CENTRAL UNIVERSITY OF PUNJAB, BATHINDA

M.Sc. in Chemical Sciences

(Medicinal Chemistry)

Session- 2020-2022

Department of Pharmaceutical Sciences and Natural Products

School of Basic and Applied Sciences

Programme Outcome

1. The programme enhances academic knowledge, increased theoretical and methodological qualifications in the field of medicinal chemistry to identify and solve complex problems in organic and medicinal chemistry independently
2. The programme enables to identify scientific problems in relation to design, syntheses and development of drugs and students will be competitive enough to work in the pharmaceutical or Biotechnological industries

Course Structure

SEMESTER 1

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr
1.	CMC.506	Organic Chemistry-I	C	4	0	0	4
2.	CMC.507	Organic Synthesis-I (Practical)	C	0	0	4	2
3.	CMC.508	Modern Spectral and Chromatography Techniques	C	4	0	0	4
4.	CMC.509	Spectral Analysis (Practical)	C	0	0	4	2
5.	CMC.510	Medicinal Chemistry-I	C	4	0	0	4
6.	CST.501	Computer Applications	CF	2	0	0	2
7.	XXX CMC.513	Inter-Disciplinary Course (IDC) (Offered by Other department) Basics of Drug Discovery (IDC) (Offered by the department) (Opt any one)	ID	2	0	0	2
Opt any one course from following electives/MOOC							
8.	CMC.511	Chemistry of Natural Products	DE	4	0	0	4
9.	CMC.512	Quantum Chemistry					
		Total		**20**	**0**	**8**	**24**

CF: Compulsory Foundation, **C**: Core, **ID**: Interdisciplinary, **DE**: Discipline elective

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

SEMESTER II

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr
1.	CMC.521	Organic Chemistry-II	C	4	0	0	4
2.	CMC.522	Organic Synthesis-II-(Practical)	C	0	0	4	2
3.	CMC.526	Computer Aided Drug Design	C	4	0	0	4
4.	CMC.524	Computer Aided Drug Design-(Practical)	C	0	0	4	2
5.	CMC.525	Advanced Spectral Analysis	C	4	2	0	5
6.	CMC.542	Seminar	SB	0	0	0	1
7.	XXX CMC.513	Inter-Disciplinary Course (IDC) (Offered by Other department) Basics of Drug Discovery (IDC) (Offered by the department) (Opt any one)	ID	2	0	0	2
		Total		**14**	**2**	**8**	**20**

CF: Compulsory Foundation, **C**: Core, **ID**: Interdisciplinary, **DE**: Discipline elective

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

SEMESTER III

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr
1	CMC.551	Research Methodology	CF	2	0	0	2
2	CMC.552	Organic Chemistry-III	C	4	0 0	0 0	4
3	CMC.553	Medicinal Chemistry-II	C	4	0	0	4
4	CMC.554	Organic Chemistry-III (Practical)	C	0	0	4	2
5	XXX CMC.558	Value added course (VAC)Offered by Other department) Modern analytical techniques (VAC)(Offered by the department) (Opt any one)	EF	1	0	0	1
6	CMC.543	Seminar	SB	0	0	0	1
7	CMC.599	Project	SB	0	0	0	6
Opt any one course from following electives/MOOC							
8	CMC.555	Current Trends in Organic Synthesis	DE	4	0	0	4
	CMC.556	Bioinorganic and Biophysical Chemistry					
	CMC.557	Nuclear Chemistry					
	Total			**15**	**0**	**4**	**24**

CF: Compulsory Foundation, **C**: Core, **ID**: Interdisciplinary, **DE**: Discipline elective

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

SEMESTER IV

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr
1	CMC.571	Organic Chemistry - IV	C	4	0	0	4
2	CMC.572	Green Chemistry	C	4	0	0	4
3	CMC.573	Medicinal Chemistry-III	C	4	0	0	4
4	CMC.574	Organic Chemistry Worksheet-I (DEC-I)	CF (DEC)	2	0	0	2
5	CMC.575	Organic Chemistry Worksheet-II (DEC-II)	CF (DEC)	2	0	0	2
6	CMC.599	Project	SB	0	0	0	6
7	XXX CMC.558	Value added course (VAC) (Offered by Other department) Modern analytical techniques (VAC) (Offered by the department) (Opt any one)	EF	1	0	0	1
		Total		**17**	0	0	**23**

Any MOOC course of 4 credits or two courses of 2 credits each may be taken

CF: Compulsory Foundation, **C**: Core, **ID**: Interdisciplinary, **DE**: Discipline elective

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

Criteria of evaluation for Theory:

A: Continuous Assessment: [25 Marks]
(i). Surprise Tests (minimum three)-Based on Objective Type Tests (10 marks)
(ii). Term paper (10 marks)
(iii). Assignments (5 marks).
B: Mid-Semester Test: Based on Subjective Type Test [25 Marks]
C: End-Semester Exam: Based on Subjective Type Test [25 Marks]
D: End-Term Exam (Final): Online Objective Type Test [25 Marks]

Semester I

Course Title: Organic Chemistry-I

Paper Code: CMC.506

L	T	P	Credits
4	0	0	4

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.
- Conceptualize difficult principles of basic organic chemistry and will apply this knowledge in drug synthesis and their interaction with receptors

Unit I **15 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, .

Unit II **15 hours**

Aliphatic nucleophilic substitution reaction: The SN^2, SN^1, mixed SN^2 and SN^1 and SET mechanism, The SN^i 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 SN^2 and SN^1 mechanisms.

Aromatic nucleophilic substitution: The SN^{Ar}, 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.

Unit III **15 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.

Unit IV **15 hours**

Addition to carbon -hetero multiple bonds: Reactivity of carbonyl group, homologation and dehomologation of carbonyl compounds, nucleophilic addition of hetero-atoms (N,O,S), conjugate addition reactions, acylation of carbonyl carbon, carbonyl cyclizations and cleavages, carboxylic acids and derivatives, decarboxylation reactions, addition of Grignard, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds, mechanism of condensation reactions involving enolates-Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions, hydrolysis of esters and amides, ammonolysis of esters.

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 Inrternational (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. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., New York.
11. Morrison, R.T., Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
12. Mukherjee, S.M. Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry.* Macmillan India Ltd., New Delhi.
13. Solomn, C.W.G, Fryble, C.B. (2009). *Organic Chemistry*. John Wiley and Sons, Inc.
14. Eliel, E. L., & Wilen, S. H. (2008). *Stereochemistry of organic compounds*. John Wiley & Sons.
15. Carey, F. A., Guiliano, R. M. (2012). *Organic Chemistry*. McGraw Hill.
16. Kofie, W., Caddick, S. (2016). *Problems in Advanced Organic Chemistry*. Auris Publishing.
17. 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:

1) Lecture
2) Demonstration
3) Group discussion
4) Tutorial
5) Problem solving
6) Self-learning

Transactional Modes:

PPT
YouTube

Course Title: Organic Synthesis –I (Practical)
Paper Code: CMC.507

L	T	P	Credits
0	0	4	2

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 glasswares 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 $NaBH_4$/$LiAlH_4$
    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., Health, 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 Cemical 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.

The following are some of the modes of classroom transaction:

1) Lecture cum demonstration
2) Group discussion
3) Experimentation
4) Problem solving
5) Self-learning

Transactional Modes:

PPT
Three dimensional models
google drive

Evaluation Criteria for Practical:

1. Continuous Assessment and Practical Note Book: **40 Marks**
2. End Term Assessment (Synopsis, Performance, Viva voce): **60 Marks**

Course Title: Modern Spectral & Chromatographic Techniques

Paper Code: CMC.508

L	T	P	Credits
4	0	0	4

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 I **15 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.

Spectroflourimetry: Theory of Fluorescence, Factors affecting fluorescence (Characterestics of drugs that can be analysed by flourimetry), Quenchers, Instrumentation and Applications of fluorescence spectrophotometer.

Flame emission spectroscopy and Atomic absorption spectroscopy: Principle, Instrumentation, Interferences and Applications.

Unit II **15 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 ^{13}C NMR. Applications of NMR spectroscopy.

Mass Spectroscopy: Principle, Theory, Instrumentation of Mass 10 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.

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

Unit III **15 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

Electrophoresis: Principle, Instrumentation, Working conditions, factors affecting separation and applications of the following: a) Paper electrophoresis b) Gel electrophoresis c) Capillary electrophoresis d) Zone electrophoresis e) Moving boundary electrophoresis f) Isoelectric focusing

Unit IV **15 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

Potentiometry: Principle, working, Ion selective Electrodes and Application of potentiometry.

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:

1) Lecture
2) Demonstration
3) Group discussion
4) Team teaching
5) Tutorial
6) Problem solving
7) Self-learning

Transaction Mode

PPT
YouTube
Three dimensional models

Course Title: Spectral Analysis (Practical)
Paper Code: CMC.509

L	T	P	Credits
0	0	4	2

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}H, ^{13}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}H, ^{13}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 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., Health, 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

1) Demonstration
2) Experimentation
3) Project Method
4) Focused group discussion
5) Tutorial
6) Problem solving

Transaction Mode

PPT
google drive
Three dimensional models
YouTube

Evaluation Criteria for Practical:

Continuous Assessment and Practical Note Book: **40 Marks**

End Term Assessment (Synopsis, Performance, Viva voce): **60 Marks**

Course Title: Medicinal Chemistry-I
Paper Code: CMC.510

L	T	P	Credits
4	0	0	4

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 I **15 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

Unit II **15 hours**

Medicinal chemistry: Definitions and objectives, Drug activity phases, Drug classification system.

Measurement and expression of drug effects: Introduction, *In-vitro* experiments, *Ex-vivo* experiments, *In-vivo* experiments.

Unit III **15 hours**

Molecular drug targets: Introduction, Non-selective cation-channels as drug targets, Direct ligand gated ion channels, Receptors with intrinsic enzyme activity, Receptors coupled to various cytosolic proteins, G-Protein coupled receptors, Nuclear receptors.

Unit IV **15 hours**

Drug targets, target identification, validation and screening: Introduction, Improving the resolution of disease etiology, Biopharmaceutical therapies, Drug target identification, Hit to lead, Clinical biomarkers.

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: Wolters Kluwer.
3. King, F. D. (2006). *Medicinal Chemistry Principles and Practice*, Royal Society of Chemistry.
4. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press.
5. Patrick, G.L. (2017). *An Introduction to Medicinal Chemistry*, Publisher: Oxford university Press, UK.
6. Singh, H., Kapoor, V.K. *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., (Latest Edition). *Burger's Medicinal Chemistry and Drug Discovery* John Wiley and 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 and tools:

1) Lecture
2) Group discussion
3) Demonstration
4) Team teaching
5) Tutorial
6) Self-learning

Transaction Mode

YouTube
PPT
Three dimensional models

Course Title: Computer Applications
Paper Code: CST.501

L	T	P	Credits
2	0	0	2

Course Objectives:
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 I **Hours: 7**

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.

UNIT II **Hours: 7**

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.

UNIT III **Hours: 8**

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.

UNIT IV **Hours: 8**

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

Transactional Modes:
PPT
Video
e-content
google drive

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/97807356694 13.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.

Elective courses

Course Title: Chemistry of Natural Products
Paper Code: CMC.511

L	T	P	Credits
4	0	0	4

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 I **15 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 β-Carotene

Unit II **15 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.

Unit III **15 hours**

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

Unit IV **15 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, ^{1}HNMR, ^{13}CNMR and MS Spectroscopy of specific drugs e.g., Penicillin, Morphine, Camphor, Vit-D, Quercetin and Digitalis glycosides.

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:

1) Lecture
2) Seminar
3) Group discussion
4) Team teaching
5) Tutorial
6) Self-learning

Transaction Mode

PPT
google drive
Three dimensional models
YouTube

Course Title: Quantum Chemistry
Paper Code: CMC.512

L	T	P	Credits
4	0	0	4

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 I **15 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.

Unit II **15 hours**

Approximate Methods: Perturbation theory for non-degenerate and degenerate states and its applications. The variation theorem and its application.

Unit III **15 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.

Unit IV **15 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.

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:

1) Lecture
2) Group discussion
3) Team teaching
4) Tutorial
5) Problem solving
6) Self-learning

Transaction Mode

PPT
YouTube
google drive

Course Code: CMC.513

L	T	P	Cr
2	-	-	2

Course Title: Basics of Drug Discovery (IDC)
Total Hours: 30

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

- Describe Lead identification and Optimization techniques
- Elaborate rational drug design and Prodrug
- Understand the concept of QSAR and Molecular Docking
- Apply QSAR and Molecular Docking for Drug Discovery

Unit I **8 Hours**

Introduction to Drug Discovery: An Overview of modern drug discovery process: Target identification, target validation, lead identification and lead optimization. Combinatorial chemistry & High throughput screening, Assay development of hit identification.

Unit II **7 Hours**

Rational Drug Design: Concept of rational drug design, Methods to derive target structures, Virtual screening, Rational Drug design Methods: Structure and Pharmacophore based Approaches. Concept of pharmacophore mapping and drug likeness.

Unit III **8 Hours**

Molecular Docking and QSAR: Concept of Molecular docking and QSAR. Rigid and Flexible Docking, scoring. Denovo drug design. 2D-QSAR and 3D-QSAR approaches along with their merits and Limitations. QSAR Statistical methods.

Unit IV **7 Hours**

Prodrug: Basic concept, Rationale of prodrug design and practical consideration of prodrug design. Prodrugs to improve patient acceptability, drug solubility, Drug absorption and distribution, site specific drug delivery and sustained drug action.

Suggested Readings:

1. Ganellin, C.R.; Roberts S. M., (1993). *Medicinal Chemistry: The Role of Organic Chemistry in Drug Research*. Publisher: Academics Press Inc.
2. Kadam, Mahadik, Bothara (2010). *Principle of Medicinal Chemistry (Volume I & II)*, Nirali publication
3. Kulkarni, V. M., Bothra, K.G., (2008). *Drug Design*, Nirali Publication.
4. Lawton, G., Witty, D.R. (2011). *Progress in Medicinal Chemistry Series. Volume 50*.
5. Lednicer, D. (2008). *Strategies for Organic Drug Synthesis and Design. (7 volume)* Publisher: John Wiley & Sons.
6. Lemke, T.L., Williams, D.A. (2012). *Foye's Principles of Medicinal Chemistry*. 7th edition.
7. Silverman R.B., (2014). *Organic Chemistry of Drug Design and Drug Action*, Publisher: Elsevier.
8. 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:

1) Demonstration
2) Group discussion
3) Tutorial

4) Self-learning

Transaction Mode

Three dimensional models
YouTube
PPT

Semester –II

Course Title: Organic Chemistry-II
Paper Code: CMC.521

L	T	P	Credits
4	0	0	4

Learning Outcomes

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

- Describe disconnection approaches applied on synthetic strategies and mechanism prediction.
- Explain the mechanism and applications of different naming reactions
- Apply photochemical reactions in drug synthesis

Unit I **15 hours**

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

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

Unit II **15 hours**

Synthetic methodologies: Synthon, 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, regioselectiviity, 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.

Unit III **15 hours**

Rearrangements: General mechanistic considerations-nature of migration, migratory aptitude, Mechanistic study of the following rearrangements: Pinacol-pinacolone, Wagner-Meerwein, Benzil-Benzillic 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 Assymetric Epoxidation, Ene, Barton, Hofmann-Loffler Fretag, Shapiro reaction, Chichibabin Reaction.

Unit IV **15 hours**

Pericyclic chemistry:

Introduction, Main features of pericyclic reactions, Classification of pericyclic reactions. Phases, nodes and symmetry properties of molecular orbitals in ethylene, 1,3-butadiene, 1,3,5- hexatriene. Allyl cation, allyl radical, pentadienyl cation and pentadienyl radical. 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. Explanation for the mechanism of cycloaddition reactions by (i) Conservation of orbital symmetry and orbital symmetry correlation diagrams (ii) Fukui Frontier Molecular Orbital (FMO) theory and (iii) Endo-exo selectivity in Diels-Alder reaction and its explanation by FMO theory. Examples of cyclo addition reactions.

Sigmatropic reactions: [1,j] and [i,j] shifts; Suprafacial and antarafacial shifts; Selection rules for [lj} shifts; Cope and Claisen rearrangements; Explanation for the mechanism of sigmatropic reactions by (i) symmetry properties of HOMO (ii) Introduction to Cheletropic reactions and the explanation of mechanism by FMO theory.

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). *Heterocyc1ic 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 Synthon 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., Guiliano, 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:

1) Lecture
2) Demonstration
3) Seminar
4) Team teaching
5) Tutorial
6) Self-learning

Transaction Mode

PPT
google drive
YouTube

Course Title: Organic Synthesis-II (Practical)

L	T	P	Credits
0	0	4	2

Paper Code: CMC.522

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}H, ^{13}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 $Pd(PPh_3)_4$ as a catalyst.

3. Exercises on identification of compounds *via* combined spectral interpretation of ^{1}H, ^{13}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 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., Health, D.C. (1999). *Macroscale and Microscale Organic Experiments, Heath, D. C*and 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

1) Demonstration
2) Focused group discussion
3) Experimentation
4) Tutorial
5) Problem solving

Transaction Mode

PPT
Three dimensional models
YouTube

Evaluation Criteria for Practical:

1. Continuous Assessment and Practical Note Book: **40 Marks**
2. End Term Assessment (Synopsis, Performance, Viva voce): **60 Marks**

Course Title: Computer Aided Drug Design

Paper Code: CMC.526

L	T	P	Credits
4	0	0	4

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 I **15 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), lipoiphilicity 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.

Unit II **15 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)

Unit III **15 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.

Unit IV **15 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.

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 Willaiams & Wikins.
12. Gore, M., & Jagtap, U. (2018). *Computational Drug Discovery and Design*. Springer Publishers.

The following are some of the modes of classroom transaction

1) Lecture
2) Demonstration
3) Group discussion
4) Team teaching
5) Tutorial

6) Self-learning

Transaction Mode

PPT
Three dimensional models
YouTube

Course Title: Computer Aided Drug Design - Practical
Paper Code: CMC.524

L	T	P	Credits
0	0	4	2

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, 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.; MarkelIn 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

1) Demonstration
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3) Experimentation
4) Tutorial
5) Problem solving

Transaction Mode

PPT
google drive
Three dimensional models
YouTube

Evaluation Criteria for Practical:

1. Continuous Assessment and Practical Note Book: **40 Marks**
2. End Term Assessment (Synopsis, Performance, Viva voce): **60 Marks**

Course Title: Advanced Spectral Analysis
Paper Code: CMC.525

L	T	P	Credits
4	2	0	5

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 I **15 Hours**

UV and IR spectroscopy: Wood ward – Fieser rule for 1,3- butadienes, cyclic dienes and α, β-carbonyl compounds and interpretation compounds of enones.
ATR-IR, IR Interpretation of organic compounds.
Raman Spectroscopy: Introduction, Principle, Instrumentation and Applications.

Unit II **15 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.

Unit III **15 Hours**

Mass Spectroscopy: Mass fragmentation and its rules, Fragmentation of important functional groups like alcohols, amines, carbonyl groups and alkanes, Meta stable ions, Mc Lafferty rearrangement, Ring rule, Isotopic peaks, Interpretation of organic compounds.
Radio immuno assay: Biological standardization, bioassay, ELISA, Radioimmuno assay of digitalis and insulin.

Unit IV **15 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

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 Willey & 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:

1) Lecture
2) Demonstration
3) Group discussion
4) Team teaching
5) Tutorial
6) Problem solving

Transaction Mode

PPT
Three dimensional models
YouTube

Course Title: Seminar
Paper Code: CMC.542

L	T	P	Credits
0	0	0	1

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

- Improve writing skills and manuscript writing
- Deliver effective PowerPoint presentation
- Response the queries

Evaluation criteria:

- Continuous assessment-50 Marks
- Response to queries- 50 Marks

Course Code: CMC.513
Course Title: Basics of Drug Discovery (IDC)
Total Hours: 30

L	T	P	Cr
2	0	0	2

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

- Describe Lead identification and Optimization techniques
- Elaborate rational drug design and Prodrug
- Understand the concept of QSAR and Molecular Docking
- Apply QSAR and Molecular Docking for Drug Discovery

Unit I **8 Hours**

Introduction to Drug Discovery: An Overview of modern drug discovery process: Target identification, target validation, lead identification and lead optimization. Combinatorial chemistry & High throughput screening, Assay development of hit identification.

Unit II **7 Hours**

Rational Drug Design: Concept of rational drug design, Methods to derive target structures, Virtual screening, Rational Drug design Methods: Structure and Pharmacophore based Approaches. Concept of pharmacophore mapping and drug likeness.

Unit III **8 Hours**

Molecular Docking and QSAR: Concept of Molecular docking and QSAR. Rigid and Flexible Docking, scoring. Denovo drug design. 2D-QSAR and 3D-QSAR approaches along with their merits and Limitations. QSAR Statistical methods.

Unit IV **7 Hours**

Prodrug: Basic concept, Rationale of prodrug design and practical consideration of prodrug design. Prodrugs to improve patient acceptability, drug solubility, Drug absorption and distribution, site specific drug delivery and sustained drug action.

Suggested Readings:

1. Ganellin, C.R.; Roberts S. M., (1993). *Medicinal Chemistry: The Role of Organic Chemistry in Drug Research*. Publisher: Academics Press Inc.
2. Kadam, Mahadik, Bothara (2010). *Principle of Medicinal Chemistry (Volume I & II)*, Nirali publication
3. Kulkarni, V. M., Bothra, K.G., (2008). *Drug Design*, Nirali Publication.
4. Lawton, G., Witty, D.R. (2011). *Progress in Medicinal Chemistry Series. Volume 50*.
5. Lednicer, D. (2008). *Strategies for Organic Drug Synthesis and Design. (7 volume)* Publisher: John Wiley & Sons.
6. Lemke, T.L., Williams, D.A. (2012). *Foye's Principles of Medicinal Chemistry*. 7th edition.
7. Silverman R.B., (2014). *Organic Chemistry of Drug Design and Drug Action*, Publisher: Elsevier.
8. 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:

1) Demonstration
2) Group discussion

3) Tutorial
4) Self-learning

Transaction Mode

Three dimensional models
YouTube
PPT

Semester –III

Course Title: Research Methodology
Paper Code: CMC.551

L	T	P	Credits
2	0	0	2

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

Unit I **7 hours**

General Research Methodology: Research, objective, requirements, practical difficulties, review of literature, study design, types of studies.

Unit II **8 hours**

General Research Methodology: Strategies to eliminate errors/bias, controls, randomization, crossover design, placebo, blinding techniques.

Unit III **7 hours**

Entrepreneurship and business development: Technical writing: Scientific writing, Writing research paper, Poster preparation and Presentation and Dissertation.

Unit IV **8 hours**

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

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

1) Lecture
2) Team teaching
3) Tutorial
4) Problem solving
5) Self-learning

Transaction Mode

PPT
YouTube

Course Title: Organic Chemistry-III
Paper Code: CMC.552

L	T	P	Credits
4	0	0	4

Learning outcome:

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

- Determine the mechanism and feasibility of a chemical reaction
- Apply principle of photochemistry in various chemical transformations
- Conceptualize various metal and non-metal reagents towards oxidation and reduction reactions

Unit I **15 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.

Unit II **15 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 π – methane rearrangement.

Photochemistry of aromatic compounds, Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction Singlet molecular oxygen reactions

Unit III **15 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-Pondorff-Verley reduction, Dissolving metal reductions, metal hydride reductions using $NaBH_4$, $LiAlH_4$, DIBAL. Wilkinson's Rh catalysis, Boron in reduction

Unit IV **15 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*.

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 Inrternational (P) Ltd., New Delhi.
5. Bansal, R.K. (2010). *Hetrocyclic Chemistry*, New Age Inrternational (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). *Heterocyc1ic 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., Guiliano, 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

1) Lecture
2) Demonstration
3) Group discussion
4) Tutorial
5) Problem solving
6) Self-learning

Transaction Mode

PPT
Three dimensional models
YouTube

Course Title: Medicinal Chemistry-II
Paper Code: CMC.553

L	T	P	Credits
4	0	0	4

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 I **15 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).

Unit II **15 Hours**

Neuromuscular blocking agents: Gallamine Triethiodide, Succinylcholine chloride, Hypoglycaemic drugs (Tolbutamide), Thyroid hormones and Antithyroid drugs (L- Thyroxine, Propylthiouracil) Pancuronium, vecuronium, rocuronium, rapacuronium, dacuronium, malouètine, 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.

Unit III **15 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).

Unit IV **15 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.*

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

1) Lecture
2) Group discussion
3) Demonstration
4) Team teaching
5) Tutorial
6) Self-learning

Transaction Mode

Three dimensional models
PPT
YouTube

Course Title: Organic Chemistry-III (Practical)
Paper Code: CMC.554

L	T	P	Credits
0	0	4	2

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}H data and ^{13}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}H data
7. Exercises of structure identifications of above synthesized compounds *via* spectral interpretation using ^{1}H data and ^{13}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}H data and ^{13}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., Health, 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 Willey & Sons.

The following are some of the modes of classroom transaction:

1) Lecture cum demonstration
2) Group discussion
3) Experimentation
4) Problem solving
5) Self-learning

Transaction Mode

Three dimensional models
PPT
google drive
YouTube

Evaluation Criteria for Practical:

1. Continuous Assessment and Practical Note Book: **40 Marks**
2. End Term Assessment (Synopsis, Performance, Viva voce): **60 Marks**

Course Code: CMC.558

L	T	P	Cr
1	0	0	1

Course Title: Modern analytical techniques (VAC)
Total Hours: 15

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

- Describe various modern analytical techniques
- Carry out Structural Elucidation of organic compounds
- Understand basics of various sophisticated instruments

Unit I **4 Hours**

UV-Visible and FT-IR spectroscopy: Basic principles and instrumentation of UV-Visible and FT-IR spectroscopy. Structural elucidation of organic compounds using UV-Visible and FT-IR spectroscopy.

Unit II **3 Hours**

NMR spectroscopy: Basic principles and instrumentation of NMR spectroscopy. Structural elucidation of organic compounds using 1-D and 2-D NMR, NOESY and COSY techniques.

Unit III **4 Hours**

Mass Spectrometry: Basic principles and instrumentation. Various fragmentation techniques and ring rule. Structural elucidation of organic compounds using mass spectrometry techniques.

Unit IV **4 Hours**

Chromatography: Basic principles and instrumentations of chromatographic techniques including HPLC, UPLC, HPTLC LC-MS and GC-MS.

Suggested Readings:

1. Kemp, W. (1991). *Organic spectroscopy* (pp. 42-51). London: Macmillan.
2. Munson, J. W. (Ed.). (1984). *Pharmaceutical analysis: modern methods* (Vol. 11). CRC Press.
3. Sethi, P. D. (1996). *HPTLC: high performance thin-layer chromatography; quantitative analysis of pharmaceutical formulations.* CBS publishers & distributors.
4. Sethi, P. D. (1985). *Quantitative analysis of drugs in pharmaceutical formulations*. CBS Publishers, New Delhi, 1997.
5. Silverstein, R. M., Webster, F. X., Kiemle, D. J., & Bryce, D. L. (2014). *Spectrometric identification of organic compounds*. John wiley & sons.
6. Skoog, D. A., Holler, F. J., & Crouch, S. R. (2017). *Principles of instrumental analysis*. Cengage learning.
7. Willard, H. H., Merritt Jr, L. L., Dean, J. A., & Settle Jr, F. A. (1988). *Instrumental methods of analysis.*

The following are some of the modes of classroom transaction:

1) Demonstration
2) Group discussion
3) Tutorial
4) Self-learning

Transaction Mode

YouTube
PPT

Course Title: Seminar
Paper Code: CMC.543

L	T	P	Credits
0	0	0	1

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

- Improve writing skills and manuscript writing
- Deliver effective PowerPoint presentation
- Response the queries

Evaluation criteria:

- Continuous assessment-50 Marks
- Response to queries- 50 Marks

Course Title: Project
Paper Code: CMC.599

L	T	P	Credits
0	0	0	6

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

- Design a research problem and prepare synopsis
- Plan and execute experiments in the laboratory
- Interpret and analyze the results

Evaluation criteria:

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

Elective courses

Course Title: Current Trends in Organic Synthesis
Paper Code: CMC.555

L	T	P	Credits
4	0	0	4

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 I **15 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

Unit II **15 hours**

Organometallic compounds

Organoboranes: Preparation of Organobornaesviz hydroboration with BH3-THF, dicylohexyl borane, disiamyl borane, theryl borane, 9-BBN and disopincamphlyel borne, functional group transformations of Organo boranes-Oxidation, protonolysis and rearrangements. Formation of carbon-carbon-bonds vizorgano boranes carbonylation.

Grignard reagents, Organo lithium, Organo zinc, Organo cadmium and Organo Copper Compounds, Organo silicon compounds for organic synthesis, Organopalladium and organostannous (Applications in coupling reactions).

Unit III **15 hours**

Reagents in organic synthesis:

Gilman'sreagent, Lithiumdiisopropylamide(LDA), DicyclohexylCarbodiimide (DDC), 1,3-Dithiane (Umpolungreagent), Trimethylsilyliodide, Bakersyeast, D.D.Q., Lead tetraacetate, Prevost Hydroxylation, Wilkinsion's catalyst, Phasetransfercatalysts:QuaternaryammoniumandPhosphoniumsalts,Crowneth ers, Merifield resin, Fenton's reagents, Ziegler-Natta catalyst, Lawson reagents, K-selecteride and L-selecteride, 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.

Unit IV **15 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.

Suggested readings:

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

1) Lecture
2) Demonstration
3) Group discussion
4) Tutorial
5) Problem solving
6) Self-learning

Transaction Mode

PPT
google drive
Three dimensional models
YouTube

Course Title: Bioinorganic Chemistry and Biophysical Chemistry
Paper Code: CMC.556

L	T	P	Credits
4	0	0	4

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 in medicinal chemistry
- Apply partition coefficient of solutes in different solvent, phenomenon of adsorption and electrochemistry

Unit I **15 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_2 and CN bridges.

Unit II **15 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.

Unit III **15 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.

Unit IV **15 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.

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. McfQuarrie, 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

1) Lecture
2) Group discussion
3) Demonstration
4) Team teaching
5) Tutorial
6) Self-learning

Transaction Mode

PPT
YouTube
google drive

Course Title: Nuclear Chemistry
Paper Code: CMC.557

L	T	P	Credits
4	0	0	4

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 I **15 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.

Unit II **15 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.

Unit III **15 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.

Unit IV **15 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

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.
12. 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

1) Lecture
2) Demonstration
3) Group discussion
4) Team teaching
5) Tutorial
6) Self-learning

Transaction Mode

PPT
YouTube

Semester-IV

Course Title: Organic Chemistry-IV
Paper Code: CMC.571

L	T	P	Credits
4	0	0	4

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

- Describe the asymmetric synthesis, chiral resolution and apply it on the resolution of chiral drugs.
- Enable to understand students to build knowledge in drug synthesis and their interaction with receptors

Unit I **15 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 and biocatalysis

Unit II **15 hours**

Reaction of ylides: Phosphorus ylide; Structure and reactivity, stabilized ylides, effects of ligands on reactivity, Witting, 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

Unit III **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 steroselective enolate formation; Enamines and metallo-enamines; Regioselectivity in generation, Application in controlling the selectivity of alkylation.

Unit IV **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

Suggested readings

1. Claydon, J., Gleeves, N., Warren, S., Wother, P.; (2001) *Organic chemistry*, Oxford University Press, UK.
2. Fieser and Fieser, (2011). *Reagents for organic synthesis*, Wiley Interscience.
3. Finar, I.L., (2012). *Organic Chemistry*, Pearson Education, UK.
4. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
5. Reich, H.J., Rigby, M., (1999). *Handbook of Reagents for Organic Synthesis Acidic and Basic Reagents,* Wiely-Interscience
6. Warren, S., (2010). *Organic synthesis: The Synthon Approach*. John wiley& Sons, New York,
7. Corey E.J., Cheng Xue-Min, (1989) *The Logic of Chemical Synthesis, Pubs*: John Wiley & Sons,.
8. FuhrhopJurgen, Penzlin Gustav, (1994) *Organic Synthesis: Concepts methods, Starting Materials*, Pubs: Verlagchemie,.
9. Devies Stephen G., (1994) *Organotransition Metal Chemistry: Application to Organic Synthesis*, Pubs: Pergamon Press.
10. Morrison J. D. (1992) (eds) *Asymmetric Synthesis*, Pubs:Academic Press.
11. Aitken R.A. and Kilenyi S.N., (1994) *Asymmetric Synthesis*, Pubs:Academic Press.
12. Garry, P. (1996) *Asymmetric Synthesis,* Pubs:Academic Press
13. Kofie, W., Caddick, S. (2016). *Problems in Advanced Organic Chemistry*. Auris Publishing.
14. 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:

1) Lecture
2) Group discussion
3) Team teaching
4) Tutorial
5) Problem solving
6) Self-learning

Transaction Mode

Three dimensional models
YouTube
PPT

Course Title: Green Chemistry
Paper Code: CMC.572

L	T	P	Credits
4	0	0	4

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 I **15 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,

Unit II **15 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.

Unit III **15 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-alkylalion, 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.

Unit IV **15 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.

Suggested Readings:

1. Ahulwalia, 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 Inclusice Approach*, Elsevier

The following are some of the modes of classroom transaction

1) Lecture
2) Demonstration
3) Group discussion
4) Team teaching
5) Tutorial
6) Self-learning

Transaction Mode

PPT
YouTube
google drive

Course Title: Medicinal Chemistry-III
Paper Code: CMC.573

L	T	P	Credits
4	0	0	4

Learning outcome:

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

- Describe various biological functions of steroids in the human body
- Conceptualize the role of opioid receptors and role of opioids as analgesic and their abuse potential, psychoactive compounds and their role in neurological disorders
- Explore the role of diuretics, cardiovascular agents, antianginals and vasodilators in different disease state

Unit I **15 Hours**

Steroids: Introduction, nomenclature, stereochemistry of cholesterol, stigmasterol, ergosterol, diosgenin, solasodine, bile acids, biosynthesis of testosterone, β-estradiol and aldosterone form cholesterol, Estrogens, SAR among estrogens, progestational agents, synthesis of progesterone from diosgenin and stigmasterol, ethisterone from dehydroepiandrosterone, oral contraceptives, SAR of progestins, **Androgens and Anabolic Agents:** Synthesis of testosterone from diosgenin, methyltestosterone from dehydroepiandrosterone, methandienone from methy1 testosterone, stanozolol from testosterone. **Aderenocorticoids:** Glucocorticoids and their SAR, mineralocorticoids, modifications in structure of hydrocortisone.

Unit II **15 Hours**

Opioid analgesics: Morphine and related drugs, synthetic modifications of morphine, codeine and thebaine, synthetic analgesics, endogenous opioid peptides, opioid antagonists, **CNS stimulants:** natural and synthetic, Methylxanthines and modified Methylxanthines, Psychopharmacological agents, Antipsychotics, Phenothiazines, **Antidepressants:** Tricyclic antidepressants, MAO inhibitors, atypical antidepressants, **Antianxiety drugs:** Meprobamate and related drugs, Benzodiazepines, Hallucinogens Hallucinogenic agents related to indoles, phenethylamines and Cannabinoids.

Unit III **15 Hours**

Diuretics carbonic anhydrase inhibitors: Thiazides and related drugs, High-ceiling diuretics. Aldosterone, antagonists, other potassium sparing diuretics, Osmotic diuretics, **Cardiovascular Agents:** cardiac glycosides, SAR, mechanism of action, toxic effects. Antihypertensive agents; introduction, ganglion blocking agents, antiadrenergic agents, drugs acting directly on smooth muscles, drugs acting on CNS. **Antianginals and vasodilators:** introduction, mechanism of smooth muscle vasodilation, esters of nitrous and nitric acid, side-effects. Antiarrhythmic and antifibrillytic drugs classification of antiarrhythmic drugs, mechanism of action, side effects. Angiotensin II receptor antagonists.

Unit IV **15 Hours**

Sulphonamides: Introduction and classification, antimicrobial spectrum, DHFR inhibitors, toxicity and side effects, reduction. **Antibiotics:** Classification, cycloserine, chloramphenicol, penicillins, cephalosporins, aminoglycosides, tetracyclines, polypeptides.

Antimycobacterial agents: Introduction, uses in therapeutics. **Antimalarials:** quinoline and analogues, 8-amino quinolines, 9-amino acridines, 4-amino quinolines, diamino pyrimidine, and biguanides and recently introduced compounds. **Antiamoebic agents:** quinoline derivatives, metal free substances, diloxanide furoate, etc. **Anthelmintic drugs** in cestode infections in trematode infections and for intestinal nematode infections, antifilarial agents, **Antiviral agents:** Introduction to DNA, RNA and retroviruses, viral application,

amantidine hydrochloride, interferones, acyclovir, idoxuridine, trifluorothymidine and vidarabine etc.

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. O. (2019). *Principles of Medicinal Chemistry*, Publisher: Wolter Kluwer
3. King, F. D. (2003). *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, New York.
5. Patrick, G.L. (2017). *An Introduction to Medicinal Chemistry*, Oxford University Press, UK.
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, UK.
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 and Sons, New York.

The following are some of the modes of classroom transaction:

1) Lecture
2) Demonstration
3) Group discussion
4) Team teaching
5) Tutorial
6) Problem solving
7) Self-learning

Transaction Mode

PPT
google drive
Three dimensional models
YouTube

Course Title: Organic Chemistry Worksheet-I (DEC-I)
Paper Code: CMC.574

L	T	P	Credits
2	0	0	2

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

- Explain IUPAC nomenclature of organic molecules
- Describe the Fundamentals of stereochemistry
- Study of reaction intermediates
- Develop skill of explaining reaction mechanisms

Unit-I **7 hours**
IUPAC nomenclature of organic molecules including regio- and stereoisomers, Aromaticity: Benzenoid and non-benzenoid compounds – generation and reactions.

Unit-II **8 hours**
Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction.

Unit-III **7 hours**
Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzynes and nitrenes.

Unit-1V **8 hours**
Organic reaction mechanisms involving addition, elimination and substitution reactions with electrophilic, nucleophilic or radical species. Determination of reaction pathways.

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 Inrternational (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. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., New York.
11. Morrison, R.T., Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
12. Mukherjee, S.M. Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry*. Macmillan India Ltd., New Delhi.
13. Roberts, J. D., & Caserio, M. C. (1977). *Basic principles of organic chemistry*. WA Benjamin, Inc..
14. Solomn, C.W.G, Fryble, C.B. (2009). *Organic Chemistry*. John Wiley and Sons, Inc..
15. Sykes, P. (1986). *A guidebook to mechanism in organic chemistry*. Pearson Education India.
16. Eliel, E. L., & Wilen, S. H. (2008). *Stereochemistry of organic compounds*. John Wiley & Sons.

The following are some of the modes of classroom transaction:

1) Demonstration
2) Group discussion
3) Tutorial
4) Self-learning

Transaction Mode

Three dimensional models
YouTube
PPT

Course Title: Organic Chemistry Worksheet-II (DEC-II)
Paper Code: CMC.575

L	T	P	Credits
2	0	0	2

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
- Elaborate Concepts in organic synthesis

Unit-I **8 hours**

Common named reactions and rearrangements – applications in organic synthesis. Organic transformations and reagents: Functional group interconversion including oxidations and reductions; common catalysts and

reagents (organic, inorganic, organometallic and enzymatic). Chemo, regio and stereoselective transformations.

Unit-II **7 hours**

Pericyclic reactions – electrocyclisation, 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)

Unit-III **8 hours**

Concepts in organic synthesis: Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups. Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. Resolution – optical and kinetic.

Unit-IV **7 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, ^{1}H & ^{13}C NMR and Mass spectroscopic techniques.

Suggested readings

1. Acheson, R.M. (1976). *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 Inrternational (P) Ltd., New Delhi.
6. Bansal, R.K. (2010). *Hetrocyclic 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 Vol. 1-3*, Springer Verlag, India.

11. Joule, J.A., Mills, K. (2010). *Heterocyc1ic 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. (2017). *Principles of Organic Synthesis*. Routledge.
20. Warren, S., (2010). *Organic synthesis: The Synthon Approach*. John Wiley & Sons, New York,
21. Warren, S., (2010). *Designing Organic synthesis: A Disconnection Approach*. John Wiley & Sons, New York.
22. Weyerstahl, P. (1996). The Logic of Chemical Synthesis. *Flavour and Fragrance Journal*, *11*(4), 261-262.
23. Silverstein, R. M., Webster, F. X., Kiemle, D. J., & Bryce, D. L. (2014). *Spectrometric Identification of Organic Compounds*. John wiley & sons.
24. Skoog, D. A., Holler, F. J., & Crouch, S. R. (2017). *Principles of Instrumental Analysis*. Cengage learning.
25. James Holler, Timothy A. Nieman. P.imprenta: Madrid, Esp.: McGRAW HILL. *Instrumental Methods of Analysis* – Willards, CBS publishers.
26. Beckett, A. H., & Stenlake, J. B. (Eds.). (1988). *Practical Pharmaceutical Chemistry: Part II*. Fourth Edition (Vol. 2). A&C Black.
27. Kemp, W. (2017). *Organic spectroscopy*. Macmillan International Higher Education.
28. Sethi, P. D. (1985). *Quantitative Analysis of Drugs in Pharmaceutical Formulations*. Unique Publishers.
29. Munson, J. W. (1984). Pharmaceutical analysis: modern methods. B. *Drugs and the Pharmaceutical Sciences*, *11*.
30. Kalsi, P. S. (2007). *Spectroscopy of Organic Compounds*. New Age International.
31. Connors, K. A. (2007). *A Textbook of Pharmaceutical Analysis*. John Wiley & Sons.

The following are some of the modes of classroom transaction:

1) Tutorial
2) Demonstration
3) Group discussion

Transaction Mode

PPT
Three dimensional models
YouTube

Course Title: Project
Paper Code: CMC.599

L	T	P	Credits
0	0	0	6

Learning outcome:

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

- Design a research problem and prepare synopsis
- Plan and execute experiments in the laboratory
- Interpret and analyze the results

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**

1) Lecture
2) Demonstration
3) Lecture cum demonstration
4) Project Method
5) Seminar
6) Group discussion
7) Focused group discussion
8) Team teaching
9) Experimentation
10) Tutorial
11) Problem solving
12) Self-learning

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

PPT
Facebook
WhatsApp
Video
Multimedia packages
TED Talks
google drive

Software tools

- Tracker
- ChemBioDraw
- Schrodinger maestro
- ppt/impress
- Blast
- Endnote

Course Code: CMC.558

L	T	P	Cr
1	0	0	1

Course Title: Modern analytical techniques (VAC)
Total Hours: 15

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

- Describe various modern analytical techniques
- Carry out Structural Elucidation of organic compounds
- Understand basics of various sophisticated instruments

Unit I **4 Hours**

UV-Visible and FT-IR spectroscopy: Basic principles and instrumentation of UV-Visible and FT-IR spectroscopy. Structural elucidation of organic compounds using UV-Visible and FT-IR spectroscopy.

Unit II **3 Hours**

NMR spectroscopy: Basic principles and instrumentation of NMR spectroscopy. Structural elucidation of organic compounds using 1-D and 2-D NMR, NOESY and COSY techniques.

Unit III **4 Hours**

Mass Spectrometry: Basic principles and instrumentation. Various fragmentation techniques and ring rule. Structural elucidation of organic compounds using mass spectrometry techniques.

Unit IV **4 Hours**

Chromatography: Basic principles and instrumentations of chromatographic techniques including HPLC, UPLC, HPTLC LC-MS and GC-MS.

Suggested Readings:

1. Kemp, W. (1991). *Organic spectroscopy* (pp. 42-51). London: Macmillan.
2. Munson, J. W. (Ed.). (1984). *Pharmaceutical analysis: modern methods* (Vol. 11). CRC Press.
3. Sethi, P. D. (1996). *HPTLC: high performance thin-layer chromatography; quantitative analysis of pharmaceutical formulations*. CBS publishers & distributors.
4. Sethi, P. D. (1985). *Quantitative analysis of drugs in pharmaceutical formulations*. CBS Publishers, New Delhi, 1997.
5. Silverstein, R. M., Webster, F. X., Kiemle, D. J., & Bryce, D. L. (2014). *Spectrometric identification of organic compounds*. John wiley & sons.
6. Skoog, D. A., Holler, F. J., & Crouch, S. R. (2017). *Principles of instrumental analysis*. Cengage learning.
7. Willard, H. H., Merritt Jr, L. L., Dean, J. A., & Settle Jr, F. A. (1988). *Instrumental methods of analysis.*

The following are some of the modes of classroom transaction:

1) Demonstration
2) Group discussion
3) Tutorial
4) Self-learning

Transaction Mode

YouTube
PPT