cephalosporin-C, cephalexin and cycloserine. Resistance to penicillins, broad spectrum penicillins – cloxacillin, methicillin, ampicillin, amoxicillin and carbenicillin. B-Lactamase inhibitors – Structural formulae and mode of action of clavulanic acid and sulbactam.
- c) **Drugs acting on specific enzymes:**  $H^+/K^+$ -ATPase inhibitors – synthesis of Omeprazole and Carbonic anhydrase inhibitors – synthesis of Acetazolamide.

#### **Unit-II**

##### **Drugs Acting on Genetic Material and Immune System**

Drugs acting on genetic material: Introduction, classification and mechanism of action.

- a) DNA-intercalating agents – Anticancer and antimalarial agents. Structural formulae of Daunomycin, Adriamycin and Amsacrine. Synthesis of Amsacrine, Nitracrine, Quinacrine and Chloroquine.
- b) DNA – Binding and nicking agents: Antiprotozoal drugs. Synthesis of Metronidazole, Dimetridazole and Tinidazole.
- c) DNA – Alkylators: Synthesis of Cyclophosphamide and Bisulphan.

*Paul*

- d) DNA – Polymerase inhibitors: Antiviral agents – Synthesis of Acyclovir and AZT.
- e) DNA – Topoisomerase inhibitors: Anti bacterial agents. Synthesis of Ciprofloxacin and Norfloxacin. Structural formulae of Iloxacin and Lomefloxacin.
- f) Inhibitors of transcribing enzymes: Anti-TB and antileprosy agents-structural formulae of Rifamycins and partial synthesis of Rifampicin.
- g) Drugs interfering with translation process: Antibacterial drugs – Structural formulae of Erythromycin, 5-Oxytetracycline and Streptomycin. Synthesis of Chloramphenicol.

**Drugs acting on immune system:** Introduction to immune system. Immunosuppressing agent – structural formula of Cyclosporin. Immunoenhancers – use of vaccines and structural formula of levamisole.

### Unit-III

#### Drugs Acting on Receptors and Ion Channels

Introduction to nervous system: structure of neuron, nerve transmission. Definition and examples of agonist, antagonist, neurotransmitters and receptors.

Drugs acting on receptors:

- a) Adrenergic receptors – Introduction and classification. A-Adrenergic-receptor agonists and antagonists – Synthesis and biological activity of Nor-adrenaline, Methyl L dopa and Tetrahydrozoline.
- B-Adrenergic-receptor – agonists and antagonists – Synthesis and pharmacological activity of Salbutamol, Terbutaline, Propranolol and Atenolol.
- b) Cholinergic-receptors: Introduction and classification. Cholinergic-receptor agonists and antagonists – Structural formulae of Nicotine, Atropine and Tubocurarine. Synthesis of Acetyl choline and Succinyl choline.
- c) Dopamine receptors: Introduction and classification. Dopamine – receptor agonists and antagonists – Biosynthesis of Dopamine. Synthesis of L-Dopa and Chlorpromazine.
- d) Serotonin receptors: Introduction and classification. Serotonin receptor agonists and antagonists – synthesis and pharmacological activity of Serotonin and Metoclopramide.
- e) Histamine receptors: Introduction and classification. Histamine receptor agonists and antagonists- synthesis and biological action of Histamine, Chlorpheniramine and Ranitidine.

Hormones and their receptors: Introduction to estrogen receptors, Structural formulae of Tamoxifen.

Drugs acting on ion channels: Introduction to ion channels, drugs acting on  $Ca^{2+}$ ,  $Na^+$  and  $Cl^-$  channels and their mode of action. Structural formulae of Tetracaine and synthesis and of Nifedipine, Diltiazem, Tetracaine and 4-aminopyridine.

### Unit-IV

#### Chiral Drugs

Introduction to chiral drugs. Three point contact model, Eutomer, Distomer and eudesmic ratio. Pfeiffer's rule. Role of chirality on biological activity: Distomers

- a) with no side effects
- b) with undesirable side effects
- c) both isomers having independent therapeutic value
- d) combination products having therapeutic advantages
- e) metabolic chirality inversion

**Pharmacological activity of some important drugs (e.g. S-Ibuprofen, Levocetazine).**

#### Suggested Reading:

1. Patrick Graham, *Introduction to Medicinal Chemistry*, 5<sup>th</sup> Ed., Oxford (1995).
2. Silverman R.B., *The Organic Chemistry of Drug Design and Drug Action*, 3<sup>rd</sup> Ed., Academic Press, (2011).
3. Foye Hollday, Thomas L. Lemke, William D.A., Vitoria F. Roche, Zito S. William, *Principles of Medicinal Chemistry*, 7<sup>th</sup> Ed., WolterKluwerLippment, (2013).
4. Nogrady T., Weaver D.F., *Medicinal Chemistry: A Molecular and Bio-Chemical Approach*, 3<sup>rd</sup> Ed., Oxford, (2005).
5. Roth Herman J., Keleman Axel, Wenger T. Beiss, Horwood Ellis, *Pharmaceutical Chemistry and Drug Synthesis*, (1988), Digitized (2008).
6. Thomas Gareth, *Medicinal Chemistry An Introduction*, 2<sup>nd</sup> Ed., Wiley (2007).
7. Ashutoshkar, *Medicinal Chemistry*, New Age International, Revised (2005).
8. Sheldon Roger A., *Chirality Technology Industrial Synthesis of Optically Active Compound*, Marcel Decker (1993).

#### Reference:

1. Wolf Manfred B., *Burger's Medicinal Chemistry and Drug Discovery*, Wiley, (2014) Digitized.
2. Hantzsch, *Comprehensive Medicinal Chemistry*, Vol. 1-5.

*Paul*



## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### MOLECULAR PHARMACOLOGY

Course Code:  
PC-704 (3 0 0)

Maximum Marks: 60 + 40 (CE)

Molecular Pharmacology  
Ability Enhancement Compulsory Course

Credit: 3

**Instruction to Paper Setters:**  
Attempt five questions

**Time: 3 hours**

**Maximum Marks: 60**

Question Paper shall contain **Five Sections**

- The student has to attempt **five questions** from five sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** to **V** shall have two questions in each section, and the student needs to attempt only one question from each section. (Section II to V shall reflect Unit I to IV of the syllabus respectively).

#### Course Objective:

1. The course intends to provide basic knowledge of the modes of action of drugs at the molecular level and pharmacological methodology.
2. It aims at detailed analysis of the mechanisms of drug action at the molecular level through the application of biochemical and molecular biological techniques.
3. Receptor binding, is studied.
4. To define the basic pharmacokinetic parameters of a drug including volume of distribution, clearance terms, extraction ratio, elimination half-life, unbound fraction and to understand how these parameters are related.

#### Course /Learning Outcomes:

Upon successful completion of the course, the student would:

- Define pharmacological terms and concepts - explain the modes of action of drug at the cellular level by describing their interactions with target proteins.
- Describe and explain the principles of absorption, distribution, metabolism and elimination of drugs.
- Describe the properties of different classes of neurotransmitter transport proteins.
- Students will be able to select the correct pharmacokinetic model based on plasma level or urinary excretion data that best describes the process of drug absorption, distribution, metabolism and elimination (ADME).

#### **Unit-I**

##### **General**

Introduction to Pharmaceutical sciences, history and development of chemotherapeutic agents, its branches, standards for drugs, naming of drugs, therapeutic index, LD50 and ED50, Pharmaceutical literature, official books, routes of drugs administration.

##### **Cell Structure & Cellular Physiology**

Sub Cellular organization, membrane processes, cell metabolism, cell division, structure and function of epithelial connective, muscular and nervous tissues, muscle contraction and properties, nerve impulse generation and transmission. Skull & skeleton.

##### **Respiratory System**

Deepa Dermal

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Structure respiratory volumes and capacities, ventilation, compliance and resistance, gaseous exchange and transport in blood, nervous and chemical regulations of respiration. Acid-base balance.

## **Unit-II**

### **Renal System**

Structure of kidney and urinary tract; nephron transport processes concentration and dilution of urine, renal control of body fluids, plasma clearances, maturation.

### **Endocrinology**

Functions of hormones and their regulation. Chemical signaling – endocrine, paracrine, autocrine, intracrine and neuroendocrine mechanisms. Chemical classification of hormones, transport of hormones in the circulation and their half-lives. Hormone therapy. General introduction to Endocrine methodology.

**Major categories of formulations, physical properties and chemical characteristics of drugs influencing their formulations.**

## **Unit-III**

### **Pharmacokinetics**

ADME (Absorption, Distribution, Metabolism-Phase I and Phase II Reactions, Excretion) of drugs, important pharmacokinetic parameters-apparent volume of distribution, bioavailability, clearance.

### **Pharmacodynamics**

Elementary idea about drug action, drug targets, neurotransmitters, the receptor role, drug receptor interactions, types of receptors-ion channel receptors, G-protein coupled receptors, kinase-linked receptors, ion channels and their control, membrane bound enzymes-activation/deactivation, design of agonists and antagonists.

## **Unit-IV**

### **Metrology:**

Introduction, units of weight and volume in both imperial and metric system, simple calculations involved in preparing solutions of solids in liquids and liquids based on imperial and metric systems, method of allegation.

**Pre Formulation Considerations:** Analytical methods for characterization of drugs, determination of  $pK_a$  value,  $pH$ , solubility profile and effect of temperature, solution and solid state stability.

### **Emulsions**

Types, identification and selection of emulgents, preparation and stability. Emphasis may be given on official products.

### **Suspensions and Mixtures**

Practical considerations, preparation of products of different categories evaluation, stability and official suspensions.

### **Semi-Solid Dosage Forms**

A brief description, preparation of ointments, creams jellies and suppositories.

### **Aerosol Dosage Forms**

Advantages, formulation and standardization.

### **Principle of Toxicology and Treatment of Poisoning**

Introduction, Toxic agents, Toxicity-acute, subacute and chronic, descriptive toxicity tests in animals, general principles of management of poisoning, antidotes, treatment of heavy metal poisoning and drugs (barbiturates, benzodiazepines, salicylates, morphine & morphine derivatives, alcohol).

### **Suggested Reading:**

1. Goodman and Gilman's *Pharmacological Basis of Therapeutics*, 12<sup>th</sup> Ed., McGraw-Hill.
2. Dandya P.C. and Kulkarni S.K., *Introduction to Pharmacology*, Vallabh Publication.

### **References:**

1. B.G. Katzung, Trevor A.J., *Basic and Clinical Pharmacology*, 3<sup>rd</sup> Ed., McGraw Hill Large Medical Publication, (2015).

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### MEDICINAL CHEMISTRY

Course Code:  
PC-706 (4 0 0)

Medicinal Chemistry  
Core Course

Maximum Marks: 60 + 40 (CE)  
Credit: 4

**Instruction to Paper Setters:**  
**Attempt five questions**

**Time: 3 hours**  
**Maximum Marks: 60**

Question Paper shall contain **Five Sections**

- The student has to attempt **five questions** from five sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II to V** shall have two questions in each section, and the student needs to attempt only one question from each section. (Section **II to V** shall reflect Unit **I to IV** of the syllabus respectively).

#### Course Objective:

1. Medicinal Chemistry course aims to gain a comprehensive understanding of the fundamental concepts related use of major classes of drugs from their chemical structures
2. It aims to interpret relationships between molecule concentration and enzyme or receptor activity.
3. Compute a molecule's pharmacokinetic parameters from  $C_p$ -time data points correlate a molecule's structure to its metabolic signalin. Prioritize the viability of weakly active molecules for potential drug development

#### Course /Learning Outcomes:

Upon successful completion of the course, the student would:

- Understand and apply the principle involved in drug action
- Correlate the pK/PD aspects of biologically active molecules
- Gain theoretical expertise in various tools employed in drug discovery
- Be able to relate the signal-chemical properties, pharmacological activities, mechanisms of action, ADME (adsorption, distribution, metabolism, and excretion), and pharmacokinetic properties of drugs to their chemical structures.
- Integrate knowledge from foundational sciences to explain how specific drugs or drug classes work and evaluate their potential value.

#### **Unit-I**

##### **Principles of Medicinal Chemistry**

Drug development, how to plan a drug, amino acids what affects bind of drug to its target. Gibbs free energy, the molecular forces: strong, weak, electrostatics, hydrogen bridges, the forces of Vander Waals. Water, entropy, degrees of freedom. Aqueous solubility; Flick's Law of diffusion; The cell membrane and lipophilicity; Partition and distribution coefficients. Isosterism and bioisosterism. Functional group modifications. Quantitative relation between structure and activity: Hammett equation and SAR. Hansch equation, log p Lipinski rule of five. Hits, leads and validated leads; specific and non-specific drug action. Lead optimization. Pharmacophores and auxophores; Minimalisation; Homologation; Branching; Ring-chain transformations.

##### **Protease Inhibitors**

Proteases – serine, wiring (cysteine), aspartic metalloproteinase (Zinc): proposed mechanisms of action, specificity and selectivity, contact various diseases. Inhibitors of proteases – a situation beyond imitation, imitation intermediate product. Examples of inhibitors of zinc proteases and development antihypertensive medications – blood (ACE inhibitors). Metalloenzymes proteases as flame retardants cancer.

##### **Cholinergic System Drugs**

Introduction, acetylcholine, conformation and the relationship between them and the activity. Agonists and antagonists of the Nicotinic and Muscarinic systems. Acetylcholine esterase: Structure and mechanism of operation, and other relevant enzymes.

Activation of the cholinergic system. Esterase blockers: Carbamates: structure, mechanism of action. Inhibitors structure. Aging process. Activation by Oximes: SAR, mechanism of action.

##### **Antibiotic**

*Handwritten signatures:* Tushar, Seera Deshpande, Javed

Beta lactams and penicillins, bond angles, structure and mechanism of action, the relationship between the structure, stability and activity. Sulfonamides, structure and activity.

#### **Peptide Drugs**

Structure of proteins, protein-drug limitations of therapeutic proteins and protein modifications, synthesize peptides and prodrugs.

#### **Inhibitors of HIV**

Viruses, HIV and drug development: Reverse transcriptase inhibitors, non-nucleosides inhibitors, and nucleosides-like inhibitors, HIV protease inhibitors and drug development based on crystallography.

### **Unit-II**

#### **Oncology**

Overview and introduction of cancer, tumorigenesis, molecular basis of cancer phenotypes, cancer-related genes, interventions in reference of targets and prevention strategies.

Antimetabolites and hormones inhibitors with chemistry and pharmacology; estrogen, progesterone and androgen receptors. DNA targeted anti-cancer drugs: DNA alkylating agents, alkylating and non-alkylating compounds interacting with the DNA minor groove, drugs targeting DNA and DNA-associated enzymes.

Anticancer drugs targeting tubulin and microtubules, signaling pathways inhibitors: kinase inhibitors, natural products in cancer prevention and therapy.

Biological and non-biological therapies of cancer; drug resistance in cancer chemotherapy, cancer chemoprevention, and anticancer drugs acting via radical species: radiotherapy and photodynamic therapy of cancer.

### **Unit-III**

#### **Tuberculosis**

Signs and symptoms; Pulmonary, Extrapulmonary. Mycobacterium tuberculosis, cell structure, Transmission and Pathogenesis. A Global Epidemic, The Medical History of Current TB Chemotherapy, The Emergence of Drug-Resistant TB, Special Challenges in TB Drug Development.

The Development of Commonly Used First-Line and Second-Line Agents for TB Therapy, Rifamycins, Isoniazid, Thioisonicotinamides and Thiosemicarbazones, Pyrazinamide, Para-Aminosalicylic Acid, Capreomycin, Aminoglycosides. Classes of Compounds in Clinical Development, Nitroimidazoles, Diarylquinolines, Oxazolidinones, Fluoroquinolones, Ethylenediamines.

Series in Preclinical Development, Benzothiazinones, Nucleosides, Macrolides, b-Lactams, Rhimino phenazines, Pyrroles, Deazapteridines. Targets based: TP Synthase Inhibitor, Translocase I Inhibitor, InhA Inhibitors, Isocitrate Lyase Inhibitors. Drug Resistance in TB and its diagnosis.

Critical Issues in TB Drug Development e.g. Cell Penetration, Animal Models for Evaluation, Pharmacological Models for Antitubercular Drugs. Clinical Development Methodologies.

### **Unit-IV**

#### **Malaria**

The Malaria Parasite and its Life-cycle; Clinical Features of Malaria, The Sporozoite, the Merozoite, and the Infected Red Cell; Parasite Ligands and Host Receptors. Antimalarial Medicines; Amino-alcohols, 4-aminoquinolines, Endoperoxides of the artemisinin family, Aniline-sulphonamides/sulphones, Diaminopyrimidines/diaminodihydrotriazines, Hydroxynaphthoquinones, Lincosamides, Tetracyclines.

Novel and Advanced Chemotypes; Spiroindolone, Aminoindole, Oxaborole, Liver Stage Acting Antimalarials; Primaquine, Tafenoquine, Bulaquine. Target-Based Optimisation; Pyrimidine Biosynthesis, Folate Biosynthesis, Deoxyuridine 50-Triphosphate Nucleotidohydrolase, Purine Biosynthesis, Degradation/Catabolic Pathways; Haemoglobin Processing, Heat Shock Proteins 70/90. Anabolism/Synthesis Pathways; Non-Mevalonate Pathway, Choline Pathway, Fatty Acids. Signalling/Proliferation Pathways; Kinases, Histone Deacetylase, DNA-Binding Bisamidines. Protein Synthesis Pathways.

#### **Drug Resistance in Malaria**

#### **Clinical Development Methodologies.**

#### **Suggested Reading:**

1. Rosenthal Philip J., *Antimalarial Chemotherapy: Mechanisms of Action, Resistance, and New Directions in Drug Discovery*, Humana Press, New Jersey, (2001).
2. Elliott Richard L., *Third World Diseases*, Springer-Verlag Berlin Heidelberg Series Volume-7, (2011).
3. Mats Wahlgren, and Peter Perlmann, *Malaria: molecular and clinical aspects*, CRC Press, (2003).
4. Elliott Richard L., *Third World Diseases*, 1<sup>st</sup> Ed., Springer-Verlag Berlin Heidelberg (2011).
5. Donald Peter R., Paul D. Van Helden, *Antituberculosis Chemotherapy*, Karger Medical and Scientific Publishers (2011).
6. Yew W. W., *Development of New Antituberculosis Drugs*, 1<sup>st</sup> Ed., Nova Science Publisher, New York, (2006).
7. Carmen Avendaño and Menéndez J. Carlos, *Medicinal Chemistry of Anticancer Drugs*, 2<sup>nd</sup> Edition, Elsevier, (2008).
8. Chemotherapeutic Agents, *Burger's Medicinal Chemistry and Drug Discovery*, 6<sup>th</sup> Edition, Volume 5, John Wiley and Sons, (2003).

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9. Bradbury Robert H. *Cancer-Topics in Medicinal Chemistry*, 1<sup>st</sup> Ed., Springer-Verlag Berlin, (2007).
10. Michelle Prudhomme. *Advances in Anticancer Agents in Medicinal Chemistry*, Vol. I & II, Bentham Science Publishers, (2013).
11. Patrick. *Introduction to Medicinal Chemistry*, 5<sup>th</sup> Ed., Oxford (2013).
12. Hantzsch. *Comprehensive Medicinal Chemistry*, Elsevier, (1995).
13. Foye William. *Principle of Medicinal Chemistry*, 7<sup>th</sup> Ed., (2012).
14. Thomas Garith. *Medicinal Chemistry: An Introduction*, 2<sup>nd</sup> Ed., Wiley (2008).
15. Thomas Nogrady. *Biochemical Approach to Medicinal Chemistry*, Oxford (2005).

**References:**

1. *Harrison's Principles of Internal Medicine*, 19<sup>th</sup> Ed., New York McGraw Hill, (2014).
2. Chan E.A. and Isman M.D., *Current Medical Treatment for Tuberculosis*, BMJ 325:1282
3. Wolf Manfred E., *Burger's Medicinal Chemistry and Drug Discovery*, 5<sup>th</sup> Ed.

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### FORMULATION CHEMISTRY

Course Code:

PC-708(A1) (2 0 0) \*\*

Formulation Chemistry

Discipline Centric Elective

Maximum Marks: 60 + 40(CE)

Credit: 2

**Instruction to Paper Setters:**

**Attempt five questions**

**Time: 3 hours**

**Maximum Marks: 60**

Question Paper shall contain **Three Sections**

- The student has to attempt **five questions** from three sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** and **III** shall have three questions in each section, and the student needs to attempt two questions from each section. (Section II and III shall reflect Unit I and II of the syllabus respectively).

#### Course Objective:

1. The course aims to identify the effective functioning of drug regulations for the new products.
2. The pharma regulatory affairs are important for knowledge of law and to equip with the educational foundation of regulatory affairs and quality education.

#### Course/Learning Outcomes:

On completion of the course the students should:

- Be able to describe basic Physico-chemical properties for solid phases, liquids and solutions.
- Be able to account for the preformulation and including characterization methods.
- Be able to account for the different dosage forms, included excipients and their function.
- Be able to account for manufacturing processes for the most common dosage forms.
- Be able to account for quality assurance and Good Manufacturing Practice (GMP) in connection with drug production.
- Having received skills in production and quality control of drug compoundings.

#### **Unit-I**

##### **Quality Control and Quality Assurance**

Definition and classification of impurities in pharmaceutical products, origin of impurities, types of impurities: process impurities, degradation impurities, and contamination impurities. Nature of impurities: organic, inorganic, and residual solvent impurities. Differences between impurities and degradation products. Impurity-drug interaction. Toxicological perspectives of impurities in pharmaceutical products: Classes of genotoxic impurity, analytical challenge of genetic toxins, determination of genotoxic impurities.

Introduction, regulatory standards for drug stability, drug decomposition mechanisms: (i) Hydrolysis and acyltransfers (ii) Oxidation (iii) Photolysis, solid state chemical decomposition: Pure drugs, drug excipient and drug-drug interaction in solid state, factors affecting drug degradation and methods of stabilization.

#### **Unit-II**

##### **Formulation Process**

Introduction to preformulation studies, Essential information helpful in designing the preformulation evaluation of new drug; Pre-formulation studies of solids, liquid, semisolid, sterile dosage forms, controlled release formulation and ocular preparations.

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Types of tables, granulation – manufacture of granules, their basic characteristic and properties, Various additives included in formulation of tablets, standardization and evaluation of tablets as per official standards. Coating of Tablets: Principles and equipment; Taste masking sugar coating; tensile strength of films, evaluation of coated tablets, defects of films.

### Processing of Capsules

Hare gelatin capsules, materials and production, Introduction of filling equipment, Soft gelatin capsules, manufacturing process, nature of capsule shell and contents, physical stability, packing and evaluation. Microencapsulation: Its importance and applications in pharmaceutical formulations, techniques and equipment for microencapsulation.

### Suggested Reading:

1. Cooper and Gunn's, *Dispensing for Pharmaceutical Students*, 12<sup>th</sup> Ed., S.J. Carter, CBS Publishers & Distributors, (2008).
2. Cooper J.W. and Gunn's, *Tutorial Pharmacy*, Carter, CBS Publishers, (2005).
3. Lachman L., Lieberman Herbert A., Kaing Joseph L., *Theory and Practice of Industrial Pharmacy*, Lea & Fabiger, 3<sup>rd</sup> Ed., (1986) Digitized (2008).
4. Bentley and Drivers, *A Textbook of Pharmaceutical Chemistry*, Oxford Press, (1969).
5. *Indian Pharmacopoeia*, Govt. of India, Ministry of Health and Family Welfare
6. *British Pharmacopoeia*
7. *Indian Patent Act*, PDF (1970).

### References:

1. ISO Annual Reports.
2. A. Osol, Remington, *The Science and Practice of Pharmacy*, 22<sup>nd</sup> Ed., Lippincultz, William and William, (2006).

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- One course to be selected among 708A1/708A2.
- The course would be offered with a minimum of 7 students.

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### HEAT AND MASS TRANSFER

Course Code:  
PC-708(A2) (2 0 0)\*\*

Heat and Mass Transfer Credit: 2  
Discipline Centric Elective

Maximum Marks: 60 + 40 (CE)

**Instruction to Paper Setters:**  
Attempt five questions

**Time: 3 hours**

**Maximum Marks: 60**

Question Paper shall contain **Three Sections**

- The student has to attempt **five questions** from three sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** and **III** shall have three questions in each section, and the student needs to attempt two questions from each section. (Section II and III shall reflect Unit I and II of the syllabus respectively).

#### Course Objective:

1. The course aims to understand the basic principles of phenomena of heat and mass transfer to develop methodologies for solving a wide variety of practical engineering problems in drug industry.

#### Course/Learning Outcomes:

- Upon successful completion of this course, the student will be able to:
- Understand the basic laws of heat transfer.
- Understand the mechanisms of heat transfer under steady and transient conditions.
- Learn and explain various modes of heat and mass transfer operations

#### **Unit-I**

##### **Heat Transfer**

Introduction, modes of heat transfer, Fourier's law of heat flow, thermal conductivity, steady state conduction. Equipment: Finned tube (extended surface) heat exchanger, plate heat exchanger, spiral heat exchanger, scraped heat exchanger and air cooled heat exchanger.

##### **Distillation**

Introduction, vapour – liquid equilibrium, partial vaporization, partial condensation, volatility, relative volatility, methods of distillation for two component systems-fractional distillation, azeotropic distillation, steam distillation, extractive distillation.

##### **Filtration**

Introduction, classification of filters, plate & frame filter presses, candle filter, filter media, filter aids, washing of filter cakes, filtration theory – constant pressure filtration, constant rate filtration, filtration cycle, centrifuges, batch top driven centrifuge, batch under driven centrifuge, disk type centrifuge.

##### **Drying**

Introduction, rate of drying, constant rate period, critical moisture content, falling rate period, equilibrium moisture, free moisture, bound and unbound moisture, drying equipment – tray dryers, drum dryers, rotary dryers, spray dryers, flash dryers.

##### **Crystallization:**

Introduction, supersaturation, modes of generation of supersaturation, nucleation, primary nucleation, secondary nucleation, crystal growth, law of crystal growth, growth rate and growth coefficients, crystallization equipment – Tank crystallizers, circulating magma – vacuum crystallizers, circulating liquid evaporator crystallizers.

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## Unit-II

### Fluid Flow:

Introduction, Newtonian and non-Newtonian fluids, viscosity, effect of temperature on viscosity, kinematic viscosity, laminar and turbulent flows, Reynolds number, Bernoulli's equation without friction, orificemeter, venturimeter, pumps, types of pumps.

### Reactors

Introduction to reactor design, ideal batch reactor, space time, space velocity, steady state mixed flow reactor, steady state plug flow reactor.

### Chemical Process Development:

Process design development, types of design process development, plant location, plant layout, plant operation and control, material handling.

### Safety and Loss Prevention:

Health and safety hazards, source of exposure, exposure evaluation, exposure hazard control, fire and explosion hazard, safety regulation, loss prevention.

### Suggested Reading:

1. Warren L. McCabe, Smith Julian C., Harriott P., *Unit Operations of Chemical Engineering*, 7<sup>th</sup> Ed. McGraw Hill, (2004).
2. Norman E. Bruce, *Chemical Reaction De Optimization and Scale Up*, 1<sup>st</sup> Ed., McGraw Hill, (2002).
3. Westreter K.R., Van Swaaij W.P.M., Beenackers AACM, *Chemical Reactor Design and Operation*, Wiley (1987).
4. Peters Max Store, *Elementary Chemical Engineering*, 2<sup>nd</sup> Ed., McGraw Hill, (1984).

### References:

1. Coulson J.M., Harker J.H. & Richardson, *Chemical Engineering: Chemical Engineering Series*, 5<sup>th</sup> Ed., Butter Worth, (2002)

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\*\*One course to be selected among 708A1/708A2

The course would be offered with a minimum of 7 students

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**CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES  
GURU GOBIND SINGH INDRAPRASTHA UNIVERSITY  
SECTOR-16C, DWARKA, NEW DELHI-110078**

**BIO-STATISTICS**

**Course Code:**  
**PC-710(A1) (2 0 0)\*\*\***

**Bio-Statistics  
Generic Elective Course**

**Maximum Marks: 60 + 40 (CE)  
Credit: 2**

**Instruction to Paper Setters:**

**Attempt five questions**

**Time: 3 hours**

**Maximum Marks: 60**

Question Paper shall contain **Three Sections**

- The student has to attempt **five questions** from three sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** and **III** shall have three questions in each section, and the student needs to attempt two questions from each section. (Section II and III shall reflect Unit I and II of the syllabus respectively).

**Course Objective:**

1. This course represents an introduction to the field and provides a survey of data and data types.
2. There are some formulae and computational elements to the course, the emphasis is on interpretation and concepts.

**Course/Learning Outcomes:**

On completion of the course the students are able to:

- Recognize and give examples of different types of data arising in public health and clinical studies
- Interpret differences in data distributions via visual displays
- Calculate standard normal scores and resulting probabilities
- Calculate and interpret confidence intervals for population means and proportions
- Interpret and explain a p-value
- Perform a two-sample t-test and interpret the results; calculate a 95% confidence interval for the difference in population means
- Select an appropriate test for comparing two populations on a continuous measure, when the two sample t-test is not appropriate
- Understand and interpret results from Analysis of Variance (ANOVA), a technique used to compare means amongst more than two independent populations
- Choose an appropriate method for comparing proportions between two groups; construct a 95% confidence interval for the difference in population proportions
- Understand and interpret relative risks and odds ratios when comparing two populations
- Understand why survival (timed to event) data requires its own type of analysis techniques

**Unit-I**

**Introduction and Scope of Biostatistics**

Use of statistics in Pharmacy. Population and sample collection. Stages of research, types of data and methods of data collections. Data arrangement and presentation, formation of table and charts.

**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.

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## Unit-II

### Measured Correlation and Regression

Experimental designing, planning of an experiment, replication and randomization. Probit analysis.

### Probability Rules:

Binomial, poison and normal distribution.

### Hypothesis Testing:

Student's 't' test, Chi square test, analysis of variance (ANOVA): 1-way, 2-way, 3-ways.

### Suggested Reading:

1. Sokal, R.R. and Rohlf, F.J. *An Introduction to Biostatistics*, W.H. Freeman and Company, (1987).
2. Bailey, N.T.J. *Statistical Methods in Biology*, 3<sup>rd</sup> Ed., English University Press, (1995).
3. Gupta S.P., *Statistical Methods*, Sultan Chand & Sons.

### References:

1. Indrayan A., *Medical Biostatistics*, 3<sup>rd</sup> Ed., Star Publisher (2012).

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- One course to be selected among 710A1/710A2/710A3.
- The course would be offered with a minimum of 7 students.



## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### BIO-ETHICS

Course Code:  
PC-710(A2) (200)\*\*\*

Maximum Marks: 60 + 40(CE)

Credit: 2

Bio-Ethics  
Generic Elective Course

#### Instruction to Paper Setters:

Attempt five questions

Time: 3 hours

Maximum Marks: 60

Question Paper shall contain **Three Sections**

- The student has to attempt **five questions** from three sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** and **III** shall have three questions in each section, and the student needs to attempt two questions from each section. (Section II and III shall reflect Unit I and II of the syllabus respectively).

#### Course Objective:

The field of bioethics will be dealt with the following five themes:

1. **Respecting Autonomy:** This deals with the importance of respecting the autonomy, or self determination, of patients and research subjects. Why is it so important? What are its limits? And what about the autonomy of doctors and nurses?
2. **Bioethics and the Human Body:** These explore issues around the human body like disability, normal and enhancing the body.
3. **Bioethics at the Beginning of Life:** This topic includes collaborative reproduction-new ways creating babies and ways building families. And some of the ethical issues they raise.
4. **Bioethics at the End of Life:** This topic deals with the other bookend of life including the persistent vegetative state, for instance and parameters to guide decision making.
5. **Global Bioethics:** It explores the bioethical issues in an increasingly globalized world including climate change, environmental justice, medical tourism and outsourcing medical research to develop countries and food securities in 21<sup>st</sup> century.

#### Course/Learning Outcomes:

On completion of the course the students are able to:

- Differentiate between ethical questions and non-moral questions. Summarize and analyze arguments for a particular ethical conclusion.
- Identify ethical issues when they arise in the context of healthcare, biotechnology, and the role of a physician.
- Form and defend a well-supported position on issues in bioethics.
- See the relevance of philosophy to the life sciences and social policy.
- Identify how very general concepts such as "person", "woman", "death" and so on work in arguments in bioethics.
- Overcome the ungrounded assumption that "anything goes" in philosophical or ethical discussion

#### Unit-I

##### Patient Autonomy

A brief historical overview of the concept, autonomy and medical paternalism, informed consent, physician truth telling, rights to refuse life-saving care, and parental rights regarding medical decisions about the children.

##### Provider Autonomy

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"Medical conscientious refusal", Autonomy Rights, Negative and Positive Rights, Obligation and Autonomy Providers, Conscientious Objection, Complicity, Institution and Complicity.

### **Disability**

Introduction, Models of Disability, Genetic Testing and Paradox of Harm, Critics of Routine Prenatal Testing, Creating a Deaf Child.

**Enhancement:** Concept of Biomedical Enhancement, Enhancement and the Ends of Medicine, Performance Enhancing Drugs, Radical Enhancement and the Human Good, Altering the Human Genome.

## **Unit II**

### **Collaborative Reproduction**

Parent, Right to be a Parent, Gamete Donation, Reproduction, Markets and Commodification, Surrogacy and Exploitation.

**Abortion:** Concept of Moral Status, Restrictive Views of Abortion, Human Dignity, Permissive Views of Abortion.

### **Death and Surrogacy Decision Making**

Ending Life Support for Other, A Definition of Death, Ending Life-Support, Surrogacy Decision Making, Futility.

**Voluntary Euthanasia:** Concept of Euthanasia, Three Approaches to the Value of Human Life, Argument from Autonomy and Beneficence, Hypocrisy.

### **Climate Change**

Cost and Options, Models of Moral Responsibility, Climate Change and Human Rights, Individual Responsibilities.

**Global Issues in Bioethics:** Medical Tourism, Bioethics Crossing Borders, Exploitation, Autonomy and Benefit, Feeding the World in 2050, Fairness and Concentration of Market Values-Horizontally concentrated and Vertically Integrated.

### **Suggested Reading:**

- 1 Moskop J.C., *Informed Consent in the Emergency Department*, Emerg Med. Clin North Am. (1999).
- 2 Derse A.R., *What part of 'No' don't you understand? Patient refusal of recommended treatment in the emergency department*, Mt. Sinai J. Med. (2005).
- 3 Thewes J. Fitz Gerald D., Sulmasy D.P., *Informed consent in emergency medicine: ethics under fire*, Emerg Med Clin North Am. (1996).
- 4 Keyes L.E., English D.K., *Cultivating conscience: learning to make end of life decisions in the emergency department*, Ann Emerg Med., (1999).
- 5 Withers E. Sklar D.P., Crandall C.S., *Impairment and Severity: how ED physicians decide to override an impaired patient's refusal*, Am J. Emerg Med. (2008)
- 6 Magauran B.G., Jr. *Risk Management for the emergency physician: competency and decision making capacity, informed consent, and refusal of care against medical advice*, Emerg Med Clin North Am. (2009).
- 7 Moskop J.C., *Informed consent and refusal of treatment: challenges for emergency physicians*, Emerg Med Clin North Am. (2006).
- 8 Arun Bhatt, *Clinical Trials and Good Clinical Practice in India*, 1<sup>st</sup> edition, D.K. Publications, Mumbai (2006).

### **References:**

1. Appelbaum P.S., *Assessment of patients, Competence to consent to treatment*, N. Engl. J. Med. (2007).
2. Derse A.R., *Ethics and the law in emergency medicine*, Emerg Med Clin N Am., (2006).
3. Lippincott Williams & Wilkins, *The Science and Practice of Pharmacy*, vol. I & II, 21<sup>st</sup> edition, Remington, Wolters Kluwer Health (India) Pvt. Ltd., New Delhi (2005).

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- One course to be selected among 710A1/710A2/710A3.
  - The course would be offered with a minimum of 7 students



## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### INTELLECTUAL PROPERTY RIGHTS

Course Code:  
PC-710(A3) (2 0 0) \*\*\*

Intellectual Property Rights  
Generic Elective Course

Maximum Marks: 60 + 40(CE)  
Credit: 2

**Instruction to Paper Setters:**  
**Attempt five questions**

**Time: 3 hours**

**Maximum Marks: 60**

Question Paper shall contain **Three Sections**

- The student has to attempt **five questions** from three sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** and **III** shall have three questions in each section, and the student needs to attempt two questions from each section. (Section II and III shall reflect Unit I and II of the syllabus respectively).

#### Course Objective

*To give an idea about IPR, registration and its enforcement.*

#### Course/Learning Outcomes:

On completion of the course the students are would have adequate knowledge of:

- The fundamental aspects of Intellectual property Rights
- Patents, patent regime in India and abroad and registration aspects
- The copyrights and its related rights and registration aspects
- The trademarks and registration aspects
- Geographical Indication (GI), Plant Variety and Layout Design Protection and their registration aspects
- Current trends in IPR and Govt. steps in fostering IPR.

#### **Unit I**

##### **Overview of Intellectual Property**

Introduction and the need for intellectual property right (IPR) - Kinds of Intellectual Property Rights: Patent, Copyright, Trade Mark, Design, Geographical Indication, Plant Varieties and Layout Design - Genetic Resources and Traditional Knowledge - Trade Secret - IPR in India : Genesis and development - IPR in abroad - Major International Instruments concerning Intellectual Property Rights: Paris Convention, 1883, the Berne Convention, 1886, the Universal Copyright Convention, 1952, the WIPO Convention, 1967, the Patent Co-operation Treaty, 1970, the TRIPS Agreement, 1994

##### **Nature of Copyright**

Subject matter of copyright: original literary, dramatic, musical, artistic works; cinematograph films and sound recordings - Registration Procedure, Term of protection, Ownership of copyright, Assignment and licence of copyright - Infringement, Remedies & Penalties - Related Rights - Distinction between related rights and copyrights

##### **Concept of Trademarks**

Different kinds of marks (brand names, logos, signatures, symbols, well known marks, certification marks and service marks) - Non Registrable Trademarks - Registration of Trademarks - Rights of holder and assignment and licensing of marks - Infringement, Remedies & Penalties - Trademarks registry and appellate board

##### **Patents**

Elements of Patentability: Novelty, Non Obviousness (Inventive Steps), Industrial Application - Non - Patentable Subject Matter - Registration Procedure, Rights and Duties of Patentee, Assignment and licence,

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Restoration of lapsed Patents, Surrender and Revocation of Patents, Infringement, Remedies & Penalties - Patent office and Appellate Board.

## Unit II

### Other forms of IP

#### Design

Design: meaning and concept of novel and original - Procedure for registration, effect of registration and term of protection

#### Geographical Indication (GI)

Geographical indication: meaning, and difference between GI and trademarks - Procedure for registration, effect of registration and term of protection

#### Plant Variety Protection

Plant variety protection: meaning and benefit-sharing and farmers' rights - Procedure for registration, effect of registration and term of protection

#### Layout Design Protection

Layout Design protection: meaning - Procedure for registration, effect of registration and term of protection

#### Current Contour

India's New National IP Policy, 2016 - Govt. of India step towards promoting IPR - Govt. Schemes in IPR - Career Opportunities in IP - IPR in current scenario with case studies

### Suggested Reading:

1. Bouchoux Deborah E., *Intellectual Property: The Law of Trademarks, Copyrights, Patents and Trade Secrets*, Cengage Learning, Third Edition, (2012).
2. Edited by Derek Bosworth and Elizabeth Webster, *The Management of Intellectual Property*, Edward Elgar Publishing Ltd., (2013).
3. GangulPrabuddha, *Intellectual Property Rights: Unleashing the Knowledge Economy*, McGraw Hill Education.

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*Tricki* , *Deena*  
*Deepa Deswal*

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- One course to be selected among 710A1/710A2/710A3.
- The course would be offered with a minimum of 7 students

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## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### SYSTEMIC PHARMACOLOGY

Course Code:  
PC-712 (2 0 0)

Systemic Pharmacology  
Skill Enhancement Course

Maximum Marks: 60 +40 (CE)  
Credit: 2

**Instruction to Paper Setters:**  
Attempt five questions

**Time: 3 hours**  
**Maximum Marks: 60**

Question Paper shall contain **Three Sections**

- The student has to attempt **five questions** from three sections.
- All sections are of 12 marks each.
- Section **I** is compulsory, and it should have objective or short answer type questions and cover the entire syllabus.
- Section **II** and **III** shall have three questions in each section, and the student needs to attempt two questions from each section. (Section II and III shall reflect Unit I and II of the syllabus respectively).

#### Course Objective:

1. The course intends to provide basic knowledge of the modes of action of drugs at the molecular level and pharmacological methodology.
2. It aims at detailed analysis of the mechanisms of drug action at the molecular level through the application of biochemical and molecular biological techniques.
3. The course aims at improving the students understanding of how drugs affect the functioning of the various body systems, so as to be able to use drugs to modify those systems and effectively monitor for adverse effects resulting from drug use at system level.

#### Course /Learning Outcomes:

Upon successful completion of the course, the student would:

- Define pharmacological terms and concepts - explain the modes of action of drug at the cellular level by describing their interactions with target proteins.
- Describe and explain the principles of absorption, distribution, metabolism and elimination of drugs.
- Insights into drug discovery will help the student to appreciate and understand how drugs are discovered and the processes that take place during the drug discovery.
- It will help in understanding the clinical utility of drugs.

#### **Unit-I**

##### **Systemic Pharmacology**

A detailed study of the mechanism of action, pharmacology and toxicology of drugs used in:

- a) ANS-Parasympathomimetics and lytics, sympathomimetics and lytics, agents acting at neuromuscular junction and ganglia.
- b) Local and general anesthetics.
- c) CNS-General anesthetics, sedatives, hypnotics. Drugs used to treat anxiety, depression, psychosis, mania, epilepsy, neurodegenerative diseases, drug dependence and addiction.
- d) CVS – Diuretics, anti ischemics, antihypertensives, antiarrhythmics, drugs for heart failure and dyslipidemia.
- e) Effect of drug on blood constituents.

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## UNIT-II

- a) Autocoid Pharmacology – A study of the mechanisms involved in the formation, release, pharmacological actions and possible physiological role of histamine, serotonin, kinins, prostaglandins, opioid autocoids and cyclic 3' – 5' AMP. Systemic pharmacology of drugs acting as agonists and antagonist to the autocoids.
- b) Immunopharmacology – Cell and biochemical mediators involved in allergy, immunomodulation and inflammation. Classification of hypersensitivity reactions and diseases involved. Therapeutic agents for allergy, asthma, COPD and other immunological diseases with emphasis on immunomodulators.
- c) GIT pharmacology – Antiulcer, prokinetics, antiemetics, antidiarrhoeal and drugs for constipation and irritable bowel syndrome.
- d) Analgesics and anti-inflammatory agents.
- e) Hormone and hormone antagonists.
- f) Antibiotics & Chemotherapeutic agents.

### Suggested Reading:

- 3. Goodman and Gilman's *Pharmacological Basis of Therapeutics*, 12<sup>th</sup> Ed., McGraw-Hill.
- 4. Dandya P.C. and Kulkarni S.K., *Introduction to Pharmacology*, Vallabh Publication.

### References:

- 2. B.G. Katzung, Trevor A.J., *Basic and Clinical Pharmacology*, 3<sup>rd</sup> Ed., McGraw Hill Large Medical Publication, (2015).

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*Rang*  
*Deepa Dasmal*  
*Bhargava*  
*A*



## CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

### PROJECT/DISSERTATION

**COURSE CODE:**  
**PC-800**

**Project/Dissertation**

**Maximum Marks: 100**  
**Credit: 8**

Dissertation work would comprise of research work carried out by each student during semester IV under the supervision of a particular faculty member. The student would carry out the review of literature on the topic of research and formulate the plan of work in consultation and in the supervision of the mentor. The student would then conduct the research experiments for the proposed work. Towards the end of semester IV, the student will compile the research work including review of literature, aims and objectives, methodology and results and discussion in the form of a dissertation in the supervision of the mentor. At the end of semester 4, students would make presentations in the presence of all faculty members and would be collectively judged by the faculty members. Marks will be assigned to each student collectively by the faculty based on his/her performance, work and continuous assessment throughout the year by the mentor.

*Paul* *Bechgal*  
*Devi*  
*K*

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#4 Credit of third semester and final to be evaluated after IV semester

*Deepa Dismal*