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

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 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.

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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 I credit, 2 hours practical class per week equals I 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.

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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.

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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.
- **PS10**: Understand structure-activity relationships to understand the mechanisms of drug action.
- **PS11:** Apply green/sustainable chemistry approach in frontier areas of synthetic pathways.
- **PS12**: 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.

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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	Digital Health Innovations and Analytics	NUES*	100			2		2
PC-652	Medicinal Chemistry (Practical)	CC	100	40	60		8	4
PC-654	Enzymology (Practical)	AECC	100	40	60		8	4
			800			18	16	26

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

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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 and Systemic Pharmacology	AECC	100	40	60	4		4
PC-706	Medicinal Chemistry	CC	100	40	60	4		4
PC-708	AI in Chemistry	DCE	100	40	60	2		2
PC-800	Project/Dissertation	CC	100		100		16	8
			500			**14**	**16**	**22**

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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
	Total	**24**	**33**				**700**

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	Digital Health Innovations and Analytics	2	2	15	25	60	100
PC-652	Medicinal Chemistry (Practical)	4	8	40		60	100
PC-654	Enzymology (Practical)	4	8	40		60	100
	Total	**26**	**34**				**800**

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Third Semester

Course Code	Nomenclature of the Paper	Credits	Teaching hours per week	Maximum Marks			Total
				Continuous Evaluation	Mid-Semester Examination	End-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
PC-799#	Project/ Dissertation	4	8				
	Total	**25**	**33**				**800**

#To be evaluated at the end of fourth semester

Fourth Semester

Course Code	Nomenclature of the Paper	Credits	Teaching hours per week	Maximum Marks			Total
				Continuous Evaluation	Mid-Semester Examination	End-Semester Examination	
PC-702	Drug Synthesis and Mechanism of Action	4	4	15	25	60	100
PC-704	Molecular and Systemic Pharmacology	4	4	15	25	60	100
PC-706	Medicinal Chemistry	4	4	15	25	60	100
PC-708	AI in Chemistry	2	2	15	25	60	100
PC-800#	Project/ Dissertation	8	16				100
	Total	**22**	**30**				**500**

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Total Marks of all Four Semesters

SEMESTER	CREDIT	MARKS
I	24	700
II	26	800
III	25	800
IV	22	500
GRAND TOTAL	**97**	**2800**

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 3rd 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 97, leaving behind NUES.

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Annexure-A

Scheme for awarding internal assessment: continuous mode

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

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

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
Less than 50 or absent	F	0

Grade B (grade point 6) 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 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:

$$SGPA = \frac{\sum_i CiGi}{\sum_I Ci}$$

$$CGPA = \frac{\sum_n \sum_i CniGni}{\sum_n \sum_i Cni}$$

Where;
Ci– number of credits for the i^{th} course.

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

Cni – number of credits of the i^{th} course of the nth semester.

Mni – marks of the i^{th} course of the nth semester.

Gni – grade points of the i^{th} course of the nth 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 CGPA x 10 shall be deemed equivalent to percentage of marks obtained by the student for the purpose of equivalence to percentage of marks.

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Semester-I	Semester-II	Semester-III	Semester-IV
PC-601: Foundation Coursein 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 Metabolism④	PC-704: Molecular and systemic Pharmacology④
PC-605: Foundation Course in Physical Chemistry ④	PC-606:Spectroscopic Studies ④	PC-705(A1):Separation Science②	PC-706: Medicinal Chemistry④
		PC-705(A2):Molecular Spectroscopy②	
PC-607: Introduction to Biomolecules③	PC-608: Enzymes ②	PC-707: Introduction to Microbiology③	PC-708: AI in Chemistry ②
	PC-610: Green Chemistry ②		
PC-651: Foundation Course Practical-I(Organic Chemistry) ⑧	PC-612: Digital Health Innovations and Analytics ②	PC-709: Concepts in Drug Design②	PC-800: Project/Dissertation (16)
PC-653: Foundation Course Practical-II (Physico-Inorganic Chemistry) ⑧	PC-652: Medicinal Chemistry Practical ⑧	PC-711: Developing Entrepreneurial Mindset②	
PC-655: Introduction to Computational Chemistry②	PC-654: Enzymology Practical⑧	PC-751: Computational Drug Design Practical④	
		PC-753: Microbiology Practical ④	
		PC-799: Project/Dissertation⑧	

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**

o : Depicts Hours

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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

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

Metal-Ligand Bonding

Crystal field theory and splitting in O*h*, T*d*, D-4*h* and C4*v* systems 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 Π – bonding). Structure and bonding in complexes containing π-acceptor ligands. Crystal field theory and splitting in O*h*, T*d*, D-4*h* and C4*v* systems. Term symbols, Russel-Saunders states, Orgel and Tanabe-Sugano diagrams, determination of D*q* and Racah 1 parameters, oxidation states and electronic absorption spectra of complex ions.

Unit-II

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, Trans effect and its application to synthesis of complexes.

Unit-III

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.

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.

Unit-IV

Introduction of nanomaterials, Preparation of nanomaterials by reduction, Sol- gel, Solvothermal synthesis, Photochemical synthesis, Electrochemical synthesis, Characterization techniques: Zeta potential, Absorption spectroscopy (UV, PL), Electron Microscopy (SEM, TEM), Dynamic Light Scattering (DLS), Atomic Force Microscopy (AFM), X-ray Diffraction (XRD).

Suggested Reading:

1. Shriver D.F., Atkins P.W. & Langford C.H., *Inorganic Chemistry*, 5th Ed., Oxford Univ. Press (2010).
2. Gupta, B.D, Elias, A J; *Basic Organometallic Chemistry, Concepts, syntheses and applications*, 2nd 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. &Wadington 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*, 4th Ed., Pearson Education (2008).
7. Cotton F.A. and Wilkinson G., *Advanced Inorganic Chemistry*, 11th Ed., Wiley & Sons, New York (1998).
8. Gilber Thomas, Kriss R.V. N. Foster& Davies G. Chemistry., 4th Ed., W.W. Norton & Co. Inc(2014).
9. Housecraft C.E. & Sharpe A.G. Inorganic Chemistry, 1st Ed., Pearson Prentice Hall, (2005).

References:

1. Hartwig J.F, Organo-transition metal chemistry: From bonding to catalysis, 1st Ed, University science books (2010).
2. Crabtree R. H., The organometallic chemistry of the transition metals, 6th Ed, Wiley (2014).
3. Eldik Rudi Van(Ed), Advances in Inorganic Chemistry, Volume62-65 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. Mcclevertry J.A.; *Comprehensive Coordination Chemistry*, Pergamon (1987, 2003).

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FOUNDATION COURSE IN ORGANIC CHEMISTRY

Course Code: **Maximum Marks: 60 + 40 (CE)**
PC-603 (4 0 0) **Foundation Course in Organic Chemistry** **Credit: 4**
Compulsory Foundation Course

Course Objective:

1. On successful completion of this module, the learner will be able to identify and explain the reaction mechanisms in organic chemistryAn examination of methods use to probe the mechanism of organic reactions and chemistry of some important reactive intermediates.
2. Topics include Nucleophillic, elecrophillic 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, carbocations 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 closer, 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_N2, S_N1, S_Ni, S_N2', S_N1' and S_Ni' 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 diazonium ions, by addition-elimination and elimination-addition mechanism (involving arynes); S_{RN} 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, Vilsmeir-Haak

reaction , Reimer-Tiemann reaction, BischlerNapieralski reaction, Pechamann reaction, Houben-Hoesch reaction, Fries rearrangement.

Aliphatic Electrophilic Substitution:
The S_E1, S_E2 and S_Ei mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and medium on the reactivity.

Mechanism of Elimination Reactions:
The El, ElcB 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, pincolpinacolone rearrangement, Demjanove rearrangement, Tiffeneau-Demjanove ring expansion, aldehyde-ketonerearrangement,dienone-phenol rearrangement and transannular rearrangements.

Suggested Reading:

1. Carey. F.A. &Sundberg, R.J. *Advanced Organic Chemistry,* 7th Ed., Parts A & B, Plenum: U.S. (2004).
2. March, J. *Advanced Organic Chemistry,* 6th 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,* 6th Ed., Pearson Education(1986).
5. Clayden Jonathan, Greeves Nick and Warren Stuart, *Organic Chemistry,* 2nd Ed., Oxford Press (2012).

References:

1. Volhardt P. and Schora N., *Organic Chemistry Structure and Function,* 5th Ed., (2007).
2. Solomons T.W.G. and Fryhle C.B., *Organic Chemistry,* 10th Ed., (2009).

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FOUNDATION COURSE IN PHYSICAL CHEMISTRY

Course Code: PC-605 (4 0 0)

Maximum Marks: 60 + 40 (CE)

Foundation Course in Physical Chemistry

Credit: 4

Compulsory Foundation Course

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.

Unit-II

Surface Chemistry and Catalysis

Deepa Semwal

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 MichealisMenten 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 Rigidrotator. 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 andvibrational 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,* 10th Ed., Oxford University Press (2013).
3. Nash, L.K. *Elements of Statistical Thermodynamics* 2nd Ed., Addison Wesley (2006) Reprint.
4. Laidler, K.J. *Chemical Kinetics* 3rd Ed., Bengamin 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,* 4th Ed. Narosa (2004).
8. Mortimer R.G., *Physical Chemistry,* 3rd Ed., Elsevier, Noida (2008).
9. Pilar, F.L. *Elementary Quantum Chemistry,* 2nd Ed., Dover Publication Inc.: N.Y. (2001).
10. Chandra A.K. *Introduction to Quantum Chemistry,* 3rd Ed., Tata McGraw Hill, (1989).
11. Glasstone Samuel, *An Introduction to Electrochemistry,* Reprint (2007).

References:

1. Glasstone Samuel S., *Physical Chemistry,* Affiliated East-West.
2. Levine I.N., *Physical Chemistry,* 6th 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).

Deepa Semwal

CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

INTRODUCTION TO BIO-MOLECULES

Course Code: PC-607 (3 0 0)

Introduction to Bio-Molecules
Skill Enhancement Course

Maximum Marks: 60 + 40 (CE)
Credit: 3

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.

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. Lehniger C., David L. Nelson and Michael M. Cox, *Principles of Biochemistry,* 6th Ed., (2013).
2. Stryer L., Freeman W.H., *Biochemistry,* 5th Ed., San Francisco, (2014).
3. Wood W.B. and Wilson J. H., Benbow R.M., and Hood L.E., *Problem Approaches in Biochemistry,* 1st 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).

Deepa Bansal

CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

FOUNDATION COURSE PRACTICAL-I (ORGANIC CHEMISTRY)

Maximum Marks: 60 + 40 (CE)

Course Code:
PC-651 (0 0 8)

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. $NaBH_4$ 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.**

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,* 5th Ed., Addison Wesley Longman (1997).
2. Harwood Laurence M., Moody Christopher J., Percy Jonathan M., *Experimental Organic Chemistry: Standard and Microscale,* 2nd Ed., Wiley-Blackwell Sevenlife, (1998).

Deepa Desai

CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

FOUNDATION COURSE PRACTICAL-II (PHYSICO INORGANIC CHEMISTRY)

Maximum Marks: 60 + 40 (CE)

Course Code:
PC-653 (0 0 8) **Foundation Course Practical-II (Physico-Inorganic Chemistry)** **Credit: 4**
Compulsory Foundation Course

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.

Nanoscience (Any Two)

1. Determine the rate constant of the redox reaction between hexacyano ferrate 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 CdSnanonparticles 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. $Hg[Co(SCN)_4]$
2. Prussian Blue and Turnbull's Blue
3. $Mn(acac)_3$
4. $[Ni(NH_3)_6]Cl_2$
5. Cis and trans $[Co(en)_2Cl_2]$
6. Bromination of Cr (III) acetylacetonato Cr $(acac)_3$. [J. Chem. Edu. 1986, 63].
7. Separation of optical isomers of cis $[Co(en)_2Cl_2]Cl$: J. Chem. Soc. 1960, 4369.
8. Preparation of copper glycine complex-cis and trans bis (glycinato)Cu(II)
9. Tris (acetylacetonato) cobaltate (III)
10. Tris (Thiourea) Copper (I) Sulphate.

Complexometric Titrations (any two)

1. Determine the strength of Zn^{2+} and Mg^{2+} in the given solution mixture by titrating it against EDTA using Erichrome black T as the indicator.

2. Determine the strength if Ca^{2+} & Mg^{2+} (as CO_3^{2-}) in the given solution mixture by titrating it against EDTA using Erichrome black T &Calcol as the indicators.
3. Estimation of Sn^{2+} as (ZnO) by titrating it against EDTA using Xylol-orange as the indicator.
4. Estimation of Zn^{2+} and Ba^{2+} mixture by back titration.
5. Determine the strength of $CuSo_4$, $5H_2O$ solution by titrating it against $Na_2S_2O_3$iodometrically.

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

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,* 8th 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,* 1st 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,* 6th Ed., Third Indian Reprint, Pearson Education Pvt. Ltd., New Delhi (2003).

Deepa Agarwal Bhagat. Parul Tuli.

CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

Course Code:
PC-655 (0 0 2)

INTRODUCTION TO COMPUTATIONAL CHEMISTRY

Maximum Marks: 60 + 40 (CE)

Credit: 1

Introduction to Computational Chemistry
Non University Examination Scheme

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 Biophyton 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, Chemsketch, 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 seuqnce databases; PDB, PIR, UniProt, EMBL, GenBank, Introduction to sequence Analysis: usage of BLAST; FASTA file format, Statastics 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.

Deepa Deswal Ishchgal. Paul Ruchi.

CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

CONFORMATIONAL ANALYSIS AND ASYMMETRIC SYNTHESIS

Maximum Marks: 60 + 40 (CE)

Course Code:
PC-602 (4 0 0) **Conformational Analysis and Asymmetric Synthesis** **Credit: 4**
Core Course

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 andasymmetric synthesis.
- Develop a fundamental understanding of the concepts of stereoisomesim, 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 polysubstitutedcyclohexanes, 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, Prostereoisomersism

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.

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, Curun-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**
   α-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 IPC_2BH and $IPCBH_2$.
4. **Chiral Catalyst Controlled Asymmetric Synthesis**
   Sharpless and Jacobsen asymmetric epoxidations. Sharpless asymmetric dihydroxylation. Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyoricatalys. Enzyme mediated enantioselective synthesis.
5. **Asymmetric Aldol Reaction**
   Diastereoselectivealdol 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 dichroissm, ORD and CD of ORD and CD curves, cotton effect. The axial haloketone rule, octant diagrams, heto structural and stereochemical problems.

Suggested Reading:

1. Lehniger C., David L. Nelson and Michael M. Cox, *Principles of Biochemistry,* 6th Ed., (2013).
2. Stryer L., Freeman W.H., *Biochemistry,* 5th Ed., San Francisco, (2014).
3. Wood W.B. and Wilson J. H., Benbow R.M., and Hood L.E., *Problem Approaches in Biochemistry,* 1st Ed., Wiley, (1974).
4. Nasipuri D., *Stereochemistry of Organic Compounds – Principles & Applications,* 2nd Ed., New Age Publication, (2005).
5. Eliel Ernest L. &Wilen Samuel H., *Stereochemistry of Organic Compounds,* 1st Ed., Wiley, (1994).
6. Kalsi P.S., *Stereochemistry: Conformation & Mechanism,* 6th Ed., New Age Pub., (2009).
7. Bassendale Alan, *The Third Dimension in Organic Chemistry,* 3rd Ed., John Wiley & Sons, (1984).
8. Stephenson G.R., Nogradi, *Asymmetric Synthesis,* 3rd Ed., John Wiley and Sons, (1984).
9. Izumi Y. & Akira Tai, *Stereo Differentiating Reactions,* 3rd Ed., Academic Press, (1977).
10. Smith M. B., *Organic Synthesis,* 3rd 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,* 2nd Ed., Elsevier, (2012).

Deepa Deswal Bhagat. Paul

CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

SYNTHETIC METHODS IN MEDICINAL CHEMISTRY (ORGANIC SYNTHESIS)

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

PC-604 (4 0 0) Synthetic Methods in Medicinal Chemistry (Organic Synthesis) Credit: 4

Core Course

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_2, PCC, PDC, Swern oxidation, Periodic acid.
b) Application of Homogenous (Wilkinsons's catalytic hydrogenation) and heterogeneous catalytic reduction, boron reagents, Birch reduction, $LiA1H_4$, $NaBH_4$ and their modifications, BH_3, DIBAL.

Unit-III

Organometallic Reagents

a) Preparation and application of the following in organic synthesis:
   (i) Grignard
   (ii) Organo lithium
   (iii)Organo copper reagents
b) Organoboranes in C-C bond formation
c) Organo silicon reagents: reactions involving β-carbocations and α-carbanions, utility of trimethylsilyl halides, cyanides and triflates.
d) Organophosphorus: witting reaction, Mitsunobu reaction + Tebbe + Sulphur elites

Carbonyl methylenation

a) Phosphorous ylide mediated olefination:
   (i) Witting 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, Stile, Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions.
2. **C=C formation reactions**
   Shapiro, Bomford-Stevens, McMurrey reactions, Julia-Lythgoeolefination and Peterson's stereoselectiveolefination.
3. **Multicomponent reactions**
   Ugi, Passerini, Biginelli, Hantzsch and Mannich reactions.
4. **Ring formation reactions**
   Pausan-Khand reaction, Bergman cyclisation, Nazerov cyclisation.
5. **Click Chemistry**
   Criteria for Click reaction, Sharplessazidescycloadditions.
6. **Metathesis**
   Grubb's 1st and 2nd 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*, 1st Ed., Reprint, Cambridge University Press, (1986).
2. Smith B. Micheal, *Organic Synthesis*, 3rd Ed., Elsevier, (2011).

References:

1. MeckieR.K., Smith D.M. &Atken R.A., *Guidebook to Organic Synthesis*, 3rd 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*, 4th Ed., Cambridge University Press, (2004).
6. House H.O. & Benjamin W.A., *Modern Synthetic Reactions*2nd Ed., (1965).

Deepa Bansal Sehgal Parul

CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

SPECTROSCOPIC STUDIES

Course Code:
PC-606 (4 0 0)

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

Spectroscopic Studies
Skill Enhancement Course

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}HNMR, ^{13}CNMR 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

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, conjugatedpolyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls.

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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, Hetro nuclei NMR-F, P.

Carbon-13 NMR Spectroscopy

Resolution and multiplicity of ^{13}C NMR, ^{1}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; α-, β-, 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*3rdEd., W.H. Freeman & Co. (1991).
2. Silverstein, R.M., Webster Francis X., Kiennle David J., Bryce David L., *Spectroscopic Identification of Organic Compounds*, 8th Ed., John Wiley & Sons (2014).
3. Pavia Donald L., Lampman Gary M. and Kriz George S., *Introduction to Spectroscopy*, 5thEd., 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*, 6th 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*, Macmillon, (1988).

8. Atta-ur-Rahman, *Nuclear Magnetic Resonance Basic Principles*, 1st 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*, 2nd Ed., Plenum Press.
3. Bovey F. and Jelinski L., *Nuclear Magnetic Resonance Spectroscopy*, Academic Press.
4. Gross, *Mass Spectrometry: A Textbook*.

Deepa Sewal Aschgal. Parul Kuchar.

CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

ENZYMES

Course Code:
PC-608 (2 0 0)

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

Enzymes
Ability Enhancement Compulsory Course

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, EadieHofstee 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 transcarbomoylase), reversible covalent modification phosphorylation (glycogen phosphorylase). Protcolytoc cleavage –zymogen. Multienzymes complex as regulatory enzymes. Occurremce 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. Balasubramananian D., *Concepts in Biotechnology,* University Press, (1996).
2. Moran Laurence A., Horton Robert A. Gray Strimgeom and Marc Perry, *Principals of Biochemistry,* Prentice Hall, (2011).
3. Dugas Herman and Penney Christopher, *Bioorganic Chemistry – A Chemical Approach to Enzyme Action,* 3rd 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,* 1st Ed., Springer (1999).

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CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

Course Code: PC-610 (2 0 0)	**GREEN CHEMISTRY** Green Chemistry **Skill Enhancement Course**	**Maximum Marks: 60 + 40 (CE)** **Credit: 2**

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

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 FinarVol II
3. Mann, J, Secondary Metabolism, 2nd Ed. Oxford Science Publication
4. Biosynthesis of Heterocycles: From Isolation to Gene Cluster, Ch:1 & Ch:2, 2015, John Wiley & Sons
5. Organic Synthesi by Michael B Smith, 4th Ed, Elsevier
6. Terahedron, 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,* 1st Ed., Springer (1999).

Deepa Semwal

CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

DIGITAL HEALTH INNOVATIONS AND ANALYTICS

Course Code: PC-612 (1 0 0)

Maximum Marks: 60 +40 (CE)

Credit: 2

Digital Health Innovations and Analytics

Non University Examination Scheme

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:

Introduction to Digital Health: Definition and scope of digital health, Historical evolution of digital health technologies, Key technologies driving digital health (e.g., IoT, AI, ML).

Digital Health Technologies: Overview of AI and ML in healthcare, Applications of IoT in health monitoring, Role of cloud computing and big data in digital health.

Data Analytics in Healthcare: Introduction to healthcare data analytics, using analytics for disease prediction and management, Practical workshop on analytics tools and software.

AI and Machine Learning Applications: Deep learning for diagnostics and patient care, Case studies on AI in genomics and proteomics, Practical sessions on building ML models for health data.

Telehealth and Mobile Health Applications: Overview of telehealth services, Technologies and platforms for mobile health, Regulatory and ethical considerations in telehealth.

Unit-II:

Augmented Reality (AR) and Virtual Reality (VR) in Healthcare: Applications of AR and VR in training and treatment, Developing AR/VR solutions for healthcare scenarios, Ethical implications of immersive technologies in health.

Digital Health Case Studies: Review of successful digital health implementations, Discussion on failures and lessons learned in digital health, Group project presentations on proposed digital health solutions.

Emerging Trends and Future of Digital Health: Discussion on future technologies in digital health, Guest lecture on innovation and entrepreneurship in digital health, Final exam.

Ethical and Social Considerations: Ethical principles in digital health, Social impacts of digital health technologies, including access and equity, Case studies on the ethical dilemmas in digital health (e.g., AI decision-making, genetic data usage).

Legal Aspects of Digital Health: Overview of regulatory frameworks governing digital health globally, Data privacy laws and compliance (e.g., GDPR, HIPAA), Intellectual property issues in digital health innovations, Discussions on recent legal cases in digital health.

Suggested Reading:-

1. Primary Textbook: "Digital Health: A Primer" by Nilmini Wickramasinghe
2. Stein, D.J., Fineberg, N.A., Chamberlain, S.R. *Mental Health in a Digital World.*
3. Marques, A., Queiros, R. (Eds.). *Digital Therapies in Psychosocial Rehabilitation and Mental Health.*
3. Additional readings and case studies will be provided throughout the course.

Deepa Dewan

CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

MEDICINAL CHEMISTRY PRACTICAL

Course Code:
PC-652 (0 0 8)

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

Medicinal Chemistry Practical
Core Course

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 β-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 euginol 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 alphà amino nitrogen of amino acid.
14. Estimation of inorganic phosphorus by Fiske-Subbarow method.

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

Experiment **Marks: 30**
Lab record & Viva-voce **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. Plummr David T., *An Introduction to Practical Biochemistry,* Tata McGraw Hill Publishing Company Ltd., New Delhi.
2. Raphel I., *Natural Products: A Laboratory Guide,* 2nd Ed. New Delhi, Elsevier.

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CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

ENZYMOLOGY

Course Code:
PC-654 (0 0 8)

Enzymology
Ability Enhancement Compulsory Course

Maximum Marks: 60 + 40 (CE)
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 Asses effect of substrate conc. (V_{max} and K_m) on enzyme activity.
5. To Asses effect of pH on enzyme activity.
6. To Asses effect of enzyme conc.
7. To Asses temperature stability of the enzyme.
8. To Asses effect of activator on enzyme activity.
9. To Asses 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	**Marks: 30**
Lab record & Viva-voce	**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)

Maximum Marks: 60 + 40 (CE)

Credit: 4

Advanced Organic Chemistry
Compulsory Foundation Course

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 compoundsand 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.

UnimolecularPyrolytic Elimination Reactions:

Cheletropic elimination, Decomposition of cyclic azo compounds, β-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-Loffler-Freytag). Photosynthesis, Phototherapy.

Unit-III

Heterocyclic Chemistry

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

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

Unit-IV

Chemistry of Fused Heterocyclic Compounds

Benzofused five membered heterocylcles with one heteroatom, e.g. indolesbenzofuran, benzothiophenes.

Chemistry of bicyclic compounds containing one or more heteroatoms.

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

Seven and large membered heterocylces: azepines, oxepines, thiepinesChemistry 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,* 1st Ed., John Wiley & Sons (1977).
4. Mukherjee S.M., *Pericyclic Reactions,* 1st Ed., Macmillon, (1980).
5. HarspoolW.M., *Aspects of Organic Photochemistry,* 1st Ed., Academic Press (1976)
6. Marchand A.P., & Lehr R.E., *Pericyclic Reactions,* 1st Ed., Academic Press (1977)
7. Turro N.J., Ramamurthy V., Scanian J.C., *Modern MolecularPhotochemistry of OrganicMolecules,* Angew Chemistry, Int. Ed., (2010).
8. Coyle D., *Introduction of Organic Photochemistry,* Wiley (1986).
9. Joule J.A. & Mills K., *Heterocyclic Chemistry,* 5th Ed., Wiley, (2010).
10. Paquett A., *Principles of Modern Heterocyclic Chemistry,* 1st Ed., Wiley, (1976), Digitized (2010).

Reference:

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

Deepa Sasmal

CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

BIOENERGETICS AND METABOLISM

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

PC-703 (4 0 0) **Bioenergetics and Metabolism** **Credit: 4**

Skill Enhancement Course

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, catabolism, anabolism

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.

Glycogen Metabolism

Glycongenesis 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.

Unit-II
Fatty Acid Oxidation
Digestion, mobilization and transport of cholesterol and triacylglycerols, fatty acid transport to mitochondira, β oxidation of saturated, unsaturated, odd and even numbered and branched chain fatty acid, regulation of fatty acid oxidation, peroxisomal oxidation, ω 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.

Unit-III
Proteins and Nucleic Acids
1. **Oxidative Degradation of Amino Acids:** Proteolysis, transamination, oxidative deamination, acetyle CoA, alpha ketoglutarate, acetoacetyle CoA, succinate, fumarate and oxaloacetate pathway. Decarbodylation, 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. 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 Synthesiss of Nucleotide Triphosphate
Biosynthesis of deoxyribonucleotides and its regulation, conversion to triphosphates,

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 StryerLubo, *Biochemistry,* 7th 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. I Longman (1998).
5. Sinden, R.P. *DNA Structure and Function,* 1st Ed., Academic Press (1994).
6. Zubay G., *Biochemistry,*4th Ed., Addison Wesley Publ. (1999).
7. Horton & others, *Principals of Biochemistry,* 5th Ed., Prentice Hall, (2011).

References:

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

Separation Science
Discipline Centric Elective

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

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:

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,* 3rd Ed., R.E. Krieger Pub., (1978).
3. Willard H.H., Merritt L.L., Dean J.A., *Instrumental Methods of Analysis,* 7th Ed., Van Nostrand, (2004).
4. Christian G.D., O'Reilly J.E., *Instrumental Analysis,* 2nd Ed., Allyn & Bacon, (1986).
5. Wendlandt W.W., *Thermal Methods of Analysis,* 2nd 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,* 2nd Ed., Sounders College Publishing, California (1990).
2. Harvey, *Modern Analytical Chemistry,* McGraw Hill. (2000).
3. Skoog, *Principles of Instrumental Analysis,* 6th 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

CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

MOLECULAR SPECTROSCOPY

Course Code: PC-705(A2) (2 0 0)*

Molecular Spectroscopy
Discipline Centric Elective

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

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.

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. BanwellC.N. *Fundamentals of Molecular Spectroscopy,* 4th Ed., Tata McGraw Hill. (2008).
2. Barrow, G.M. *Introduction to Molecular Spectroscopy* McGraw-Hill (1962).
3. Chang, R. *Basic Principles of Spectroscopy,* 2nd 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,* 1st Ed., Allyl and Bacon (1977).

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

Deepa Desmal Paul

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

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 physiologyand 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 Loch, 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.

Deepa Bansal

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, Archaebacterial cell wall, Gram and acid fast staining mechanisms, lipopolyssaccharide (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 catergories, Culture media: components of media, natural and sunthetic 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 phages (lambda phage).

Fungi

Fungi General characteristics of fungi including habitat, distribution, nutritional requirements, fungal cell ultra-structure, thallusorganization 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.

Deepa Dewal Bengal. Paul Tucu.

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

References:

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

Deepa Deswal

CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

CONCEPTS IN DRUG DESIGN*

Course Code:
PC-709 (2 0 0)

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

Concepts in Drug Design*
Core Course

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

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; Discriptors 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,* 3rd Edition, Academic Press, (2014).
3. Charifson P.S., *Practical Applications of Computer Aided Drug Design,* Marcel Deckker, (1997).
4. Cohen N.C., *Molecular Modeling in Drug Design,* Online.
5. Goodman J., *Chemical Applications of Molecular Modeling,* RSC, (2004).
6. GunerO.F.,*PharmacophorePerceptio, Development and use in Drug Design,* International University, (2000).
7. Lemke Thomas L. and William David A., *Berger'sMedicinal Chemistry and Drug Design,* 6th 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, 7th Edition, Wiley, (2010).
10. Korolkovas A. and Burckhalter J.H., *Essentials of Medicinal Chemistry,* John Wiley, (1976).
11. VeerapandionPandi, *Structure Based Drug Design,* Monograph, Vol. II and III, Academic Press.

References:

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

Deepa Deswal

CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

Course Code: PC-711 (2 0 0)	**Developing Entrepreneurial Mindset** **Developing Entrepreneurial Mindset** **Non-University Examinational Subject**	**NUES*** **Credit: 2**

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).
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

CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

COMPUTATIONAL DRUG DESIGN PRACTICAL

Maximum Marks: 60 + 40 (CE)

Course Code:
PC-751 (0 0 4)

Computational Drug Design Practical **Credit: 2**
Core Course

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)

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

Experiment **Marks: 30**
Lab record & Viva-voce **Marks: 5+15**

References:

1. Internet, Documentation of Software.

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 β-galactosidase.

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

Experiment **Marks: 30**
Lab record & Viva-voce **Marks: 5+15**

Suggested Reading:

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

References:

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

Deepa Dewan Paul Sehgal

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

CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

DRUG SYNTHESIS AND MECHANISM OF ACTION

Course Code: **Maximum Marks: 60 + 40**

(CE)PC-702 (4 0 0) **Drug Synthesis and Mechanism of Action** **Credit: 4**

Core Course

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, Syntheis of sulfomethoxazole, sulfodoxine, sulfaguanidine and dapsone. Diaminopyrimidines – trimethoprim, bacterial resistance of sulfonamides and drug synergism.

b) **Drugs acting on cell wall:** Structure of bacterial cell wall, β-Lactam antibiotics – mechanism of action of penicillins and cephalosporins. Synthesis of pencillin-G and cephalosporin-C, cephalexin and cycloserine. Resistance to pencillins, broad spectrum penicillins – cloxacillin, methicillin, ampicillin, amoxicillin and carbenicillin. B-Lactamase inhibitors –Structural formulae and mode of action of clavulanic acid and sulbactum.

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 Amscarine, 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.

d) DNA – Polymerase inhibitors: Antiviral agents – Synthesis of Acyclovier and AZT.

e) DNA – Topoisomerase 60nhibitors: Anti bacterial agents. Synthesis of Ciprofloxacin and Norfloxacin. Structural formulae of loxacin and Lomefloxacin.
f) Inhibitors of transcribing enzymes: Anti-TB and antileprosy agents-strcutural 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 Chloromycetin.

Drugs acting on immune system: Introduction to immune system. Immunosupressing agent – structural formula of Cyclosporin. Immunoenhancers – use of vaccines and structural formula of levamisol.

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 Tetrazosin.
   B-Adrenergic-receptor – agonists and antagonists – Synthesis and pharmacological activity of Salbutamol, Tetrabutalin, 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, Chloropheneramine 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, Diltiazen, Tetracine 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, Levocetrazine).

Suggested Reading:

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

Deepa Sewal

CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

MOLECULAR AND SYNTHETIC PHARMACOLOGY

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

Course Code:
PC-704 (3 0 0)

Molecular Pharmacology
Ability Enhancement Compulsory Course

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 Pharmacology and Toxicology

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, routs of drugs administration.

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

Principle of Toxicology and Treatment of Poisoning

Introduction, Toxic agents, Toxicity-acute, subacture and chronic, descriptive toxicity tests in animals, general principles of management of poisoning, treatment of heavy metal , antidotes

Unit-II

Systemic Pharmacology I

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

a) **ANS**-Parasympathomimetics and lytics, sympathomimetics and lytics, agents

b) **CNS**-General anesthetics, sedatives, hypnotics. Drugs used to treat anxiety, depression, psychosis, mania, epilepsy, neurodegenerative diseases, drug dependence and addiction Local and general anesthetics.

c) **CVS** – Diuretics, anti ischemic, antihypertensive, antiarrythmics, drugs for heart failure and dyslipidiemia. Effect of drug on blood constituents.

Unit-III

Systemic Pharmacology II

a) **Autocoid and anti inflammatory drugs** – A study of the mechanisms involved in the formation,release, pharmacological actions and possible physiological role of histamine, serotonin, kinins, prostaglandins, opioidautocoids and cyclic 3' – 5' AMP. Systemic pharmacology of drugs acting as agonists and antagonist to the autocoids. Analgesics and anti-inflammatory agents.

b) **Respiratory and Immuno pharmacology** –General considerations of immune system Immunomodulators (Biological Response modifiers). Classification of hypersentitivity 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) Harmone and Chemotherapeutic agents

Unit-IV

Molecular Pharmacology

Drug receptors. Classification and properties of receptors. Receptors for physiological regulatory molecules. Regulation of receptors. Quantization of drug-receptors interactions. Molecular biology of different types of drug-receptors. Structures, types and functions of membrane ion channels. Cellular mechanism of signal transduction and second messenger systems.

Suggested Reading:

1. Goodman and Gilman's *Pharmacological Basis of Therapeutics*, 12th Ed., McGraw-Hill.
2. Dandya P.C. and Kulkarni S.K., *Introduction to Pharmacology,* Vallabh Publication.
3. Srivastava AK, Verma PK and Dumka VK (Eds). 2013. Veterinary Toxicology. Satish Serial Publishing House, New Delhi
4. Essentials of veterinary pharmacology and therapeutics- Sandhu H.S
5. Rang & Dale's pharmacology

References:

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

Deepa Deswal

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

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

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; Fick's Law of diffusion; Lipinski rule of five. Hits and leads, specific and non-specific drug action. Lead optimization. Pharmacophores and auxophores; Homologation; Branching; Ring-chain transformations. Protease Inhibitors: Proteases- serine, wiring (cysteine), aspartic metalloproteinase (Zinc): proposed mechanisms of action, Inhibitors of HIV Viruses, Reverse transcriptase inhibitors, non-nucleosides inhibitors, and nucleosides-like inhibitors

Unit-II

Oncology

Overview and introduction of cancer, tumorigenesis, molecular basis of cancer phenotypes, cancer-related genes, 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 DNAminor groove, drugs targeting DNA and DNA-associated enzymes.

Anticancer drugs targeting tubulin and microtubules, 64ignaling 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.

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, Rhiminophenazines, Pyrroles, Deazapteridines. Targets based; TP Synthase Inhibitor, Translocase I Inhibitor, InhA Inhibitors, IsocitrateLyase Inhibitors. Drug Resistance and specialal challenges in TB and is diagnosis.

Unit-IV

Malaria

The Malaria Parasite and its Life-cycle; Clinical Features of Malaria, The Sporozoite, the Merozoite. Antimalarial Medicines; Amino-alcohols, 4-aminoquinolines, Endoperoxides of the artemisinin family, Aniline-sulphonamides/sulphones,Diaminopyrimidines/diamino-dihydrotriazines,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, Purine Biosynthesis. Drug Resistance and Clinical development methodologies in Malaria

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*, 1st 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*; 1st Ed., Nova Science Publisher, New York, (2006).
7. CarmenAvendaño and Menéndez J. Carlos, *Medicinal Chemistry of Anticancer Drugs*, 2nd Edition, Elsevier, (2008).
8. Chemotherapeutic Agents, *Burger's Medicinal Chemistry and Drug Discovery*, 6th Edition, Volume 5, John Wiley and Sons, (2003).

Deepa Semwal Rajesh. Paul Tiwari

CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

AI IN CHEMISTRY

Maximum Marks: 60 + 40(CE)

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

AI in Chemistry

Discipline Centric Elective

Credit: 2

Course Objective:

1. Introduce the basic concepts of using chemical structure databases.
2. To provide students with skills and knowledge to apply computational techniques to analyse and model chemical data for drug design and discovery.

Course/Learning Outcomes:

On completion of the course the students should be able to:

1. Apply the application of Python and machine learning tools within a chemistry context, to enable you to tackle a broad range of data-intensive chemistry problems and research challenges.
2. Gain skills to analyse the properties of small molecules.
3. Design the biological targets and properties of the small molecule under investigation.
4. Better understanding of the drug discovery and development process.
5. Apply the concepts to create novel leads.

Unit-I

An Introduction to Python Programming: Working with Python, An interpreter for python, Relational operators, Logical operators, Bitwise operators, Variables and assignment Statements, Keywords, Script mode. Control structures, Debugging, Strings, String manipulations, Regular Expressions, Built-in Functions, I/O Functions, Importing user defined modules, Command-line arguments, Mutable and Immutable objects, Recursion.

Basic concepts of Cheminformatics: Application of and modern prospective of Cheminformatics. Representation and manipulations of 2D and 3D structures of chemical compounds, molecular descriptors, and calculations of physical and chemical data, calculation of structural deciphers, In silico representation of chemical information (SMILES, IchI, SDF, MOL, PDB, PDBQT, etc). Molecular drawing of chemical structures and reactions, interactive visualization.

Unit-II

Combinatorial Chemistry: Combinatorial chemistry technologies & libraries, Solution phase synthesis, High-Throughput Synthesis and Screening, Target-oriented synthesis: Designing organic synthesis, Retrosynthetic analysis, disconnection approach, linear and convergent synthesis. Diversity-oriented synthesis: concept of forward-synthetic analysis, appendage diversity, skeletal diversity, stereo-chemical diversity, complexity and diversity.

Suggested Reading:

1. Cooper and Gunn's, *Dispensing for Pharmaceutical Students,* 12th 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, 3rd 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,* 22nd 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.

CENTRE OF EXCELLENCE IN PHARMACEUTICAL SCIENCES

PROJECT/DISSERTATION

COURSE CODE:
PC-800

Project/Dissertation

MaximumMarks: 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.

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