

**CENTRAL UNIVERSITY OF PUNJAB**



**M.Sc. in Chemical Sciences  
(Medicinal Chemistry)**

**Session- 2021-2023**

# **Department of Pharmaceutical Sciences and Natural Products**

## **Graduate attributes for M. Sc. Chemical Sciences (Medicinal Chemistry)**

Graduate attributes are statements that describe what students are expected to know and do by the time of graduation. After completing M.Sc. in Medicinal Chemistry, the graduates will have quality-conscious service providing attribute by adopting the knowledge of spectral analysis and chromatographic techniques in manufacturing and R & D of drugs. They will be able to implement the role of Computer-Aided Drug Design (CADD) in the modern drug discovery & development process and its applicability in higher studies and at the industrial level. They will be able to apply the knowledge in process chemistry for the development of synthetic methodologies, including green chemistry, peptide chemistry, retro-synthesis for making the drugs affordable to the public. They will have the ability to create, select and apply appropriate techniques, resources and modern analytical tools to identify, formulate, and solve problems of medicinal chemistry and will develop attribute to become self-reliant in Active Pharmaceutical Ingredients (APIs) by the development of scale-up of APIs and intermediates, unit operations and industrial safety guidelines. Moreover, the program will help them make their career in academic, research, and industry.

# Course Structure

## SEMESTER 1

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr
1.	CMC.506	Organic Chemistry-I	C	3	0	0	3
2.	CMC.507	Organic Synthesis-I (Practical)	SB	0	0	4	2
3.	CMC.508	Modern Spectral and Chromatography Techniques	C	3	0	0	3
4.	CMC.509	Spectral Analysis (Practical)	SB	0	0	4	2
5.	CMC.510	Medicinal Chemistry-I	C	3	0	0	3
6.	CMC 511	Chemistry of Natural Products	C	3	0	0	3
7.	XXX	Inter-Disciplinary Course (Offered by Other department)	ID	2	0	0	2
	CMC 512	Basics of Drug Discovery (Offered by the department)					
<b>Opt any one course from following electives</b>							
8.	CMC.513	Current Trends in Organic Synthesis	DE	3	0	0	3
9.	CMC.514	Quantum Chemistry					
10.	CHM.509	Inorganic Chemistry-1					
11.	CHM.511	Physical Chemistry – I					
		<b>Total</b>		<b>17</b>	<b>0</b>	<b>8</b>	<b>21</b>

**CF:** Compulsory Foundation, **C:** Core, **ID:** Interdisciplinary, **DE:** Discipline elective, **SB:** Skill based, **EF/VB:** Elective foundation/Value based

**L: Lectures T: Tutorial P: Practical Cr: Credits**

**MOOC:** MOOC may be taken up 40% of the total credit (excluding dissertation credits). MOOC may be taken in lieu of any course but content of that course should match minimum 70%.

## SEMESTER II

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr
1.	CMC.521	Organic Chemistry-II	C	3	0	0	3
2.	CMC.522	Organic Synthesis-II-(Practical)	SB	0	0	4	2
3.	CMC.523	Fundamentals of Computer Aided Drug Design	C	3	0	0	3
4.	CMC.524	<i>In silico</i> Drug Design-(Practical)	SB	0	0	4	2
5.	CMC.525	Advanced Spectral Analysis	C	3	0	0	3
6.	CMC. 526	Medicinal Chemistry-II	C	3	0	0	3
7.	CMC.527	Process Chemistry	CF	3	0	0	3
8.	XXX  CMC.528	Value added course (VAC) offered by other department Modern analytical techniques offered by our department	VAC	2	0	0	2
<b>Opt any Course from following electives</b>							
9.	CMC.529	Green Chemistry	DE	3	0	0	3
10.	CMC.530	Nuclear Chemistry					
11.	CHM.521	Inorganic Chemistry – II					
12	CHM.523	Physical Chemistry – II					
		<b>Total</b>		<b>20</b>	<b>0</b>	<b>8</b>	<b>24</b>

Discipline elective, **SB**: Skill based, **EF/VB**: Elective foundation/Value based  
**L: Lectures T: Tutorial P: Practical Cr: Credits**

**MOOC**: MOOC may be taken up 40% of the total credit (excluding dissertation credits). MOOC may be taken in lieu of any course but content of that course should match minimum 70%.

### SEMESTER III

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr
1.	CMC.551	Research Methodology & Biostatistics	CF	3	0	0	3
2.	CMC.552	Organic Chemistry-III	C	3	0	0	3
3.	CMC.553	Organic Synthesis-III-(Practical)	SB	0	0	4	2
4.	CMC. 554	Entrepreneurship	CF	1	0	0	1
5.	CMC. 555	Organic Chemistry Worksheet	CF	2	0	0	2
6.	CMC. 556	Computer Applications	C	3	0	0	3
7.	CMC. 600	Research Proposal	SB	0	0	8	4
<b>Opt any elective course from the following</b>							
8.	CMC.557	Logics of Organic Synthesis	DE	3	0	0	3
9.	CMC.558	Bioinorganic and Biophysical Chemistry					
10.	CHM.525	Molecular Spectroscopy					
11.	CHM.551	Inorganic Chemistry-III					
	<b>Total</b>			<b>15</b>	<b>0</b>	<b>12</b>	<b>21</b>

Discipline elective, **SB**: Skill based, **EF/VB**: Elective foundation/Value based  
**L: Lectures T: Tutorial P: Practical Cr: Credits**

**MOOC**: MOOC may be taken up 40% of the total credit (excluding dissertation credits). MOOC may be taken in lieu of any course but content of that course should match minimum 70%.

### SEMESTER IV

<b>S. No.</b>	<b>Paper Code</b>	<b>Course Title</b>	<b>Course Type</b>	<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
1	CMC.600	Dissertation	SB	0	0	40	20
		<b>Total</b>		<b>0</b>	<b>0</b>	<b>40</b>	<b>20</b>

Discipline elective, **SB**: Skill based, **EF/VB**: Elective foundation/Value based  
**L: Lectures T: Tutorial P: Practical Cr: Credits**

### Examination Pattern

	Core, Discipline Elective, Compulsory Foundation, Value Added and Interdisciplinary Courses		Discipline Enrichment Course		Entrepreneurship Course	
	Marks	Evaluation	Marks	Evaluation	Marks	Evaluation
Internal Assessment	25	Various	-	-	-	-
Mid-semester test (MST)	25	Subjective	50	Objective	25	Objective
End-semester test (EST)	50	Subjective (70%) Objective (30%)	50	Objective	25	Subjective

**Objective Questions-** one word answers, fill-in the blank, sentence completion, true/false, MCQs'

**Subjective Questions-**The subjective type will include very short answer (1-2 lines), short answer (one paragraph), essay type with restricted response, and essay type with extended response

**Internal assessment-** any two or more of the given methods (Surprise Tests, one sentence summary, classroom assignments, home work assignments, term paper).

### Evaluation Criteria for Practical

Item	Practical Note book and continuous evaluation	Synopsis	Performance	Viva voce
Marks	40	10	20	30

### Evaluation Criteria for Dissertation

Dissertation Proposal (Third Semester)			Dissertation (Fourth Semester)		
	Marks	Evaluation		Marks	Evaluation
Supervisor	50	Dissertation proposal and presentation	Supervisor	50	Continuous assessment (regularity in work, mid-term evaluation) dissertation report, presentation, final viva-voce

HoD and senior-most faculty of the department	50	Dissertation proposal and presentation	External expert, HoD and senior-most faculty of the department	50	Dissertation report (30), presentation (10), final viva-voce (10)
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Evaluation pattern similar to fourth semester dissertation will apply for internship where supervisor will award 50% marks and external co-supervisor, HoD and senior-most faculty will award 50% marks.

### Semester 1

**Course Title: Organic Chemistry-I**

**Paper Code: CMC.506**

L	T	P	Credits
3	0	0	3

**Course Hours: 45h**

#### Learning Outcomes:

After completing this course, the learner will be able to:

- Describe disconnection approaches applied on synthetic strategies and mechanism prediction.
- Conceptualize difficult principles of basic organic chemistry and will apply this knowledge in drug synthesis and their interaction with receptors

#### Unit 1

**12 hours**

**Synthetic methodologies:** Synthons, Synthetic equivalent, Functional group interconversion (FGI), Functional group addition, Functional group elimination, Criteria for selection of target, Linear and convergent synthesis, Retrosynthetic analysis and synthesis involving chemoselectivity, Regioselectivity, Reversal of Polarity (Umpolung), Synthesis of cyclic molecules, Strategic bond: Criteria for disconnection of strategic bonds, Importance of the order of events in organic synthesis. One group and two group C-X disconnections in 1,2-, 1,3-, 1,4 & 1,5-difunctional compounds, One group C-C disconnections, alcohol and carbonyl compounds, regioselectivity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis, Two group C-C disconnections, Diels-Alder



reaction, 1,3-difunctionalised compounds, Control in carbonyl condensation, 1,5-difunctionalised compounds.

- Learner will be engaged in Group discussion to explain disconnection approaches in synthesis

## Unit 2

11 hours

**Aliphatic nucleophilic substitution reaction:** The  $S_N2$ ,  $S_N1$ , mixed  $S_N2$  and  $S_N1$  and SET mechanism, The  $S_Ni$  mechanism. Nucleophilic substitution at an allylic, aliphatic and vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile, regioselectivity, competition between  $S_N2$  and  $S_N1$  mechanisms.

**Aromatic nucleophilic substitution:** The  $S_NAr$ , bimolecular displacement mechanism and benzyne mechanism, reactivity effect of substrate structure, leaving group and attacking nucleophile.

**Aromatic electrophilic substitution:** The arenium ion mechanism, orientation and reactivity, energy profile diagrams, *ortho/para* ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles, Diazonium coupling, Vilsmeier–Haack reaction.

- Learner will be engaged in Molecular models to explain the stereochemistry in substitution reactions

## Unit 3

10 hours

**Elimination reactions:** E2, E1 and E1cB mechanisms and their spectrum, orientation of the double bond, effects of substrate structures, attacking base, the leaving group and the medium, mechanism and orientation in pyrolytic elimination.

**Addition to carbon-carbon multiple bonds:** Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, addition of halogen polar reagents to alkenes, Regio- and chemoselectivity, orientation and reactivity, hydroboration, epoxidation and hydroxylation.

- Learner will be engaged in Molecular models to explain the stereochemistry in elimination reactions

## Unit 4

12 hours

**Heterocyclic chemistry:** Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles, Aromatic heterocycle, Non-aromatic heterocycle: Bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles and their synthesis

(a) Three-membered and four-membered heterocycles: synthesis and reactions of aziridines, oxiranes, thiranes, azetidines, oxetanes and thietanes.

(b) Five membered heterocycles containing two heteroatoms (S,N,O): Diazoles, imidazole, pyrazole, oxazoles and thiazoles.

(c) Benzo-fused five-membered and six membered heterocycles: Synthesis and reactions of indoles, benzofurans and benzimidazoles, benzothiazoles.

(d) Six-membered heterocycles with heteroatom: Synthesis and reactions of pyrylium salts and pyrones, coumarins, chromones, pyridine, pyrimidine *etc.*

• Learner will be engaged in using ball and stick models and web mediated activity to explain heterocyclic Chemistry

### **Suggested Readings:**

1. Clayden, J., Greeves, N., Warren, S., Wothers, P. (2012). *Organic chemistry* Organic Chemistry Oxford press.

2. Finar, I.L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, UK. F

3. Mc Murry J., *Organic Chemistry*, Asian Book Pvt. Ltd, New Delhi

4. Smith, M. B. (2013). *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*. John Wiley & Sons.

5. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., New Delhi-110002.

6. Bansal, R. K., (2010). *A text book of Organic Chemistry*, New Age International (P) Ltd., New Delhi.

7. Bansal R.K., (2010). *Organic Reaction Mechanism*, New Age International (P) Ltd., New Delhi.

8. Kalsi, P.S., (2010). *Organic Reactions and Their Mechanisms*. New Age International Pub., New Delhi.

9. Kalsi, P.S., (2010). *Stereochemistry: Conformation and Mechanism*, New Age International (p) Ltd. New Delhi.

10. Morrison, R.T., Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of

India, New Delhi.

11. Mukherjee, S.M. Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry*. Macmillan India Ltd., New Delhi.
12. Eliel, E. L., & Wilen, S. H. (2008). *Stereochemistry of organic compounds*. John Wiley & Sons.
13. Carey, F. A., Giuliano, R. M. (2012). *Organic Chemistry*. McGraw Hill.
14. Kofie, W., Caddick, S. (2016). *Problems in Advanced Organic Chemistry*. Auris Publishing.
15. Solomons, T. W. G., Fryhle, C. B., Snyder, S. A. (2017). *Solomons' Organic Chemistry*. John Wiley & Sons.
16. Acheson, R.M. (1976). *An Introduction to the Chemistry of Heterocyclic Compounds*, Wiley India Pvt. Ltd.
17. Gupta R.R., Kumar M., Gupta V. (2010). *Heterocyclic Chemistry-II Five Membered Heterocycles Vol. 1-3*, Springer Verlag, India.
18. Warren, S., (2010). *Organic Synthesis: The Synthron Approach*. John Wiley & Sons, New York,
19. Warren, S., (2010). *Designing Organic Synthesis: A Disconnection Approach*. John Wiley & Sons, New York.

**The following are some of the modes of classroom transaction**

- Lecture
- Group discussion
- Demonstration
- Team teaching
- Tutorial
- Self-learning

**Transaction Mode**

- PPT
- YouTube
- Google drive
- Google meet

**Course Title: Organic Synthesis –I (Practical)**

<b>L</b>	<b>T</b>	<b>P</b>	<b>Credits</b>
0	0	4	2

**Paper Code: CMC 507**

**Course Hours: 60h**

**Learning Outcomes:**

After completing this course, the learner will be able to:

- Interpret stereochemistry of organic compounds
- Explain the handling, storage and disposal of hazardous chemicals and their Material safety data sheets (MSDS)
- Monitor the progress of chemical reactions by thin layer chromatography
- Purify a given organic compound through crystallization, fractional distillation or column chromatography

**Course content:**

1. Awareness to various glassware and plasticwares used in the organic synthesis.
2. Demonstration of Stereochemical aspects of the compounds through molecular models
3. Awareness to handling, storage and disposal of hazardous chemicals and their Material safety data sheets (MSDS).
4. Thin layer chromatography: Monitoring the progress of chemical reactions, identification of unknown organic compounds by comparing the  $R_f$  values of known standards, preparative TLC for separation of mixtures
5. Purification of a given organic compound through crystallization, fractional distillation or column chromatography.
6. **Organic Synthesis:** Single or multi- steps synthesis of organic compounds. Aspects such as conversion, yield, selectivity, effluent treatment, atom economy, etc. should be paid attention. TLC should be used to monitor the reaction. (attempt any five)
  - a) Synthesis of an anticancer stilbene via Wittig reaction
  - b) Synthesis of chalcones via Claisen-Schmidt condensation.
  - c) Preparation of vanillyl alcohol from vanillin
  - d) Reduction of 3-nitroacetophone using  $\text{NaBH}_4/\text{LiAlH}_4$
  - e) Preparation of bromohydrin from methylstyrene
  - f) Preparation of aniline from nitrobenzene
  - g) Synthesis of ethyl *N*-butylacetoacetate by A.E.E. condensation
  - h) Cannizzaro reaction: 4-chlorobenzaldehyde as substrate.
  - i) Preparation of Iodoxybenzoic acid (IBX) and its application in oxidation.
  - j) Preparation of pyridine chlorochromate (PCC) and its application in oxidation.
  - k) Multistep synthesis of phenytoin.

### **Suggested Readings:**

1. Adams, R., Johnson, J.R., Wilcox, C.F. (1970). *Laboratory Experiments in Organic Chemistry*, The Macmillan Limited, London.
2. Mann, F. G. (2009). *Practical Organic Chemistry*. Pearson Education India.
3. Pasto, D.P., Johnson, C., Miller, M. (2010). *Experiments and Techniques in Organic Chemistry*, Prentice Hall.
4. Roberts, R.M., Gilbert, J.C., Rodewald, L.B., Wingrove, A.S. (1969). *An Introduction to Modern Experimental Organic Chemistry*, Ranehart and Winston Inc., New York.
5. Vogel, A.I. (latest edition). *Text Book of Practical Organic Chemistry*, Pearson
6. Williamson, K.L., Heath, D.C. (1999). *Macroscale and Microscale Organic Experiments*, Heath, D. C & Co., Lexington, MA.
7. Armarego, W. L., & Chai, C. (2012). *Purification of Laboratory Chemicals*. Butterworth-Heinemann.
8. Young, J. A. (Ed.). (1991). *Improving Safety in the Chemical Laboratory: a Practical Guide*. Wiley.

9. Zercher, C. A. (2010). *Organic Syntheses*. John Wiley & Sons.
10. Leonard, J., Lygo, B., Procter, G. (2013). *Advanced Practical Organic Chemistry*. CRC Press.

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- Experimentation
- Group discussion
- Demonstration
- Self-learning

**Transaction Mode**

- PPT
- YouTube
- Google drive
- Google meet

**Course Title: Modern Spectral & Chromatographic Techniques**

**Paper Code: CMC.508**

**Course Hours: 45h**

L	T	P	Credits
3	0	0	3

**Learning Outcomes**

After completing this course, the learner will be able to:

- Conceptualize general principle and theory of spectroscopy
- Describe the concept and instrumentation of UV-Vis, IR, NMR, Mass and Chromatographic techniques
- Solve the spectra of compounds
- Separate different constituents of mixture by chromatographic techniques

**Unit 1**

**12 hours**

### **UV-Visible spectroscopy**

Introduction, Theory, Laws, Instrumentation associated with UV-Visible spectroscopy, Choice of solvents and solvent effect and Applications of UV-Visible spectroscopy, Difference/ Derivative spectroscopy.

### **IR spectroscopy**

Theory, Modes of Molecular vibrations, Sample handling, Instrumentation of Dispersive and Fourier – Transform IR Spectrometer, Factors affecting vibrational frequencies and applications of IR spectroscopy, Data Interpretation, Theory of NIR.

### **Spectrofluorimetry**

Theory of Fluorescence, Factors affecting fluorescence, Quenchers, Applications of fluorescence spectrophotometer, Instrumentation

- Learner will be provided hands on training to different instruments like UV, IR and spectrofluorimetry.

## **Unit 2**

**12 hours**

### **NMR spectroscopy**

Quantum numbers and their role in NMR, Principle, Instrumentation, Solvent requirement in NMR, Relaxation process, NMR signals in various compounds, Chemical shift, Factors influencing chemical shift, Spin-Spin coupling, Coupling constant, Nuclear magnetic double resonance, Brief outline of principles of FT-NMR and <sup>13</sup>C NMR, Applications of NMR spectroscopy

### **Mass Spectroscopy**

- Principle, Theory, Instrumentation of Mass Spectroscopy, Different types of ionization like electron impact, chemical, field, FAB and MALDI, APCI, ESI, APPI Analyzers of Quadrupole and Time of Flight, Mass fragmentation and its rules, Meta stable ions, Isotopic peaks and Applications of Mass spectroscopy.
- Learner will be provided NMR and mass spectra for the characterization of compounds.

## **Unit 3**

**11 hours**

### **Chromatography**

Principle, apparatus, instrumentation, chromatographic parameters, factors affecting resolution, isolation of drug from excipients, data interpretation and applications of the following: Thin Layer chromatography, High Performance Thin Layer Chromatography, Ion exchange chromatography, Column chromatography, Gas chromatography, High Performance Liquid chromatography, Ultra High Performance Liquid chromatography, Affinity chromatography, Gel Chromatography

- Learner will be provided experience of chromatography by using different

techniques like TLC, Column, HPLC, HPTLC and GC.

#### **Unit 4**

**10 hours**

#### **Thermal Techniques**

Principle, thermal transitions and Instrumentation (Heat flux and power-compensation and designs), Modulated DSC, Hyper DSC, experimental parameters (sample preparation, experimental conditions, calibration, heating and cooling rates, resolution, source of errors) and their influence, advantage and disadvantages, pharmaceutical applications. Differential Thermal Analysis (DTA): Principle, instrumentation and advantage and disadvantages, pharmaceutical applications, derivative differential thermal analysis (DDTA). TGA: Principle, instrumentation, factors affecting results, advantage and disadvantages, pharmaceutical applications

- Learner will be provided Web based learning to explain thermal techniques

#### **Suggested readings**

1. Silverstein, R. M., Webster, F. X., Kiemle, D. J., & Bryce, D. L. (2014). *Spectrometric Identification of Organic Compounds*. John Wiley & Sons.
2. Skoog, D. A., Holler, F. J., & Crouch, S. R. (2018). *Principles of Instrumental Analysis*. Singapore: Cengage Learning Asia Pte Ltd.
3. Willard, H. H. (2012). *Instrumental methods of analysis*. New Delhi: CBS.
4. Beckett, A. H., & Stenlake, J. B. (Eds.). (1988). *Practical Pharmaceutical Chemistry: Part II*, A&C Black.
5. Kemp, W. (1991). *Organic Spectroscopy* (pp. 42-51). London: Macmillan.
6. Sethi, P. D. (1985). *Quantitative Analysis of Drugs in Pharmaceutical Formulations*. Unique Publishers.
7. Munson, J. W. (Ed.). (1984). *Pharmaceutical Analysis: Modern Methods* (Vol. 11). CRC Press.
8. Kalsi, P. S. (2007). *Spectroscopy of Organic Compounds*. New Age International.
9. Connors, K. A. (2007). *A Textbook of Pharmaceutical Analysis*. John Wiley & Sons.
10. McHale, J. L. (2017). *Molecular Spectroscopy*. CRC Press.
11. Kromidas, S. (2017). *The HPLC Expert Possibilities and Limitations of Modern High Performance Liquid Chromatography*. John Wiley and Sons.

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- Lecture
- Group discussion
- Demonstration



- Tutorial
- Self-learning

### **Transaction Mode**

- PPT
- YouTube
- Google drive
- Google meet

**Course Title: Spectral Analysis (Practical)**

<b>L</b>	<b>T</b>	<b>P</b>	<b>Credits</b>
0	0	4	2

**Paper Code: CMC.509**

**Course Hours: 60h**

### **Learning Outcomes**

After completing this course, the learner will be able to:

- Develop knowledge skills and understanding of structure elucidation of unknown compounds *via* spectral interpretation of  $^1\text{H}$ ,  $^{13}\text{C}$  NMR, IR, UV and Mass.
- Independently operate analytical instruments such as FT-IR, UV-vis spectrophotometer, GC-MS, and HPLC

### **Course content**

- Estimation of elements and functional groups in organic natural compounds
- Analysis of organic compounds by UV Vis spectrophotometer
- Experiments based on Column chromatography

- Experiments based on HPLC
- Experiments based on Gas Chromatography
- Characterization of organic compounds using TLC, melting point,  $^1\text{H}$ ,  $^{13}\text{C}$  NMR, IR, UV and Mass.
- Isolation, characterization like melting point, mixed melting point, molecular weight determination, functional group analysis, co-chromatographic technique for identification of isolated compounds and interpretation of UV and IR data

### **Suggested Readings**

1. Adams, R., Johnson, J.R., Wilcox, C.F. (1970). *Laboratory Experiments in Organic Chemistry*, The Macmillan Limited, London.
2. Mann and Saunders. (2009). *Practical Organic Chemistry*, Pearson.
3. Pasto, D.P., Johnson, C., Miller, M. (2010). *Experiments and Techniques in Organic Chemistry*, Prentice Hall.
4. Roberts, R.M.; Gilbert, J.C.; Rodewald, L.B.; Wingrove, A.S. (1969). *An introduction to Modern Experimental Organic Chemistry*, Ranehart and Winston Inc., New York.
5. Vogel, A.I. (latest edition). *Text Book of Practical Organic Chemistry*, Pearson
6. Williamson, K.L., Heath, D.C. (1999). *Macroscale and Microscale Organic Experiments*, Heath, D.C and Co., Lexington, MA.
7. Armarego, W. L., & Chai, C. (2012). *Purification of Laboratory Chemicals*. Butterworth-Heinemann.
8. Young, J. A. (Ed.). (Latest Edition). *Improving Safety in the Chemical Laboratory: a Practical Guide*. Wiley.
9. Findeisen, M., (2013). *50 And More Essential NMR Experiments: A Detailed Guide*. John Willey & Sons.
10. Kromidas, S. (2017). *The Hplc Expert Possibilities and Limitations of Modern High Performance Liquid Chromatography*. John Wiley and Sons.

### **The following are some of the modes of classroom transaction**

- Experimentation
- Group discussion
- Demonstration

### **Transaction Mode**

- YouTube
- PPT
- Google meet

**Course Title: Medicinal Chemistry-I**  
**Paper Code: CMC.510**  
**Course Hours: 45h**

<b>L</b>	<b>T</b>	<b>P</b>	<b>Credits</b>
3	0	0	3

### **Learning Outcomes**

After completing this course, the learner will be able to:

- Interpret basics concepts of drugs, their effects and screening.
- Describe drugs interaction with various types of enzymes and receptors
- Conceptualize the process of drug discovery and its progress

### **Unit 1** **10 hours**

**History of drug discovery** Introduction, Drug discoveries, Recent trends in drug discovery, Enzymes as drug targets, Membrane transporters as drug targets, Voltage-gated ion channels as drug targets

- Learner will be engaged in group discussion to explain history of drug discovery

### **Unit 2** **11 hours**

**Drug discovery:**

Stages of drug discovery, lead discovery; identification, validation and diversity of drug targets

### **Biological drug targets**

Receptors, types, binding and activation, theories of drug receptor interaction, drug receptor interactions, agonist vs antagonists, artificial enzymes.

### **Measurement and expression of drug effects**

Introduction, *In-vitro* experiments, *Ex-vivo* experiments, *In-vivo* experiments.

- Learner will be explained about drug interaction and target through molecular modeling studies

## **Unit 3**

**12 hours**

### **Prodrug Design and Analog design**

#### **Prodrug design**

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

#### **Combating drug resistance**

Causes for drug resistance, strategies to combat drug resistance in antibiotics and anticancer therapy, Genetic principles of drug resistance.

#### **Analog Design**

Introduction, Classical & Non classical, Bioisosteric replacement strategies, rigid analogs, alteration of chain branching, changes in ring size, ring position isomers, design of stereo isomers and geometric isomers, fragments of a lead molecule, variation in inter atomic distance.

- Learner will be engaged in Web based training to familiarize with prodrug and analog design

## **Unit 4**

**12 hours**

- a) Medicinal chemistry aspects of the following class of drugs Systematic study, SAR, Mechanism of action and synthesis of new generation molecules of following class of drugs:
- b). Anti-hypertensive drugs, Psychoactive drugs, Anticonvulsant drugs, H1 & H2 receptor antagonist, COX1 & COX2 inhibitors, Adrenergic & Cholinergic agents, Antineoplastic and Antiviral agents.
- c). Stereochemistry and Drug action: Realization that stereo selectivity is a pre-requisite for evolution. Role of chirality in selective and specific therapeutic agents. Case studies, enantioselectivity in drug adsorption, metabolism, distribution and elimination.

- Learner will be engaged in Group discussion to explain SAR, Mechanism of action and synthesis of drugs

### **Suggested Readings:**

1. Foye, W. C. (2019). *Principles of Medicinal Chemistry*, Publisher: Wolters Kluwer.
2. King, F. D. (2006). *Medicinal Chemistry Principles and Practice*, Royal Society of Chemistry.
3. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press.
4. Patrick, G.L. (2017). *An Introduction to Medicinal Chemistry*, Publisher: Oxford university Press, UK.
5. Singh, H., Kapoor, V.K. *Medicinal and Pharmaceutical Chemistry* Vallabh Prakashan, Delhi.
6. Smith, H.J. (2006). *Introduction to the Principles of Drug Design and Action*, Taylor and Francis.
7. Wermuth, C.G. (2009). *The Practice of Medicinal Chemistry*, Academic Press (Elsevier).
8. Wolff, M E, Ed., (Latest Edition). *Burger's Medicinal Chemistry and Drug Discovery* John Wiley and Sons, New York.
9. Ferrant, E., (2011). *New Synthetic Technologies In Medicinal Chemistry*. Royal Chemical Society.
10. Medicinal Chemistry by Burger, Vol I –VI.
11. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, 12<sup>th</sup> Edition, Lppincott Williams & Wilkins, Woltess Kluwer (India) Pvt.Ltd, New Delhi.
12. Comprehensive Medicinal Chemistry – Corwin and Hansch.
13. Computational and structural approaches to drug design edited by Robert M Stroud and Janet. F Moore

### **The following are some of the modes of classroom transaction**

- Lecture
- Group discussion
- Demonstration
- Team teaching

### **Transaction Mode**

- Molecular Models
- PPT
- YouTube
- Software for *In silico* study
- Google meet

**Course Title: Chemistry of Natural Products**

**Paper Code: CMC.511**

**Course Hours: 45h**

L	T	P	Credits
3	0	0	3

### Learning Outcomes

After completing this course, the learner will be able to:

- Describe various types of natural products
- Conceptualize the role of natural products in living organisms, their biosynthesis and will have a greater understanding of organic synthesis
- Explain the role of natural products in drug discovery and development

### Unit 1

**12 hours**

**Terpenoids and carotenoids:** Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Geraniol, Menthol and  $\beta$ -Carotene

- Learner will be engaged in molecular models to explain the structure and stereochemistry of terpenoids.

**Unit 2****11 hours**

**Alkaloids:** Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following: Ephedrine, Nicotine and Morphine

- Learner will be able to explain chemical tests for the identification of plant alkaloids

**Unit 3****10 hours**

**Steroids:** Occurrence, nomenclature, basic skeleton and stereochemistry, Structure determination and synthesis of cholesterol, partial synthesis of Testosterone and Progesterone, Chemical tests for steroids

- Learner will be engaged in molecular models to explain the structure and stereochemistry of steroids.

**Unit 4****12 hours**

**Flavonoids:** Introduction, isolation and purification of flavonoids, General methods of structural determination of flavonoids; Structural elucidation of quercetin

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

- Learner will be provided spectral data for the identification of above mentioned natural compounds.

**Suggested Readings**

1. Bhat, S.V., Nagasampagi, B.A., Meenakshi, S. (2013). *Natural Product Chemistry & Applications*, Narosa Publishing House, New Delhi.
2. Bhat, S.V., Nagasampagi, B.A., Sivakumar, M. (2005), *Chemistry of Natural Products*. Narosa Publishing House, New Delhi.
3. Brahamchari, G. (2009). *Natural Product: Chemistry, Biochemistry and Pharmacology*. . Narosa Publishing House, New Delhi.
4. Cseke, L.J. (2009). *Natural Products from plants*. CRC Press, Taylor and Francis, US.
5. Dewick, P.M. (2009). *Medicinal Natural Products: A Biosynthetic Approach*. Willey & Sons, UK.
6. Finar, I.L. (2006). *Organic Chemistry: Stereochemistry and the Chemistry of Natural Products*. Dorling Kindersley Pvt. Ltd., India.
7. Peterson, F., Amstutz, R. (2008). *Natural Compounds as drugs*. Birkhauser Verlay.
8. Thomson, R.H. (2008). *The Chemistry of Natural Products*, Springer.

9. Singh, J., Ali, S. M., Singh, J. (2010) *Natural Products Chemistry*. Pragati Books.
10. Xu, R., Ye, Y., Zhao, W., (2011). *Introduction to Natural Products Chemistry*. CRC Press.
11. Rehman, A., (2015). *Studies in Natural Products Chemistry*, Elsevier Books.

**The following are some of the modes of classroom transaction**

- Lecture
- Group discussion
- Demonstration
- Tutorial

**Transaction Mode**

- PPT
- YouTube
- Google meet

**Course Title: Basics of Drug Discovery**

L	T	P	Credits
3	-	0	3

**Paper Code: CMC.512**

**Course Hours: 45h**

**Learning outcome:** Students who successfully complete this course will be able to

- Apply the knowledge of drug-receptor interactions for understanding drug mechanism
- Utilize the knowledge of ligand interactions with the active site of receptor in novel drug design and discovery
- Apply the knowledge of QSAR for novel drug designing

**Unit 1**

**11 hours**

**Interactions of enzyme/receptor with drug molecules:** Chirality and drug action; Covalent, ion-dipole, hydrogen bonding, C-H hydrogen bonding, dihydrogen bonding, van der waals interactions and the associated energies, Receptor & biological response, Drug-receptor interactions, receptor theories and drug action, Occupancy theory, rate theory, induced fit theory, macromolecular perturbation theory, activation-aggregation theory, Topological and stereochemical consideration.

**Theoretical Aspects of Drug Action:** Drug distribution, Active transport, Passive transport, The Ferguson Principle Physicochemical Parameters and



Pharmacological Activity-Solubility, Partition Coefficient, Surface Activity, pKa, Ionisation, Stereochemical Factors, Bio-isosterism.

- Learner will be engaged in molecular modeling to explain drug interactions and online ADME calculation softer for determination of pharmacokinetic parameters.

## Unit 2

12 hours

**Enzyme kinetics in drug action:** Mechanisms of enzyme catalysis, Electrostatic catalysis and desolvation, Covalent catalysis, acid-base catalysis, strain / distortion in enzyme catalysis, Coenzyme catalysis, Theories of enzyme inhibition and inactivation, Enzyme activation of drugs-prodrugs.

**Drug metabolism:** Metabolic Processes- Phase-I (Oxidation, Reduction & Hydrolysis) and Phase-II (Glucuronide Conjugation, Acetylation, Methylation, Sulphate Conjugation, Conjugation with amino acids and Mercapturic acid formation), Routes of Elimination, Factors Affecting Metabolism–Genetic Factors, Physiological Factors, Pharmaceutical Factors, Drug Interactions.

- Learner will be engaged in group discussion about enzyme kinetics and drug metabolism

## Unit 3

12 hours

**SAR studies, Lead modification and Drug Design:** Lead modification strategies; Bioisosterism, variation of alkyl substituents, chain homologation and branching, Variation of aromatic substituents, Extension of structure, Ring expansion or contraction, Ring variation, Variation in position of hetero atoms, Ring fusion, Simplification of the lead, Rigidification of lead; Discovery of oxaminquine, salbutamol, cimitidine and captopril. Structure-Activity Relationship studies in sulfa drugs, benzodiazepines, barbiturates, and taxol analogs. Principles of prodrug design, Serendipitous discovery of leads e.g. Penicillin and librium, sildenafil.

**In silico methods:** Introduction to Quantitative Structure Activity Relationship (QSAR) studies. 2-D QSAR, QSAR parameters. 3-D QSAR, CoMFA and CoMSIA. Molecular docking, Pharmacophore mapping and virtual screening.

- Learner will be provided web based training to familiarize SAR and *in silico* studies for drug design

## Unit 4

10 hours

**Combinatorial synthesis and chiral drugs:** Introduction, Combinatorial approach, Combinatorial library, Solid phase synthesis, resins, linkers. Parallel synthesis; Haughton's tea bag procedure, Automated parallel synthesis, Mix and Split combinatorial synthesis, Structure determination of active compounds, Synthesis

of heterocyclic combinatorial libraries, Analytical characterization of synthetic organic libraries.

- Learner will be engaged in web based training to explain Combinatorial synthesis of chiral drugs.

**Suggested Readings:**

1. Ellis, G.P., West, G. B. (1983). *Progress in Medicinal Chemistry Series*. Elsevier Science.
2. Foye, W.O.; Lemke, T. L.; Williams, D. A. (Latest Edition). *Principles of Medicinal Chemistry*, Indian Ed. Waverly, Pvt. Ltd. New Delhi.
3. Ganellin, C.R.; Roberts S. M., (1993). *Medicinal Chemistry: The Role of Organic Chemistry in Drug Research*. Publisher: Academics Press Inc.
4. Kadam, Mahadik, Bothara (2010). *Principle of Medicinal Chemistry (Volume I & II)*, Nirali publication
5. Kulkarni, V. M., Bothra, K.G., (2008). *Drug Design*, Nirali Publication.
6. Lawton, G., Witty, D.R. (2011). *Progress in Medicinal Chemistry Series. Volume 50*.
7. Lednicer D., Laster A. M. (1998). *The Organic Chemistry of Drug Synthesis(3 Volumes)* John Wiley & Sons.
8. Lednicer, D. (2008). *Strategies for Organic Drug Synthesis and Design. (7 volume)* Publisher: John Wiley & Sons.
9. Lemke, T.L., Williams, D.A. (2012). *Foye's Principles of Medicinal Chemistry*. 7th edition.
10. Silverman R.B., (2014). *Organic Chemistry of Drug Design and Drug Action*, Publisher: Elsevier.
11. Wilson, C.O.; Block, J.H.; Gisvold, O.; Beale, J. M. Wilson and Gisvold's (2003) *Textbook of Organic Medicinal and Pharmaceutical Chemistry*. Lippincott Willaiams & Wikins.

**The following are some of the modes of classroom transaction**

- Lecture
- Group discussion
- Demonstration
- Team teaching
- Tutorial
- Self-learning

**Transaction Mode**

- PPT
- YouTube
- Google drive
- Google meet

### **Elective courses**

**Course Title: Current Trends in Organic Synthesis**

**Paper Code: CMC.513**

**Course Hours: 45h**

<b>L</b>	<b>T</b>	<b>P</b>	<b>Credits</b>
3	0	0	3

### **Learning Outcomes:**

After completing this course, the learner will be able to:

- Explain the role of free radicals in chemical transformation
- Conceptualize the importance of organometallic compounds and their application
- Apply the knowledge of various reagents for the synthesis of target molecules and will also acquire knowledge of some important C-C, and C-N bond formation reactions

### **Unit 1**

**11 hours**

#### **Free radical reactions**

Types of free radical reactions, free radical substitution mechanism at an aromatic substrate, neighbouring group assistance, Reactivity for aliphatic and aromatic substrates at a bridgehead,

Reactivity in the attacking radicals, the effect of solvents on reactivity, Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation. Coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction, Free Radical Rearrangement, Hunsdiecker reaction

- Learner will be engaged in Group discussion to explain free radical reactions.

## Unit 2

12 hours

### Organometallic compounds

Organoboranes: Preparation of Organoboranes viz hydroboration with BH<sub>3</sub>-THF, dicyclohexyl borane, disiamyl borane, theryl borane, 9-BBN and disopinacamphyl borane, functional group transformations of Organoboranes-Oxidation, protonolysis and rearrangements. Formation of carbon-carbon-bonds viz organoboranes carbonylation. Grignard reagents, Organolithium, Organozinc, Organocadmium and Organocopper Compounds, Organosilicon compounds for organic synthesis, Organopalladium and organostannous (Applications in coupling reactions).

- Learner will be used web based learning to understand organometallic compounds and their uses

## Unit 3

12 hours

### Reagents in organic synthesis:

Gilman's reagent, Lithium diisopropylamide (LDA), Dicyclohexyl Carbodiimide (DDC), 1,3-Dithiane (Umpolung reagent), Trimethylsilyliodide, Baker's yeast, D.D.Q., Lead tetraacetate, Prevost Hydroxylation, Wilkinson's catalyst, Phase transfer catalysts: Quaternary ammonium and Phosphonium salts, Crown ethers, Merfield resin, Fenton's reagents, Ziegler-Natta catalyst, Lawson reagents, K-selectride and L-selectride, Sodium cyanoborohydride, 9-BBN, IBX, Manganese dioxide, Fetizon reagent, Dioxiranes, Ceric ammonium nitrate, Tebbe reagent, Corey-Nicolaou reagent, Mosher's reagent, use of Os, Ru, and Tl reagents.

- Learner will be used web based learning to understand the applications of reagents in organic synthesis

## Unit 4

10 hours

**New synthetic reactions:** Baylis-Hillman reaction, Biginelli reaction, Mukaiyama aldol reaction, Mitsunobu reaction, McMurrey reaction, Julia-Lythgoe olefination, and Peterson's stereoselective olefination, Buchwald-Hartwig coupling, Eishenmosher-Tanabe fragmentation and Shapiro reaction, Stork-enamine reaction Aza-Cope, Aza-Wittig reaction, BINAL and BINAP assisted reactions. Ugi reaction, Robinson-Gabriel synthesis, Strecker amino acid synthesis Vilsmeier-Haack reaction, Wohl-Ziegler reaction.

- Molecular models will be used to explain the stereochemistry of new synthetic reactions.

### **Suggested readings:**

1. Finar, I.L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, UK.
2. Finar, I.L., (2012). *Organic Chemistry Vol. 2: Stereochemistry and The Chemistry of Natural Products*, Pearson Education, UK.
3. Fleming (1999). *Pericyclic Reactions*, Oxford University Press, Oxford.
4. Fleming (2010). *Molecular Orbitals and Organic Chemical Reactions*, John Wiley & Sons.
5. Jie Jack Li, (2009). *Name Reactions: A collection of detailed Reaction Mechanism*, Publisher: Springer-verlag.
6. Kalsi, P.S., (2010). *Organic Reactions and Their Mechanisms*, New Age International Pub., New Delhi.
7. Kalsi, P.S., (2010). *Stereochemistry: Conformation and Mechanism*, New Age International (p) Ltd., New Delhi.
8. Lowry, T.H., Richardson K.S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc.
9. Mc Murry, J., *Organic Chemistry*, Asian Book Pvt Ltd, New Delhi
10. Morrison, R.T., Boyd, R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
11. Mukherjee, S.M., Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
12. Reinhard Bruckner, (2001). *Advanced Organic Chemistry: Reaction Mechanism*, Academic Press.
13. Smith, M. B. (2013). *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*. John Wiley & Sons.
14. Solomn, C.W.G, Fryble, C.B. (2003). *Organic Chemistry*, John Wiley & Sons, Inc., New York.
15. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, US.
16. W. Carruthers, (2004). *Some Modern Methods of Organic Synthesis*, Cambridge Uni. Press, UK.

### **The following are some of the modes of classroom transaction**

- Lecture
- Group discussion
- Demonstration

### **Transaction Mode**

- PPT
- YouTube
- Google meet

**Course Title: Quantum Chemistry**

L	T	P	Credits
3	0	0	3

**Paper Code: CMC.514**

**Course Hours: 45h**

### **Learning Outcomes**

After completing this course, the learner will be able to:

- Describe quantum chemical description of chemical bonding, reactivity and their applications in molecular spectroscopy and inorganic chemistry
- Explain Electronic and Hamiltonian operators for molecules.
- Utilize Quantum chemical description of angular momentum and term symbols for a one and many-electron systems.
- Conceptualize Born-Oppenheimer approximation, the Pauli principle, Hund's rules, Hückel theory and the variation principle

### **Unit 1**

**12 hours**

**Fundamental Background:** Postulates of quantum mechanics, Eigen values and Eigen functions, operators, hermitian and unitary operators, some important theorems. Schrodinger equation-particle in a box (1D, 3D) and its application, potential energy barrier and tunneling effect, one-dimensional harmonic oscillator and rigid rotor, Particle in a Ring, Hydrogen Atom.

- Learner will apply Schrodinger equation for particle in 1D and 3D

**Unit 2** **10 hours**

**Approximate Methods:** Perturbation theory for non-degenerate and degenerate states and its applications, Variation theorem and its application.

- Web based approach will be used to explain perturbation and variation theory

**Unit 3** **12 hours**

**Angular Momentum:** Ordinary angular momentum, Eigen functions and Eigen values for angular momentum, Addition of angular momenta, Spin, Anti-symmetry and Pauli exclusion principle.

**Electronic Structure of Atoms:** Electronic configuration, Russell-Saunders terms and Coupling Schemes, Magnetic Effects: Spin-orbit Coupling and Zeeman Splitting, the self-consistent field method, Hartree-Fock SCF method for molecules.

- Learner will apply Angular momentum and Pauli exclusion principle to solve numerical problems

**Unit 4** **11 hours**

**Born-Oppenheimer Approximation:** LCAO-MO and VB treatments of the  $H_2^+$  and  $H_2$ , Hybridization and valence MOs of  $H_2O$  and  $NH_3$ . Huckel Theory of acyclic and cyclic conjugated systems, Bond Order and Charge Density Calculations.

- Learner will be engaged in web based learning to explain Born-Oppenheimer approximation concept

**Suggested Readings:**

1. Levine, I.N. *Quantum Chemistry*, 2016, Pearson Educ., Inc. New Delhi.
2. Chandra, A.K. 1994, *Introductory Quantum Chemistry*, Tata McGraw Hill.
3. Prasad, R.K., 2009, *Quantum Chemistry*, New Age Science.
4. Mc Quarrie, D. A. (2011). *Quantum Chemistry*. Viva Publishers.
5. Murrell, J.N. Kettle S.F.A. and Tedder, J. M. Valence Theory, 1965, John Wiley.
6. Lowe, J. P. and Peterson, K. 2006, *Quantum Chemistry*, Academic Press.

**The following are some of the modes of classroom transaction**

- Demonstration
- Group discussion
- Lecture
- Self-learning

### Transaction Mode

- Google meet
- PPT
- YouTube

### Semester -II

**Course Title: Organic Chemistry-II**

**Paper Code: CMC.521**

**Course Hours: 45h**

L	T	P	Credits
3	0	0	3

### Learning Outcomes

After completing this course, the learner will be able to:

- Interpret the stereochemistry, spatial arrangement of atoms/groups and apply it on the course of reactions and mechanism prediction.
- Explain the mechanism and applications of different naming reactions
- Apply principle of photochemistry in various chemical transformations

### Unit 1

**12 hours**

**Stereochemistry:** IUPAC nomenclature of organic molecules, Elements of symmetry, Chirality, Projection formulae [Flywedge, Fischer, Newman and Saw horse], Configurational and conformational isomerism in acyclic and cyclic compounds; Stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity, racemic mixture and their resolution, Configurational notations of simple molecules, D/L, R/S, E/Z and *cis/trans* configurational notations, Threo and erythro isomers, Methods of resolution, Optical purity, Enantiotopic and diastereotopic atoms, groups and faces, Stereospecific and stereoselective synthesis, Asymmetric synthesis, Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), Chirality due to helical shape, Stereochemistry of the compounds



containing nitrogen, sulphur and phosphorus, Conformational analysis of cyclic compounds such as cyclopentane, cyclohexane, cyclohexanone derivatives, decalins, 1,2-; 1,3-, 1,4-disubstituted cyclohexane derivatives and D-Glucose, Effect of conformation on the course of rate of reactions, Effect of conformation on reactivity, Conformation of sugars, strain due to unavoidable crowding.

- Learner will be engaged in Molecular models and online modeling tools to explain the stereochemistry of compounds

## Unit 2

11 hours

**Rearrangements:** General mechanistic considerations-nature of migration, migratory aptitude, Mechanistic study of the following rearrangements: Pinacol-pinacolone, Wagner-Meerwein, Benzil-Benzilic acid, Favorskii, Arndt-Eister synthesis, Neber, Beckmann, Hofmann, Curtius, Schmidt, Baeyer-Villiger, Shapiro reaction, Carroll, Claisen, Cope, Gabriel-Colman, Smiles and Sommelet-Hauser rearrangements.

**Selective Name Reactions:** Aldol, Perkin, Stobbe, Dieckmann Condensation, Reimer-Tiemann, Reformatsky Grignard reactions, Diels-Alder reaction, Robinson Annelation, Michael addition, Mannich reaction, Stork-enamine, Sharpless Asymmetric Epoxidation, Ene, Barton, Hofmann-Löffler Fretag, Shapiro reaction, Chichibabin Reaction.

- Learner will be engaged in Group discussion to explain rearrangement and name reactions.

## Unit 3

10 hours

**Photochemistry:** Franck-Condon principle, Jablonski diagram, Singlet and triplet states, Photosensitization, Quantum efficiency, Photochemistry of carbonyl compounds, Norrish type-I and type-II cleavages, Paterno-Buchi reaction, Photoreduction, Di  $\pi$  - methane rearrangement. Photochemistry of aromatic compounds, Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction Singlet molecular oxygen reactions

- Learner will be engaged in web based learning to explain photochemical reactions

## Unit 4

12 hours

**Pericyclic Chemistry:** Main features of pericyclic reactions, Classification of pericyclic reactions, Thermal and photochemical pericyclic reactions.

Electrocyclic reactions: Conrotation and disrotation, Electrocyclic closure and opening in  $4n$  and  $4n+2$  systems. Woodward-Hoffmann selection rules for electrocyclic reactions. Explanation for the mechanism of electrocyclic reactions by (i) symmetry properties of HOMO of open chain partner (ii) Conservation of orbital symmetry and orbital symmetry correlation diagrams and (iii) Huckel-Mobius aromatic and antiaromatic transition state method. Examples of electrocyclic reactions.

Cycloaddition reactions: Suprafacial and antarafacial interactions.  $\pi^2 + \pi^2$  and  $\pi^4 + \pi^2$  cycloadditions. Cycloreversions. Stereochemical aspects in supra-supra, supra-antara, antara-supra and antara-antara  $\pi^2 + \pi^2$  and  $\pi^4 + \pi^2$  cycloadditions. Diels-Alder reaction. Woodward-Hoffmann Selection rules for cycloaddition reactions. Sigmatropic reactions: [1,j] and [i,j] shifts; Suprafacial and antarafacial shifts; Selection rules for [l,j] shifts; Cope and Claisen rearrangements

- Learner will be engaged in web based learning to explain cycloaddition, electrocyclic and sigmatropic reactions

### Suggested Readings

1. Morrin Acheson, R. (2008) *An Introduction to the Chemistry of heterocyclic compounds*. Wiley India Pvt. Ltd.
2. Clayden, J., Greeves, N., Warren, S., Wothers, P. (2012). *Organic Chemistry*. Oxford press.
3. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., India.
4. Bansal, R. K., (2012). *Organic Reaction Mechanism*, New Age International (P) Ltd., New Delhi.
5. Bansal, R. K., (2007). *A Text Book of Organic Chemistry*, New Age International (P) Ltd., New Delhi.
6. Bansal, R.K. (2010). *Heterocyclic Chemistry*, New Age International (P) Ltd., New Delhi.
7. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B*, Springer.
8. Finar, I. L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, UK.
9. Gilchrist, T.L. (1997). *Heterocyclic Chemistry*, Longman, Prentice Hall, US.
10. Gupta R.R., Kumar M., Gupta V. (2010). *Heterocyclic Chemistry-II Five Membered Heterocycles*, Springer Verlag, India.
11. Joule, J.A., Mills, K. (2010). *Heterocyclic Chemistry*, Blackwell Publishers, New York.
12. Kalsi P. S., (2010). *Organic Reactions and Their Mechanisms*, New Age International Publication, New Delhi.
13. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc, US.
14. Morrison, R.T., Boyd R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
15. Mukherjee S. M., Singh S. P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
16. R. Katritzky, (2010). *Handbook of Heterocyclic Chemistry* Elsevier, UK.

17. Smith, M. B. (2013). *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*. John Wiley & Sons.
18. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, US.
19. Norman, R.O.C.; Coxon, J.M. *Principles of Organic Synthesis*, Blackie Academic & Professional.
20. Warren, S., (2010). *Organic Synthesis: The Synthons Approach*. John Wiley & Sons, New York,
21. Warren, S., (2010). *Designing Organic Synthesis: A Disconnection Approach*. John Wiley & Sons, New York.
22. Corey E.J., Cheng Xue-Min, (1989) *The Logic of Chemical Synthesis*, Pubs: John Wiley & Sons,
23. Carey, F. A., Giuliano, R. M. (2012). *Organic Chemistry*. McGraw Hill.
24. Kofie, W., Caddick, S. (2016). *Problems in Advanced Organic Chemistry*. Auris Publishing.
25. Solomons, T. W. G., Fryhle, C. B., Snyder, S. A. (2017). *Solomons' Organic Chemistry*. John Wiley & Sons.
26. Fleming (1999). *Pericyclic Reactions*, Oxford University Press, Oxford.

**The following are some of the modes of classroom transaction**

- Lecture
- Group discussion
- Demonstration
- Team teaching

**Transaction Mode**

- PPT
- Google meet
- YouTube

**Course Title: Organic Synthesis-II (Practical)**

**Paper Code: CMC.522**

**Course Hours: 60h**

L	T	P	Credits
0	0	4	2

### Learning Outcomes

After completing this course, the learner will be able to:

- Differentiate mixture of *ortho* and *para* as well as cis/trans mixture by column chromatography
- Describe Multi-Step Synthesis of Organic Compounds
- Identify compounds *via* combined spectral interpretation of  $^1\text{H}$ ,  $^{13}\text{C}$  NMR, IR, UV and Mass along with 2-D NMR spectra.

### Course content

1. Separation and purification of organic compounds by column chromatography: Separation of mixture of *ortho* and *para* mixture and cis/trans mixture. The column chromatography should be monitored by TLC.

2. **Multi-Step Synthesis of Organic Compounds:** The exercise should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques. (Any five)

- a) Synthesis of isoxazole derivatives via 1,3-dipolar cycloaddition.
- b) Synthesis of pyrazole derivatives from chalcones.
- c) Synthesis of an antihypertensive drug-propranolol via epoxide ring opening reaction.
- d) Synthesis of Diltiazem (a calcium channel blocker) via Darzen condensation, a key step in its synthesis.
- e) Protection and deprotection of alcohols and amines.
- f) Preparation of Triphenyl Carbinol from Bromobenzene (Grignard's reaction)

- g) Preparation of allylic alcohols via Baylis-Hillman reaction using DABCO as a catalyst under neat condition and their characterization through various spectroscopic techniques.
- h) Preparation of homoallyl alcohols via Barbier type reaction under aqueous condition using Indium as a catalyst.
- i) Suzuki reaction of 3,4-dimethoxy phenyl boronic acid with aryl halides using Pd(PPh<sub>3</sub>)<sub>4</sub> as a catalyst.
3. Exercises on identification of compounds *via* combined spectral interpretation of <sup>1</sup>H, <sup>13</sup>C NMR, IR, UV and Mass along with 2-D NMR spectra.

### **Suggested Readings**

1. Adams, R.; Johnson, J.R.; Wilcox, C.F. (1970). *Laboratory Experiments in Organic Chemistry*, The Macmillan Limited, London.
2. Mann and Saunders. (2009). *Practical organic chemistry*, Pearson.
3. Pasto, D.P., Johnson, C., Miller, M. (2010). *Experiments and Techniques in Organic Chemistry*, Prentice Hall.
4. Roberts, R.M.; Gilbert, J.C.; Rodewald, L.B.; Wingrove, A.S. (1969). *An introduction to Modern Experimental Organic Chemistry*, Ranehart and Winston Inc., New York.
5. Vogel, A.I. (Latest edition). *Text book of practical organic chemistry*, Pearson
6. Williamson, K.L., Heath, D.C. (1999). *Macroscale and Microscale Organic Experiments*, Heath, D. Cand Co., Lexington, MA.
7. Findeisen, M., (2013). *50 And More Essential NMR Experiments: A Detailed Guide*. John Willey & Sons.

### **The following are some of the modes of classroom transaction**

- Experimentation
- Group discussion
- Demonstration
- Self-learning

### **Transaction Mode**

- PPT
- YouTube
- Google drive
- Google meet

**Course Title: Fundamentals of Computer Aided Drug Design**

**Paper Code: CMC.523**

**Course Hours: 45h**

L	T	P	Credits
3	0	0	3

**Learning outcome:**

After completing this course, the learner will be able to:

- Describe the role of CADD in drug discovery
- Design and develop new drug like molecules
- Work with molecular modelling software's to design new drug molecules

**Unit 1**

**12 hours**

**Introduction to Computer Aided Drug Design (CADD):** History, different techniques and applications. Quantitative Structure Activity Relationships: Basics. History and development of QSAR: Physiochemical parameters and methods to calculate physiochemical parameters: Hammett equation and electronic parameters ( $\sigma$ ), lipophilicity effects and parameters ( $\log P$ ,  $\pi$ -substituent constant), steric effects (Taft steric and MR parameters) Experimental and theoretical approaches for the determination of these physiochemical parameters. Hansch analysis, Free Wilson analysis and relationship between them, Advantages and disadvantages: Deriving 2D-QSAR equations. 3D- QSAR approaches and contour map analysis. Statistical methods used in QSAR analysis and importance of statistical parameters.

- Learner will be engaged in group discussion to explain 2D-QSAR, 3D-QSAR and importance of statistical parameters

**Unit 2**

**11 hours**

**Molecular Modeling and Docking:**

- a) Molecular and Quantum Mechanics in drug design.
- b) Energy Minimization Methods: comparison between global minimum conformation and bioactive conformation.
- c) Molecular docking and drug receptor interactions: rigid docking, flexible docking and extra-precision docking. Agents acting on enzymes such as DHFR, HMG-CoA reductase and HIV protease, choline esterase (AChE & BchE)
  - Learner will be engaged in molecular modeling of compounds

### Unit 3

10 hours

#### Molecular Properties and Drug Design:

- a) Prediction and analysis of ADMET properties of new molecules and its importance in drug design.
- b) De novo drug design: Receptor/enzyme-interaction and its analysis, Receptor/enzyme cavity size prediction, predicting the functional components of cavities, Fragment based drug design.
- c) Homology modelling and generation of 3D-structure of protein.
  - Learner will study Molecular model to explain interactions between ligand and drug target

### Unit 4

12 hours

**Pharmacophore Mapping and Virtual Screening:** Concept of pharmacophore, pharmacophore mapping, identification of Pharmacophore features and Pharmacophores modelling; Conformational search used in pharmacophore mapping. In-silico Drug Design and Virtual Screening Techniques. Similarity based methods and Pharmacophore based screening, structure based In-silico virtual screening protocols.

- Learner will be engaged in Pharmacophore band structure based *In-silico* virtual screening protocols

#### Suggested Readings

1. Ellis, G.P., West, G. B. (1983). *Progress in Medicinal Chemistry Series*. Elsevier Science.
2. Foye, W.O., Lemke, T. L., Williams, D. A. (2019). *Principles of Medicinal Chemistry*, Indian Ed. Waverly, Pvt. Ltd. New Delhi.
3. Ganellin, C.R.; Roberts S. M., (1993). *Medicinal Chemistry: The Role of Organic Chemistry in Drug Research*. Publisher: Academics Press Inc.
4. Kadam, Mahadik, Bothara (2010). *Principle of Medicinal Chemistry (Volume I & II)*, Nirali publication

5. Kulkarni, V. M., Bothra, K.G., (2008). *Drug Design*, Nirali Publication.
6. Lawton, G., Witty, D.R. (2011). *Progress in Medicinal Chemistry Series. Volume 50*.
7. Lednicer D., Laster A. M. (1998). *The Organic Chemistry of Drug Synthesis(3 Volumes)* John Wiley & Sons.
8. Lednicer, D. (2008). *Strategies for Organic Drug Synthesis and Design. (7 volume)* Publisher: John Wiley & Sons.
9. Lemke, T.L., Williams, D.A. (2012). *Foye's Principles of Medicinal Chemistry*.
10. Silverman R.B., (2014). *Organic Chemistry of Drug Design and Drug Action*, Publisher: Elsevier.
11. Wilson, C.O.; Block, J.H.; Gisvold, O.; Beale, J. M. Wilson and Gisvold's (2003) *Textbook of Organic Medicinal and Pharmaceutical Chemistry*. Lippincott Williams & Wikins.
12. Gore, M., & Jagtap, U. (2018). *Computational Drug Discovery and Design*. Springer Publishers.

**The following are some of the modes of classroom transaction**

- Lecture
- Group discussion
- Demonstration
- Team teaching
- Tutorial
- Self-learning

**Transaction Mode**

- PPT
- YouTube
- Molecular modeling software
- Google drive
- Google meet



**Course Title: *In silico* Drug Design - Practical**

L	T	P	Credits
0	0	4	2

**Paper Code: CMC.524**

**Course Hours: 60h**

**Learning outcome:**

After completing this course, the learner will be able to:

- Determine log P, MR, hydrogen bond donors and acceptors of selected drugs using softwares
- Calculate ADMET properties of drug molecules and its analysis using software's
- Describe Pharmacophore modeling
- Perform 2D and 3D-QSAR based experiments
- Perform virtual screening and Homology Modelling based experiments

**Course content:**

Following practicals utilizing the available softwares such as ChemBio Draw, Autodock, Schrodinger, or any other online freeware, etc. need to be conducted.

- 1) Determination of log P, MR, hydrogen bond donors and acceptors of selected drugs using softwares
- 2) Calculation of ADMET properties of drug molecules and its analysis using softwares
- 3) Pharmacophore modeling
- 4) 2D-QSAR based experiments
- 5) 3D-QSAR based experiments
- 6) Docking study based experiment
- 7) Virtual screening based experiment
- 8) Homology Modelling based experiments.
- 9) Practical based on 2D and 3D-QSAR of drug molecules.
- 10) Docking and virtual screening based experiments.



## **Suggested Readings**

1. León, D.; MarkellIn S. (2006). *In silico Technologies in Drug Target Identification and Validation*. by Taylor and Francis Group, LLC.
2. Kubiny, H. *QSAR: Hansch Analysis and Related Approaches. Methods and Principles in Medicinal Chemistry*. Publisher Wiley-VCH
3. Gubernator, K.; Böhm, H. *Structure-Based Ligand Design. Methods and Principles in Medicinal Chemistry*. Publisher Wiley-VCH
4. Parrill, A. H.; Reddy, M R. *Rational Drug Design. Novel Methodology and Practical Applications*.
5. Turner J. R. *New Drug Development Design, Methodology and Analysis*. John Wiley & Sons, Inc., New Jersey.
6. Gore, M., & Jagtap, U. (2018). *Computational Drug Discovery and Design*. Springer Publishers.

## **The following are some of the modes of classroom transaction**

- Experimentation
- Demonstration
- Focused group discussion
- Problem solving

## **Transaction Mode**

- PPT
- Google drive
- Three-dimensional models
- YouTube
- Google meet

**Course Title: Advanced Spectral Analysis**

**Paper Code: CMC.525**

**Course Hours: 45h**

L	T	P	Credits
3	0	0	3

**Learning outcome:**

After completing this course, the learner will be able to:

- Describe hyphenated analytical instrumental techniques for identification, characterization and quantification of drugs. Instruments dealt are LC-MS, GC-MS, ATR-IR, DSC etc.
- Interpret NMR, Mass and IR spectra of various organic compounds

**Unit 1**

**12 hours**

**UV and IR spectroscopy:** Woodward – Fieser rule for 1,3-butadienes, cyclic dienes and carbonyl compounds and interpretation of enones.

**ATR-IR,** IR Interpretation of organic compounds, NIR Applications.

**Raman Spectroscopy:** Introduction, Principle, Instrumentation and Applications.

- Learner will calculate  $\lambda_{\max}$  for conjugated diene and enone derivatives

**Unit 2**

**12 hours**

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

**Thermal methods of analysis:** Introduction, principle, instrumentation and application of DSC, DTA and TGA.

- Learner will be provided spectra for the identification of compounds

**Unit 3**

**11 hours**

**Mass Spectroscopy:** Mass fragmentation and its rules, Fragmentation of important functional groups like alcohols, amines, carbonyl groups and alkanes, Meta stable ions, McLafferty rearrangement, Ring rule, Isotopic peaks, Interpretation of organic compounds.

- Learner will apply Mass fragmentation rules for identification of compounds containing functional group

**Unit 4**

**10 hours**

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

- Learner will be engaged in Learning experience of chromatography by

using different techniques like TLC, Column, HPLC, HPTLC and GC

### **Suggested Readings:**

1. Silverstein, R. M., Webster, F. X., Kiemle, D. J., & Bryce, D. L. (2014). *Spectrometric Identification of Organic Compounds*. John Wiley & Sons.
2. Skoog, D. A., Holler, F. J., & Crouch, S. R. (2017). *Principles of Instrumental Analysis*. Cengage Learning.
3. Willard, H. H., Merritt Jr, L. L., Dean, J. A., & Settle Jr, F. A. (1988). *Instrumental Methods and Analysis*.
4. Kemp, W. (1991). *Organic Spectroscopy* (pp. 42-51). London: Macmillan.
5. Sethi, P. D. (1996). *HPTLC: High Performance Thin-layer Chromatography; Quantitative Analysis of Pharmaceutical Formulations*. CBS Publishers & Distributors.
6. Sethi, P. D. (1985). *Quantitative Analysis of Drugs in Pharmaceutical Formulations*. CBS Publishers, New Delhi, 1997.
7. Munson, J. W. (Ed.). (1984). *Pharmaceutical Analysis: Modern Methods* (Vol. 11). CRC Press.
8. Findeisen, M., (2013). *50 And More Essential Nmr Experiments: A Detailed Guide*. John Wiley & Sons.
9. Kromidas, S. (2017). *The Hplc Expert Possibilities and Limitations of Modern High Performance Liquid Chromatography*. John Wiley and Sons

### **The following are some of the modes of classroom transaction**

- Lecture
- Group discussion
- Demonstration
- Problem solving

### **Transaction Mode**

- PPT
- YouTube
- Google meet

**Course Title: Medicinal Chemistry-II**

**Paper Code: CMC.526**

**Course Hours: 45h**

L	T	P	Credits
3	0	0	3

**Learning outcome:**

After completing this course, the learner will be able to:

- Interpret basics concepts of drugs, their effects and screening.
- Describe drugs interaction with various types of enzymes and receptors
- Conceptualize the mechanism of action and SAR studies of drug molecules.

**Unit 1**

**12 hours**

Physicochemical and stereochemical aspects: In relation to biological activity, Drug receptor interaction, Adrenergic hormones and Drugs including biosynthesis, storage, release and metabolism of catecholamines (Andrenaline, Isoprenaline, Salbutamol, Amphetamine, Naphazoline), Cholinergics and Anticholinesterases including biosynthesis, storage and metabolism of acetylcholine (Methacholine Chloride, Neostigmine Bromide), Antispasmodic and Antiulcer Drugs (Cyclopentolate, Propantheline Bromide, Benzhexol), Antiparkinsonism Drugs (Apomorphine).

- Learner will be engaged in Web based learning to study Physicochemical and Stereochemical aspect of drugs

**Unit 2**

**12 hours**

Neuromuscular blocking agents: Gallamine Triethiodide, Succinylcholine chloride, Hypoglycaemic drugs (Tolbutamide), Thyroid hormones and Antithyroid drugs (L-Thyroxine, Propylthiouracil) Pancuronium, vecuronium, rocuronium, rapacuronium, dacturionium, malouëtine, duador, dipyrandium, pipecuronium, chandonium. Anticoagulants and haemostatic agents: Warfarin, Phenindione, Oxytocics (includes discussion on Ergot alkaloids) (Ergometrine). Antihistamines including discussion on Sodium cromoglycate (Mepyramine, Diphenhydramine, Chlorpheniramine, Promethazine). Non-steroidal anti-inflammatory drugs and anti-gout drugs: Indomethacin, Phenylbutazone, Allopurinol, Probenecid.

- Learner will be engaged in Molecular modeling study to understand neuromuscular blocking reagent

**Unit 3**

**11 hours**

General Anaesthetic Agents: Introduction, medicinal aspects of anaesthetics, mode of action, gases and volatile liquid anaesthetics, intravenous anaesthetics or fixed anaesthetics, toxicity of general anaesthetics (Divinyl ether, Ethyl chloride, Cyclopropane, Thiopentone Sodium).

Local Anaesthetic Agents: Introduction, Structure-activity relationships, benzoic acid derivatives, aminobenzoic acid derivatives, lidocaine derivatives, miscellaneous,

toxicity, mode of action (Benzocaine, Procaine Hydrochloride, Lidocaine Hydrochloride).

- Learner will be engaged in web based study to understand aesthetic reagent

#### **Unit 4**

**10 hours**

Sedatives-Hypnotics: Introduction, classification of sedative-hypnotics, structure-activity relationships, barbiturates, amides and imides, alcohols and their carbamate derivatives, aldehydes and their derivatives, mode of action, pharmacological properties and side effects (Barbitone, Phenobarbitone, Cyclobarbitone, Pentobarbitone Sodium, Thiopentone Sodium), non-barbiturates (Official drugs).

Anticonvulsants: Introduction, epilepsy and its types, SAR, barbiturates (official products), hydantoins, Oxazolidinediones, Succinamides; miscellaneous drugs, (Phenytoin Sodium, Troxidone), Antipsychotic agents: introduction, SAR and drugs like chlorpromazine, prochlorperazine, *etc.*

- Learner will be engaged in group discussion to understand the structures of different sedatives and hypnotics and anticonvulsants.

#### **Suggested Readings**

1. Delgado, J. N. and Remers W A, Ed. (2010). *Wilson & Gisvold's Textbook of Organic and Pharmaceutical Chemistry*, J. Lippincott Co., Philadelphia.
2. Foye, W. C. (2019). *Principles of Medicinal Chemistry*, Publisher: Wolter Kluwer.
3. King, F. D. (2006). *Medicinal Chemistry Principles and Practice*, Royale Society of Chemistry, London.
4. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press, UK.
5. Patrick, G.L. (2017). *An Introduction to Medicinal Chemistry*, Oxford University PressUS.
6. Singh, H., Kapoor, V.K. (Latest Edition). *Medicinal and Pharmaceutical Chemistry* Vallabh Prakashan, Delhi.
7. Smith, H.J. (2006). *Introduction to the Principles of Drug Design and Action*, Taylor and Francis.
8. Wermuth, C.G. (2009). *The Practice of Medicinal Chemistry*, Academic Press (Elsevier).
9. Wolff, M E, Ed., (2010). *Burger's Medicinal Chemistry and Drug Discovery* John Wiley & Sons, New York.
10. Ferrant, E., (2011). *New Synthetic Technologies In Medicinal Chemistry*. Royal Chemical Society.

**The following are some of the modes of classroom transaction**

- Lecture
- Group discussion
- Demonstration
- Self-learning

**Transaction Mode**

- PPT
- YouTube
- Google drive
- Google meet



**Course Title: Process Chemistry**

**Paper Code: CMC.527**

**Course Hours: 45h**

L	T	P	Credits
3	0	0	3

**Learning outcome:**

After completing this course, the learner will be able to:

- The strategies of scale up process of APIs and intermediates
- The various unit operations and various reactions in process chemistry

**Unit 1**

**12 hours**

**Process chemistry**

Introduction, Synthetic strategy, Stages of scale up process: Bench, pilot and large scale process. In-process control and validation of large scale process. Case studies of some scale up process of APIs. Impurities in API, types and their sources including genotoxic impurities

- Learner will be provided training involving case studies on scale up of APIs.

**Unit 2**

**12 hours**

**Unit operations**

*Extraction:* Liquid equilibria, extraction with reflux, extraction with agitation, counter current extraction.

*Filtration:* Theory of filtration, pressure and vacuum filtration, centrifugal filtration,

*Distillation:* azeotropic and steam distillation

*Evaporation:* Types of evaporators, factors affecting evaporation.

*Crystallization:* Crystallization from aqueous, non- aqueous solutions factors affecting crystallization, nucleation. Principle and general methods of Preparation of polymorphs, hydrates, solvates and amorphous APIs.

- Learner will be engaged in group discussion to understand Extraction, filtration, distillation, evaporation and crystallization processes

**Unit 3**

**11 hours**

**Unit Processes - II**

**Reduction:** Catalytic hydrogenation, Heterogeneous and homogeneous catalyst; Hydrogen transfer reactions, Metal hydrides. Case study on industrial reduction process.

**Fermentation:** Aerobic and anaerobic fermentation.

Production of

Antibiotics; Penicillin and Streptomycin,

Vitamins: B2 and B12

Statins: Lovastatin, Simvastatin

### **Reaction progress kinetic analysis**

Streamlining reaction steps, route selection, Characteristics of expedient routes, characteristics of cost-effective routes, reagent selection, families of reagents useful for scale-up.

- Learner will be engaged in group discussion to understand unit processes for reduction, fermentation and reaction progress kinetic analysis

### **Unit 4**

**10 hours**

### **Industrial Safety**

MSDS (Material Safety Data Sheet), hazard labels of chemicals and Personal Protection Equipment (PPE)

Fire hazards, types of fire & fire extinguishers

Occupational Health & Safety Assessment Series 1800 (OHSAS-1800) and ISO-14001 (Environmental Management System), Effluents and its management

- Learner will be provided Awareness about industrial safety protocols

### **Suggested Readings**

1. Process Chemistry in the Pharmaceutical Industry: Challenges in an Ever- Changing Climate-An Overview; K. Gadamasetti, CRC Press.
2. Pharmaceutical Manufacturing Encyclopedia, 3<sup>rd</sup> edition, Volume 2.
3. Medicinal Chemistry by Burger, 6<sup>th</sup> edition, Volume 1-8.
4. W.L. McCabe, J.C Smith, Peter Harriott. Unit operations of chemical engineering, 7th edition, McGraw Hill
5. Polymorphism in Pharmaceutical Solids. Dekker Series Volume 95 Ed: H G Brittain (1999)
6. Regina M. Murphy: Introduction to Chemical Processes: Principles, Analysis, Synthesis
7. Peter J. Harrington: Pharmaceutical Process Chemistry for Synthesis: Rethinking the Routes to Scale-Up
8. P.H.Groggins: Unit processes in organic synthesis (MGH)
9. F.A.Henglein: Chemical Technology (Pergamon)
10. M.Gopal: Dryden's Outlines of Chemical Technology, WEP East-West Press
11. Clausen, Mattson: Principle of Industrial Chemistry, Wiley Publishing Co.,
12. Lowenheim & M.K. Moran: Industrial Chemicals
13. S.D. Shukla & G.N. Pandey: A text book of Chemical Technology Vol. II, Vikas Publishing House
14. J.K. Stille: Industrial Organic Chemistry (PH)
15. Shreve: Chemical Process, Mc Grawhill.
16. B.K.Sharma: Industrial Chemistry, Goel Publishing House
17. ICH Guidelines

18. United States Food and Drug Administration official website [www.fda.gov](http://www.fda.gov)  
**The following are some of the modes of classroom transaction**

- Lecture
- Group discussion
- Demonstration
- Team teaching

**Transaction Mode**

- PPT
- YouTube
- Google drive
- Google meet

**Course Title: Modern analytical techniques**

**Paper Code: CMC.528**

**Course Hours: 45h**

L	T	P	Credits
3	0	0	3

### Learning Outcomes

After completing this course, the learner will be able to:

- Conceptualize general principle and theory of spectroscopy
- Describe the concept and instrumentation of UV-Vis, IR, NMR, Mass and Chromatographic techniques
- Solve the spectra of compounds
- Separate different constituents of mixture by chromatographic techniques

#### Unit 1

**12 hours**

**UV-Visible spectroscopy:** Introduction, Theory, Laws, Instrumentation associated with UV-Visible spectroscopy, Choice of solvents and solvent effect and Applications of UV-Visible spectroscopy, Difference/ Derivative spectroscopy.

**IR spectroscopy:** Theory, Modes of Molecular vibrations, Sample handling, Instrumentation of Dispersive and Fourier – Transform IR Spectrometer, Factors affecting vibrational frequencies and Applications of IR spectroscopy, Data Interpretation, Theory of NIR.

- Learner will be provided Hands on training to different instruments like UV Spectrophotometer, IR and spectrofluorimetry

#### Unit 2

**12 hours**

**NMR spectroscopy:** Quantum numbers and their role in NMR, Principle, Instrumentation, Solvent requirement in NMR, Relaxation process, NMR signals in various compounds, Chemical shift, Factor influencing chemical shift, Spin-Spin coupling, Coupling constant, Nuclear magnetic double resonance, Brief outline of principles of FT-NMR and <sup>13</sup>C NMR. Applications of NMR spectroscopy.

- Learner will be provided NMR spectra's for the characterization of compounds

#### Unit 3

**11 hours**

**Mass Spectroscopy:** Principle, Theory, Instrumentation of Mass Spectroscopy, Different types of ionization like electron impact, chemical, field, FAB and MALDI, APCI, ESI, APPI Analyzers of Quadrupole and Time of Flight, Mass fragmentation and its rules, Meta stable ions, Isotopic peaks and Applications of Mass spectroscopy.

- Learner will be provided mass spectra's for the characterization of compounds

#### **Unit 4**

**10 hours**

**Chromatography:** Principle, apparatus, instrumentation, chromatographic parameters, factors affecting resolution, isolation of drug from excipients, data interpretation and applications of the following: Thin Layer chromatography, High Performance Thin Layer Chromatography, Ion exchange chromatography, Column chromatography, Gas chromatography, High Performance Liquid chromatography, Ultra High Performance Liquid chromatography, Affinity chromatography, Gel Chromatography

- Learner will be provided experience of chromatography by using different techniques like TLC, Column, HPLC, HPTLC and GC

#### **Suggested Readings**

1. Silverstein, R. M., Webster, F. X., Kiemle, D. J., & Bryce, D. L. (2014). *Spectrometric Identification of Organic Compounds*. John Wiley & Sons.
2. Skoog, D. A., Holler, F. J., & Crouch, S. R. (2018). *Principles of Instrumental Analysis*. Singapore: Cengage Learning Asia Pte Ltd.
3. Willard, H. H. (2012). *Instrumental methods of analysis*. New Delhi: CBS.
4. Beckett, A. H., & Stenlake, J. B. (Eds.). (1988). *Practical Pharmaceutical Chemistry: Part II*, A&C Black..
5. Kemp, W. (1991). *Organic Spectroscopy* (pp. 42-51). London: Macmillan.
6. Sethi, P. D. (1985). *Quantitative Analysis of Drugs in Pharmaceutical Formulations*. Unique Publishers.
7. Munson, J. W. (Ed.). (1984). *Pharmaceutical Analysis: Modern Methods* (Vol. 11). CRC Press.
8. Kalsi, P. S. (2007). *Spectroscopy of Organic Compounds*. New Age International.
9. Connors, K. A. (2007). *A Textbook of Pharmaceutical Analysis*. John Wiley & Sons.
10. McHale, J. L. (2017). *Molecular Spectroscopy*. CRC Press.
11. Kromidas, S. (2017). *The HPLC Expert Possibilities and Limitations of Modern High Performance Liquid Chromatography*. John Wiley and Sons.

#### **The following are some of the modes of classroom transaction**

- Lecture
- Group discussion
- Demonstration
- Team teaching
- Self-learning

#### **Transaction Mode**

- PPT
- YouTube
- Google meet

### **Elective Course**

**Course Title: Green Chemistry**

**Paper Code: CMC.529**

**Course Hours: 45h**

L	T	P	Credits
3	0	0	3

### **Learning outcome**

After completing this course, the learner will be able to:

- Describe various aspects of green chemistry for sustainable development
- Utilize ionic liquids and solid supported reaction conditions to reduce or eliminate use of volatile organic solvents
- Utilize MW and sonicator in organic synthesis

### **Unit 1**

**12 hours**

**Introduction to green chemistry:** History, need and goals. Green chemistry and sustainability, dimensions of sustainability, limitations/obstacles in pursuit of the goals of green chemistry. Opportunities for the next generation of materials designers to create a safer future. Basic principles of green chemistry: Atom economy and scope, Prevention/Minimization of hazardous/toxic products, designing safer chemicals, Selection of appropriate auxiliary substances (solvents, separation agents etc), use of renewable starting materials, Avoidance of unnecessary derivatization-careful use of blocking/protection groups. Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents, designing biodegradable products,

- Learner will be engaged in Group discussion to explain Green Chemistry Principles

### **Unit 2**

**11 hours**

Prevention of chemical accidents, Strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes. Development of accurate and reliable sensors and monitors for real time in process monitoring.

- Learner will be provided web based learning for prevention of chemical accident and minimization of hazardous products

### **Unit 3**

**12 hours**

**Approaches to green synthesis:** Basic principles of green synthesis. Different approaches to green synthesis, Use of green reagents in green synthesis: polymer supported reagents, polymer supported peptide coupling reagents. Green catalysts,

Phase-transfer catalysts in green synthesis. Advantages of PTC, Reactions to green synthesis, Application of PTCs in C-alkylation, N-alkylation, S-alkylation. Darzens reaction, Williamsons synthesis, Wittig reaction, Click Chemistry. Use of Crown ethers in esterification, saponification, anhydride formation, aromatic substitution and elimination reactions. Water and ionic liquids as green solvents.

- Learner will be engaged in Group discussion to explain the use of PTC and crown ethers

#### **Unit 4**

**10 hours**

**Microwave induced and ultrasound assisted green synthesis:** Introduction to synthetic organic transformation under microwave (i) Microwave assisted reactions in water (ii) Microwave assisted reactions in organic solvents. (iii) Microwave solvent free reactions Ultrasound assisted reactions: Introduction, substitution reactions, addition, oxidation, reduction reactions. Biocatalysts in organic synthesis: Introduction, Biochemical oxidation and reductions.

- Learner will be engaged in Web based learning to Perform Microwave induced and ultrasound assisted reactions

#### **Suggested Readings:**

1. Ahluwalia, V.K.; Kidwai M. (2004). *New Trends in Green Chemistry*, Springer
2. Anastas, P.T.; Warner J. C. (2000). *Green Chemistry, Theory and Practical*. Oxford University Press.
3. Grieco, P.A. (1997). *Organic Synthesis in Water*. Publisher: Kluwer Academic.
4. Matlack, A. (2010). *Introduction to green chemistry*. CRC Press.
5. Ahluwalia, V. K. (2011). *Green Chemistry: Greener Alternatives to Synthetic Organic Transformations*. Alpha Science International.
6. Torok, B.; Dransfield, T. (2018). *Green Chemistry: An Inclusive Approach*, Elsevier

#### **The following are some of the modes of classroom transaction**

- Lecture
- Group discussion
- Demonstration
- Self-learning

#### **Transaction Mode**

- PPT
- YouTube
- Google drive

- Google meet

**Course Title: Nuclear Chemistry**

L	T	P	Credits
3	0	0	3

**Paper Code: CMC.530**

**Course Hours: 45h**

**Learning outcome:**

After completing this course, the learner will be able to

- Explain the nuclear structure and its stability
- Describe nuclear reactions and different fission model

**Unit 1 10 hours**

**Nuclear Structure and Stability**

Binding energy, empirical mass equation, nuclear models, the liquid drop model, the shell model, the Fermi gas model & collective nuclear model, nuclear spin, parity & magnetic moments of odd mass numbers nuclei.

- Learner will be provided models to explain structure and stability of nucleus

**Unit 2 12 hours**

**Nuclear reaction**

Introduction, Production of projectiles, nuclear cross section, nuclear dynamics, threshold energy of nuclear reaction, Coulomb scattering, potential barrier, potential well, formation of a compound nucleus, Nuclear reactions, direct Nuclear reactions, heavy ion induced nuclear reactions, photonuclear reactions.

**Nuclear fission**

Liquid drop model of fission, fission barrier and threshold, fission cross section, mass energy and charge distribution of fission products, symmetric and Asymmetric fission, decay chains and delayed neutrons.

- Learner will be provided Web based learning to understand nuclear fission reactions

**Unit 3 12 hours**

**Reactor Theory**

Nuclear fission as a source of energy, Nuclear chain reacting systems, critical size of a reaction, research reactors, graphite moderated, heterogeneous, enriched uranium reactors, light water moderated, heterogeneous, enriched uranium reactors, water boilers enriched aq. Homogeneous reactors, Thermonuclear reactors, gamma interactions, shielding and health protection. Reactors in India.

**Nuclear Resources in India**

Uranium and Thorium resources in India and their extractions, Heavy water manufacturing in India.



- Learner will be engaged in group discussion to understand reactor theory and natural resources in India

#### **Unit 4**

**11 hours**

#### **Elements of Radiation Chemistry**

Radiation Chemistry, Interaction of radiation with matter, Passage of neutrons through matter, Interaction of gamma radiation with matter, Units for measuring radiation absorption, Radiolysis of water, Free radicals in water radiolysis, Radiolysis of some aqueous solutions

- Learner will be provided Web based learning to understand radiation chemistry and interaction of gamma radiation

#### **Suggested readings:**

1. Friedlander, G., Kennedy, J. W., & Macias, E. S. (1981). *Nuclear and radiochemistry*. John Wiley & Sons.
2. Harvey, B. G. (1962). *Introduction to Nuclear Physics and Chemistry*. Soil Science, 94(4), 274.
3. Haissinsky, M. (1964). *Nuclear chemistry and its applications*. Addison-Wesley Pub. Co.
5. Choppin, G. R., Liljenzin, J. O., & Rydberg, J. (2002). *Radiochemistry and Nuclear Chemistry*. Butterworth-Heinemann.
6. Friedlander, G., Kennedy, J. W., & Macias, E. S. (1981). *Nuclear and Radiochemistry*. John Wiley & Sons.
7. Kanne, W. R. (1961). *Basic Principles of Nuclear Science and Reactors*. Journal of the American Chemical Society, 83(2), 508-508.
8. Darmstadter, J., Landsberg, H. H., & Morton, H. C. (1983). *Energy, today and tomorrow: living with uncertainty*. Prentice Hall.
9. Kenneth: Nuclear Power Today, Tomorrow: ELBS
10. Arnikar, H. J. (1995). *Essentials of nuclear chemistry* (No. 1653). New Age International.
11. Cottingham, W. N., Greenwood, D. A., & Greenwood, D. A. (2001). *An Introduction to Nuclear Physics*. Cambridge University Press.

#### **The following are some of the modes of classroom transaction**

- Lecture
- Demonstration
- Tutorial
- Self-learning

#### **Transaction Mode**

- PPT
- YouTube
- Google meet

## Semester -III

**Course Title: Research Methodology & Biostatistics**

L	T	P	Credits
3	0	0	3

**Paper Code: CMC.551**

**Course Hours: 45h**

### Learning Outcomes:

After completing this course, the learner will be able to:

- Define an appropriate research problem
- Describe the objectives based on literature search.
- Prepare poster and dissertation work
- To apply biostatistics in research problem

### Unit 1

**12 hours**

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

- Learner will be engaged in literature search and study design

### Unit 2

**11 hours**

**Technical writing:** Scientific writing, Writing research paper, Poster preparation and Presentation and Dissertation.

- Learner will be engaged in scientific writing, poster presentation and dissertation

### Unit 3

**10 hours**

**Library:** Classification systems, e-Library, Reference management, Web-based literature search-engines

- Learner will be engaged in web based literature search engine

### Unit 4

**12 hours**

**Biostatistics:** Definition, application, sample size, importance of sample size, factors influencing sample size, dropouts, statistical tests of significance, type of significance tests, parametric tests (students "t" test, ANOVA, Correlation coefficient, regression), non-parametric tests (wilcoxon rank tests, analysis of variance, correlation, chi square test), null hypothesis, P values, degree of freedom, interpretation of P values.

- Learner will be engaged in Web based learning to explain concepts of biostatistics in research problem

**Suggested Readings:**

1. Gupta, S. (2005). *Research methodology and statistical techniques*, Deep & Deep Publications (p) Ltd. New Delhi.
2. Kothari, C. R. (2008.) *Research Methodology(s)*, New Age International (p) Limited. New Delhi
3. Best J. W., Khan J. V. (Latest Edition) *Research in Education*, Prentice Hall of India Pvt. Ltd.
4. *Safe Science: Promoting a Culture of Safety in Academic Chemical Research*; National Academic Press, www.nap.edu.
5. Creswell, D., & Creswell, J. W. (2017). *Research Design: Qualitative, Quantitative, and Mixed Methods Approaches*.

**The following are some of the modes of classroom transaction**

- Lecture
- Group discussion
- Demonstration

**Transaction Mode**

- PPT
- YouTube
- Google drive

**Course Title: Organic Chemistry-III****Paper Code: CMC.552****Course Hours: 45h**

L	T	P	Credits
3	0	0	3

**Learning outcome:**

After completing this course, the learner will be able to:

- Determine the mechanism and feasibility of a chemical reaction
- Describe the asymmetric synthesis, chiral resolution and apply it on the resolution of chiral drugs.
- Conceptualize various metal and non-metal reagents towards oxidation and reduction reactions

**Unit 1****11 hours**

**Reaction mechanism, structure and reactivity:** Types of mechanisms, types of reactions, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, Potential energy diagrams, Transition states and intermediates, Kinetics and non-kinetics method, Isotopes effects, Effect of structure on reactivity; Resonance, inductive, electrostatic and steric effect, quantitative treatment, the Hammett equation and linear free energy relationship, Substituent and reaction constants, Taft equation.

- Learner will be engaged in Group discussion to explain reaction mechanism

**Unit 2****10 hours**

**Asymmetric synthesis,** chiral pools, chiral catalysis: Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. Resolution – optical and kinetic, Chemo- regio- and stereoselective transformations, Organocatalysis

- Learner will be engaged in Molecular models to explain the stereochemistry in asymmetric reaction

**Unit 3****12 hours**

**Metal and non-metal mediated oxidation and reductions:** Mechanism, Selectivity, Stereochemistry and applications of oxidation reactions, Oppenauer, Baeyer-Villiger, Oxidation reactions using DDQ, NBS, leadtetraacetate, selenium dioxide, DCC, PCC, CAN, Cr and Mn reagents, periodic acid, Osmium tetroxide, Swern oxidations, Hydroboration, Dehydrogenation, Ozonolysis, Epoxidations using peracids. Mechanism, selectivity, stereochemistry and applications of catalytic

hydrogenations using Pd, Pt and Ni catalysts, Clemmensen reduction, Wolff-Kishner reduction, Meerwein-Ponndorf-Verley reduction, Dissolving metal reductions, metal hydride reductions using NaBH<sub>4</sub>, LiAlH<sub>4</sub>, DIBAL. Wilkinson's Rh catalysis, Boron in reduction

- Learner will be engaged in web mediated activity to explain different reagents in chemical synthesis

#### Unit 4

12 hours

**Reaction of ylides:** Phosphorus ylide; Structure and reactivity, stabilized ylides, effects of ligands on reactivity, Wittig, Wittig-Horner and Wadsworth, Emmons reactions-mechanistic realization; E/Z selectivity for olefin formation, Schlosser modification: Peterson's olefin synthesis. Sulphur Ylides; Stabilized and non-stabilized ylides: Thermodynamically and kinetically controlled reactions with carbonyl compounds, regio- and stereo-selective reactions

- Learner will be engaged in Molecular models to explain the reaction of ylides and their E/Z selectivity

#### Suggested Readings

1. Acheson, R.M. (1976). *An Introduction to the Chemistry of Heterocyclic Compounds*, Wiley India Pvt. Ltd.
2. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., India.
3. Bansal, R. K., (2012). *Organic Reaction Mechanism*, New Age International (P) Ltd., New Delhi.
4. Bansal, R. K., (2007). *A Text Book of Organic Chemistry*, New Age International (P) Ltd., New Delhi.
5. Bansal, R.K. (2010). *Heterocyclic Chemistry*, New Age International (P) Ltd., New Delhi.
6. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B*, Springer.
7. Finar, I. L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, UK.
8. Gilchrist, T.L. (1997). *Heterocyclic Chemistry*, Longman, Prentice Hall, US.
9. Gupta R.R., Kumar M., Gupta V. (2010). *Heterocyclic Chemistry-II Five Membered Heterocycles Vol. 1-3*, Springer Verlag, India.
10. Joule, J.A., Mills, K. (2010). *Heterocyclic Chemistry*, Blackwell Publishers, New York.
11. Kalsi, P. S., (2008). *Stereochemistry: Conformation and Mechanism*, New Age International (P) Ltd., India.
12. Kalsi P. S., (2014). *Organic Reactions and Their Mechanisms*, New Age International Publication, New Delhi.

13. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., US.
14. Morrison, R.T., Boyd R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
15. Mukherjee S. M., Singh S. P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
16. R. Katritzky, (2010). *Handbook of Heterocyclic Chemistry* Elsevier, UK.
17. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
18. Kalsi, P. S., (2008). *Stereochemistry: Conformation and Mechanism*, New Age International (P) Ltd., India
19. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., US.
20. Morrison, R.T., Boyd R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
21. Mukherjee S. M., Singh S. P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
22. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
23. Carey, F. A., Giuliano, R. M. (2012). *Organic Chemistry*. McGraw Hill.
24. Kofie, W., Caddick, S. (2016). *Problems in Advanced Organic Chemistry*. Auris Publishing.
25. Solomons, T. W. G., Fryhle, C. B., Snyder, S. A. (2017). *Solomons' Organic Chemistry*. John Willey & Sons.

**The following are some of the modes of classroom transaction**

- Lecture
- Group discussion
- Demonstration
- Self-learning

**Transaction Mode**

- PPT
- YouTube
- Google meet

**Course Title: Organic Synthesis-III-(Practical)**

L	T	P	Credits
0	0	4	2

**Paper Code: CMC.553**

**Course Hours: 60h**

**Learning outcomes:** After completing this course, the learner will be able to

- Synthesize 5, 6, and 7 membered heterocyclics compounds and their characterization
- Describe Metal catalyzed reactions
- Interpret of UV, IR,  $^1\text{H}$  data and  $^{13}\text{C}$  NMR, IR, UV and Mass spectral data

**Course contents:**

1. Synthesis of 5, 6, and 7 membered heterocyclics using conventional heating or microwave heating
2. Experiments involving photochemical reactions
3. Experiments involving metal catalyzed reaction
4. Exercises of structure identifications of above synthesized compounds *via* spectral interpretation using UV data
5. Exercises of structure identifications of above synthesized compounds *via* spectral interpretation using IR data
6. Exercises of structure identifications of above synthesized compounds *via* spectral interpretation using  $^1\text{H}$  data
7. Exercises of structure identifications of above synthesized compounds *via* spectral interpretation using  $^1\text{H}$  data and  $^{13}\text{C}$  NMR
8. Exercises of structure identifications of above synthesized compounds *via* spectral interpretation using Mass
9. Exercises of structure identifications of above synthesized compounds *via* spectral interpretation using combined data of UV, IR,  $^1\text{H}$  data and  $^{13}\text{C}$  NMR, IR, UV and Mass.

**Suggested Readings:**

1. Adams, R., Johnson, J.R., Wilcox, C.F. (1970). *Laboratory Experiments in Organic Chemistry*, The Macmilan Limited, London.

2. Mann and Saunders. (2009). *Practical organic chemistry*, Pearson.
3. Pasto, D.P., Johnson, C., Miller, M. (2010). *Experiments and Techniques in Organic Chemistry*, Prentice Hall.
4. Roberts, R.M., Gilbert, J.C., Rodewald, L.B. Wingrove, A.S. (1969). *An introduction to Modern Experimental Organic Chemistry*, Ranehart and Winston Inc., New York.
5. Vogel, A.I. (latest edition). *Text Book of Practical Organic Chemistry*, Pearson
6. Williamson, K.L., Heath, D.C. (1999). *Macroscale and Microscale Organic Experiments*, Heath, D.C and Co., Lexington, MA.
7. Armarego, W. L., & Chai, C. (2012). *Purification of Laboratory Chemicals*. Butterworth-Heinemann.
8. Young, J. A. (Ed.). (Latest Edition). *Improving Safety in the Chemical Laboratory: a Practical Guide*. Wiley.
9. Kofie, W., Caddick, S. (2016). *Problems in Advanced Organic Chemistry*. Auris Publishing.
10. Solomons, T. W. G., Fryhle, C. B., Snyder, S. A. (2017). *Solomons' Organic Chemistry*. John Wiley & Sons.

**The following are some of the modes of classroom transaction**

- Experimentation
- Group discussion
- Demonstration
- Self-learning

**Transaction Mode**

- PPT
- YouTube
- Google drive
- Google meet



**Course Title: Entrepreneurship**

L	T	P	Credits
1	0	0	1

**Paper Code: CMC. 554**

**Course Hours: 15h**

**Learning Outcomes:** After completing this course, the learner will be able to:

- Understand the basic concepts of entrepreneur, entrepreneurship and its importance.
- Aware of the issues, challenges and opportunities in entrepreneurship.
- Develop capabilities of preparing proposals for starting small businesses.
- Know the availability of various institutional supports for making a new start-up.

**Unit 1**

**3 hours**

Introduction to entrepreneur and entrepreneurship; Characteristics of an entrepreneur; Characteristics of entrepreneurship; entrepreneurial traits and skills; innovation and entrepreneurship; Types of entrepreneurial ventures; enterprise and society in Indian context; Importance of women entrepreneurship

- Learner will be engaged in Group discussion to explain the concept of entrepreneurship

**Unit 2**

**4 hours**

Promotion of a venture – Why to start a small business; How to start a small business; opportunity analysis, external environmental analysis, legal requirements for establishing a new unit, raising of funds, and establishing the venture - Project report preparation – format for a preliminary project report, format for a detailed/final project report.

- Learner will interact with Entrepreneurs to understand how to start small business

**Unit 3**

**5 hours**

Launching and Organising An Enterprise: Environment scanning – Information, sources, schemes of assistance, problems. Enterprise selection, market assessment, enterprise feasibility study, SWOT Analysis. Resource mobilisation - finance,

technology, raw material, site and manpower. Costing and marketing management and quality control. Feedback, monitoring and evaluation.

- Learner will be engaged in Group discussion to explain about resource mobilization, costing and marketing management

#### **Unit 4**

**3 hours**

Preparing Project Proposal to Start On New Enterprise Project work – Feasibility report; Planning, resource mobilisation and implementation.

- Learner will be engaged to prepare project proposal to start new enterprise

#### **Suggested Readings:**

1. Arora, Renu (2008). *Entrepreneurship and Small Business*, Dhanpat Rai & Sons Publications.
2. Chandra, Prasaaan (2018). *Project Preparation, Appraisal, Implementation*, Tata Mc-Graw Hills.
3. Desai, Vasant (2019). *Management of a Small Scale Industry*, Himalaya Publishing House.
4. Jain, P. C. (2015). *Handbook of New Entrepreneurs*, Oxford University Press.
5. Srivastava, S. B. (2009). *A Practical Guide to Industrial Entrepreneurs*, Sultan Chand & Sons.
6. Akhauri, M.M.P.(1990): *Entrepreneurship for Women in India*, NIESBUD, New Delhi.
7. Hisrich, R.D & Brush, C.G.(1996) *The Women Entrepreneurs*, D.C. Health & Co., Toranto.
8. Hisrich, R.D. and Peters, M.P. (1995): *Entrepreneurship – Starting, Developing and Managing a New Enterprise*, Richard D., Inwin, INC, USA.
9. Meredith, G.G. etal (1982): *Practice of Entrepreneurship*, ILO, Geneva.
10. Patel, V.C. (1987): *Women Entrepreneurship – Developing New Entrepreneurs*, Ahmedabad EDII.

#### **The following are some of the modes of classroom transaction**

- Group discussion
- Lecture
- Demonstration
- Team teaching

#### **Transaction Mode**

- PPT
- YouTube
- Google drive
- Google meet

**Course Title: Organic Chemistry Worksheet**

L	T	P	Credits
2	0	0	2

**Course Code: CMC. 555**

**Course Hours: 30h**

**Learning outcome**

After completing this course, the learner will be able to:

- Conceptualize the mechanism of Pericyclic reactions
- Characterized structure of organic compounds
- Develop Analytical skills

**Unit 1**

**15 hours**

Pericyclic reactions – electrocycloisatation, cycloaddition, sigmatropic rearrangements and other related concerted reactions. Principles and applications of photochemical reactions in organic chemistry. Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatoms (O, N, S)

- Learner will be engaged in Web based learning to understand the concept of photochemical and thermal assisted reactions

**Unit 2**

**15 hours**

Chemistry of natural products: Carbohydrates, proteins and peptides, fatty acids, nucleic acids, terpenes, steroids and alkaloids. Biogenesis of terpenoids and alkaloids. Structure determination of organic compounds by IR, UV-Vis, <sup>1</sup>H & <sup>13</sup>C NMR and Mass spectroscopic techniques.

- Learner will be provided Spectra's of natural products to characterize the structure of compounds

**Suggested readings**

1. Clayden, J., Greeves, N., Warren, S., Wothers, P. (2012). *Organic Chemistry*. Oxford press.
2. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., India.

3. Bansal, R. K., (2012). *Organic Reaction Mechanism*, New Age International (P) Ltd., New Delhi.
4. Bansal, R. K., (2007). *A text book of Organic Chemistry*, New Age International (P) Ltd., New Delhi.
5. Bansal, R.K. (2010). *Heterocyclic Chemistry*, New Age International (P) Ltd., New Delhi.
6. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B*, Springer.
7. Finar, I. L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, UK.
8. Gilchrist, T.L. (1997). *Heterocyclic Chemistry*, Longman, Prentice Hall, US.
9. Gupta R.R., Kumar M., Gupta V. (2010). *Heterocyclic Chemistry-II Five Membered Heterocycles Vol. 1-3*, Springer Verlag, India.
10. Joule, J.A., Mills, K. (2010). *Heterocyclic Chemistry*, Blackwell Publishers, New York.
11. Kalsi P. S., (2010). *Organic Reactions and Their Mechanisms*, New Age International Publication, New Delhi.
12. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., US.
13. Morrison, R.T., Boyd R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
14. Mukherjee S. M., Singh S. P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
15. Sethi, P. D. (1985). *Quantitative Analysis of Drugs in Pharmaceutical Formulations*. Unique Publishers.
16. Munson, J. W. (1984). *Pharmaceutical analysis: modern methods. B. Drugs and the Pharmaceutical Sciences, 11*.
17. Kalsi, P. S. (2007). *Spectroscopy of Organic Compounds*. New Age International.
18. Connors, K. A. (2007). *A Textbook of Pharmaceutical Analysis*. John Wiley & Sons.

**The following are some of the modes of classroom transaction**

- Lecture
- Group discussion
- Demonstration
- Tutorial
- Self-learning

### Transaction Mode

- PPT
- YouTube
- Google drive
- Google meet

**Course Title: Computer Applications**

**Paper Code: CMC.556**

**Course Hours: 45h**

L	T	P	Credits
3	0	0	3

### Learning outcomes:

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

- Use different operating system and their tools easily.
- Use word processing software, presentation software, spreadsheet software and latex.
- Explain networking and internet concepts.
- Use computers in every field like teaching, industry and research.

### Unit 1

**10 hours**

**Computer Fundamentals:** Introduction to Computer, Input devices, Output Devices, Memory (Primary and Secondary), Concept of Hardware and Software, C.P.U., System bus, Motherboard, Ports and Interfaces, Expansion Cards, Ribbon Cables, Memory Chips, Processors, Software: Types of Software, Operating System, User Interface of popular Operating System, Introduction to programming language, Types of Computer.

- Learner will be engaged in group discussion to understand fundamentals and type of computer

### Unit 2

**11 hours**

**Computer Network:** Introduction to Computer Network, Types of Network: LAN, WAN and MAN, Topologies of Network, Internet concept, WWW.

**Word Processing:** Text creation and Manipulation; Table handling; Spell check, Hyper-linking, Creating Table of Contents and table of figures, Creating and tracking comments, language setting and thesaurus, Header and Footer, Mail Merge, Different views, Creating equations, Page setting, Printing, Shortcut keys.

- Learner will be provided web based learning to understand computer network and word processing

**Unit 3****12 hours**

**Presentation Tool:** Creating Presentations, Presentation views, working on Slide Transition, Making Notes Pages and Handouts, Drawing and Working with Objects, Using Animations, Running and Controlling a Slide Show, Printing Presentations, and Shortcut keys.

**Spread Sheet:** Entering and editing data in cell, Basic formulas and functions, deleting or inserting cells, deleting or inserting rows and columns, printing of Spread Sheet, Shortcut keys.

- Learner will be engaged in to prepare power point presentation for their seminar and dissertation

**Unit 4****12 hours**

**Use of Computers in Education and Research:** Data analysis tools, e-Library, Search engines related to research, Research paper editing tools like Latex.

- Learner will use e-library, search engines for writing proposal and manuscripts.

**Suggested Readings:**

1. Sinha, P.K. *Computer Fundamentals*. BPB Publications.
2. Goel, A., Ray, S. K. 2012. *Computers: Basics and Applications*. Pearson Education India.
3. Microsoft Office Professional 2013 Step by Step  
<https://ptgmedia.pearsoncmg.com/images/9780735669413/samplepages/9780735669413.pdf>
4. Gookin, D. (2013). *Word 2013 for dummies*. John Wiley & Sons.
5. Harvey, G. (2016). *Excel 2016 for dummies*. John Wiley & Sons.
6. Bott, E., Siechert, C., & Stinson, C. (2009). *Windows 7 inside out*. Pearson Education.

**The following are some of the modes of classroom transaction**

- Lecture
- Group discussion
- Demonstration
- Tutorial
- Self-learning

**Transaction Mode**

- PPT
- YouTube
- Google meet

**Course Title: Project Proposal**  
**Paper Code: CMC. 600**

L	T	P	Credits
0	0		4

**Learning outcome:**

After completing this course, the learner will be able to:

- Designing of research problem and prepare synopsis
- Preparation of synopsis for Project
- Planning of experiments

**Evaluation criteria:**

- Literature survey/background information
- Organization of content
- Physical presentation
- Questions and answers
- Report evaluation

The following are some of the **modes of classroom transaction**

- Lecture cum demonstration
- Project Method
- Seminar
- Group discussion

The following **tools** can be used in **different transactional modes:**

PPT

TED Talks

Video

google drive

Multimedia packages

**Software tools**

- Tracker

- ChemBioDraw
- Schrodingermaestro/AutoDck
- ppt
- BLAST
- Endnote



## Elective Course

**Course Title: Logics of Organic Synthesis**

**Paper Code: CMC.557**

**Course Hours: 45h**

L	T	P	Credits
3	0	0	3

## Learning Outcomes

After completing this course, the learner will be able to:

- Explain the reactions of different reaction intermediates
- Conceptualized the concept of Regio- and stereo-selectivity in enolate generation
- Explain protection and de-protection of functional groups

### Unit 1 15 hours

**Reactive intermediates:** Generation, structure and reactions of carbocation, carbanion, free radicals, carbenes, nitrenes, benzyne, classical and non-classical carbocations, phenonium ions and norbornyl system, neighboring group participation.

**Aromaticity:** Benzenoid and non-benzenoid compounds – generation and reactions.

- Learner will be engaged in group discussion to explain reactive intermediates and concept of aromaticity

### Unit 2 15 hours

**Alkylation:** Enolates: Regio- and stereo-selectivity in enolate generation. “O” versus “C” alkylation, Effect of solvent, Counter cation and Electrophiles; Symbiotic effect; Thermodynamically and kinetically controlled enolate formations; Various transition state models to explain stereoselective enolate formation; Enamines and metallo-enamines; Regioselectivity in generation, Application in controlling the selectivity of alkylation.

- Learner will be engaged in Web base learning to understand the concepts of enolates

### Unit 3 15 hours

#### **Protection and deprotection of various functional groups:**

Protection of alcohols by ether, silyl ethers and ester formations and their deprotection, Protection of 1, 2 diols- by acetal, ketal and carbonate formation and their deprotection, Protection of amines by acetylation, benzylation, benzyloxy carbonyl, t-butoxycarbonyl, fmoc, triphenyl methyl groups and their deprotection, Protection of carbonyls by acetal and ketal formation and their deprotection, Protection of carboxylic acids by ester formation and their deprotection

- Learner will be engaged in group discussion to explain protective and de-protection of functional groups

### **Suggested Readings:**

1. Clayden, J., Greeves, N., Warren, S., Wothers, P. (2012). *Organic chemistry Organic Chemistry* Oxford press.
2. Finar, I.L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, UK.
3. Mc Murry J., *Organic Chemistry*, Asian Book Pvt. Ltd, New Delhi
4. Smith, M. B. (2013). *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*. John Wiley & Sons.
5. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., New Delhi-110002.
6. Bansal, R. K., (2010). *A text book of Organic Chemistry*, New Age International (P) Ltd., New Delhi.
7. Bansal R.K., (2010). *Organic Reaction Mechanism*, New Age International (P) Ltd., New Delhi.
8. Kalsi, P.S., (2010). *Organic Reactions and Their Mechanisms*. New Age International Pub., New Delhi.
9. Kalsi, P.S., (2010). *Stereochemistry: Conformation and Mechanism*, New Age International (p) Ltd. New Delhi.
10. Morrison, R.T., Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
11. Mukherjee, S.M. Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry*. Macmillan India Ltd., New Delhi.
12. Eliel, E. L., & Wilen, S. H. (2008). *Stereochemistry of organic compounds*. John Wiley & Sons.
13. Carey, F. A., Giuliano, R. M. (2012). *Organic Chemistry*. McGraw Hill.
14. Kofie, W., Caddick, S. (2016). *Problems in Advanced Organic Chemistry*. Auris Publishing.

### **The following are some of the modes of classroom transaction**

- Lecture
- Group discussion
- Demonstration

### **Transaction Mode**

- PPT
- YouTube

- Google drive

**Course Title: Bioinorganic Chemistry and Biophysical Chemistry**

**Paper Code: CMC.558**

**Course Hours: 45h**

L	T	P	Credits
3	0	0	3

**Learning outcome:**

Students who successfully complete this course will be able to

- Describe stereo-chemical aspects of metal complexes and their application in medicinal chemistry
- Apply the phenomenon of reaction kinetics and their applications
- Apply partition coefficient of solutes in different solvent, phenomenon of adsorption and electrochemistry

**Unit 1**

**12 hours**

**Isomerism:** Ligand field theory and molecular orbital theory; nephelauxetic series, structural distortion and lowering of symmetry, electronic, steric and Jahn-Teller effects on energy levels, conformation of chelate ring, structural equilibrium, Magnetic properties of transition metal ions and free ions present, Effects of L-S coupling on magnetic properties, Temperature independent paramagnetism (TIP) in terms of crystal field theory CFT and molecular orbital theory (MOT), Quenching of orbital angular momentum by crystal fields in complexes in terms of splitting. Effect of spin-orbit coupling and A, E & T states mixing, first order and second order Zeeman effects, Spin paired and spin-free equilibria in complexes magnetic properties of polynuclear complexes involving OH, NH<sub>2</sub> and CN bridges.

- Learner will be engaged in Group discussion to explain Jahn-Taylor effect, Zeeman effect and CFT theory

**Unit 2**

**11 hours**

**Transition Metal Complexes:**

Introduction, Potential energy diagram and reactivity of metal complexes, ligand substitution reactions, substitution reactions mechanisms, labile and Inert metal complexes, Acid hydrolysis, Factors affecting acid hydrolysis, Base hydrolysis, Conjugate base mechanism, Anation reaction. Substitution reactions

in square planar complexes, Trans effect, Mechanism of the substitution reaction Reactions without metal ligand bond cleavage, electron transfer processes outer and inner sphere. The Marcus theory, doubly bridged inner-sphere transfer, other electron transfer reactions; two electron transfers, Non-complementary reaction, Ligand exchange via electron exchange, reductions by hydrated electrons. Applications of metal complexes in Medicinal Chemistry.

- Learner will be engaged in Group discussion to explain Potential energy diagram and reactivity of Transition metal complexes

### Unit 3

10 hours

**Chemical Kinetics:** Empirical rate laws and temperature dependence; complex reactions; steady state approximation; determination of reaction mechanisms; collision theory; Potential energy surfaces; transition state theory (statistical and classical treatment); unimolecular reactions and Lindemann mechanism; Solution kinetics factors affecting reaction rate in solution. Effect of solvent and ionic strength (primary salt effect) on the rate constant. Secondary salt effects.

- Learner will be engaged in Web base learning to understand the concepts of chemical kinetics

### Unit 4

12 hours

**Chemical Equilibrium:** Gibbs energy is a minimum with respect to the extent to the extent of reaction, Equilibrium constant is a function of temperature, Standard Gibbs energies of formation is used to calculate Equilibrium constant, Direction of reaction spontaneity, Van't Hoff equation, Molecular partition functions and related thermodynamic data.

**Adsorption:** Adsorption of solids, Gibbs adsorption isotherm, BET adsorption isotherm: estimation of surface area of solids, Langmuir and Fredulich Isotherms, catalysis.

- Learner will be engaged in Web base learning to understand the concepts of Chemical equilibrium and adsorption

### Suggested Books

1. Drago, R. S. (1992). *Physical methods for chemists*.
2. Ebsworth, E.A.V., Rankin, D.W.H., Cracock, S. *Structural Methods in Inorganic Chemistry*, ELBS, 1987.
3. Cotton, F.A., Lippard, S.J. *Progress in Inorganic Chemistry*, Vol. 8, Vol. 15, Wiley Internationals.
4. Huheey, James E. (1993). *Inorganic Chemistry: Principles of Structure and Reactivity*, Harper Collins College Publishers.
5. Glasstone, S. (1951). *Textbook of physical chemistry*. Tata McGraw-Hill, 2007.
6. Kapoor, K. L. (2006). *Text Book of Physical Chemistry*, Macmillan Publishers.

7. Tinoco, I., Sauer, K., Wang, J. C., Puglisi, J. D., Harbison, G., & Rovnyak, D. (1995). Physical chemistry: principles and applications in biological sciences (Vol. 552, p. 553). Englewood Cliffs, NJ Prentice Hall.
8. McQuarrie, D. A. (1997). Physical Chemistry A molecular approach (No. 539 M34).
9. Moore, J. W., & Pearson, R. G. (1961). Kinetics and mechanism. John Wiley & Sons.
10. Glasstone, S. (1951). Textbook of Physical Chemistry.
11. T. Engel, and P. Reid (2012) Physical Chemistry, Prentice-Hall.

**The following are some of the modes of classroom transaction**

- Lecture
- Group discussion
- Demonstration

**Transaction Mode**

- PPT
- YouTube
- Google drive

## Semester IV

**Course Title: Dissertation**

**CMC. 600**

**Course Hours:**

<b>L</b>	<b>T</b>	<b>P</b>	<b>Credits</b>
0	0	40	20

### **Learning outcome:**

After completing this course, the learner will be able to:

- Plan and execute experiments in the laboratory
- Interpret and analyze the results

### **Evaluation criteria:**

- Experimentation in laboratory
- Interpretation of result
- Physical presentation
- Questions and answers
- Report evaluation

The following are some of the **modes of classroom transaction**

- 1) Lecture
- 2) Demonstration
- 3) Project Method
- 4) Seminar
- 5) Group discussion

The following **tools** can be used in **different transactional modes:**

PPT

Multimedia packages

google drive

### **Software tools**

- Tracker
- ChemBioDraw
- Schrodinger maestro/or any freeware
- ppt/impress
- BLAST
- Endnote

