Annexure I
W.E.F. 2017-18
Centre for Pharmaceutical Sciences and Natural Products

M.Sc. in Chemical Sciences (Medicinal Chemistry)
Duration of the Course: **Two Years**

SEMESTER 1

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	Weightage (%)				E
								A	B	C	D	
1	CMC.501	Computer Applications	FC	2	-	-	2	10	15	15	10	50
2	CMC.506	Organic Chemistry-I	CC	4	1	-	4	25	25	25	25	100
3	CMC.507	Organic Synthesis-I (Practical)	CC	-	-	4	2	-	-	-	-	50
4	CMC.508	Modern Spectral and Chromatography Techniques	CC	4	1	-	4	25	25	25	25	100
5	CMC.509	Spectral Analysis (Practical)	CC	-	-	4	2	-	-	-	-	50
6	CMC.510	Medicinal Chemistry-I	EC	4	1	-	4	25	25	25	25	100
7	CMC.597-Seminar-I	Seminar	FC	-	-	-	2	-	-	-	-	50
8	XXX	Inter-Disciplinary (IDC) Course (Opt any one from other Centres)	EC	2	-	-	2	10	15	15	10	50
		Total		**16**	**3**	**8**	**22**					**550**

FC: Foundation Course, **CC**: Core Course, **EC**: Elective Course

A: Surprise Tests: (Based on Objective Type Tests), and internal assessment including term paper and assignments.

B: Mid-Semester Test – I: Based on Subjective Type Test

C: Mid-Semester Test – II: Based on Subjective Type Test

D: End-Term Exam (Final): Online Objective Type Test

E: Total Marks

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

SEMESTER 2

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	Weightage (%)				E
								A	B	C	D	
1	CMC.521	Organic Chemistry-II	CC	4	1	-	4	25	25	25	25	100
2	CMC.522	Organic Synthesis-II-(Practical)	CC	-	-	4	2	-	-	-	-	50
3	CMC.523	Medicinal Chemistry-II	EC	4	1	-	4	25	25	25	25	100
4	CMC.524	Basics of Drug Design and Drug Action	EC	4	1	-	4	25	25	25	25	100
5	CMC.525	Computer Aided Drug Design-(Practical)	CC	-	-	4	2	-	-	-	-	50
6	CMC.597-Seminar-II	Seminar	FC	-	-	-	2	-	-	-	-	50
7	XXX	Inter-Disciplinary Course (ID) (Opt any one from other Centres)	EC	2	1	-	2	10	15	15	10	50
Opt any one course from following elective courses												
8	CMC.526	Chemistry of Natural Products	EC	4	-	-	4	25	25	25	25	100
	CMC.527	Quantum Chemistry										
		Total		**18**	**4**	**8**	**24**					**600**

FC: Foundation Course, **CC**: Core Course, **EC**: Elective Course

A: Surprise Tests (Based on Objective Type Tests), and internal assessment including term paper and assignments.

B: Mid-Semester Test – I: Based on Subjective Type Test

C: Mid-Semester Test – II: Based on Subjective Type Test

D: End-Term Exam (Final): Online Objective Type Test

E: Total Marks

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

SEMESTER 3

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	Weightage (%)				E
								A	B	C	D	
1	CMC.551	Organic Chemistry-III	EC	4	1	-	4	25	25	25	25	100
2	CMC.552	Medicinal Chemistry-III	CC	4	1	-	4	25	25	25	25	100
3	CMC.553	Organic Chemistry-III (Practical)	EC	-	-	4	2	-	-	-	-	50
4	CMC.554	Green Chemistry	CC	4	1	-	4	25	25	25	25	100
5	CMC.555	Bioorganic Chemistry	CC	4	1	-	4	25	25	25	25	100
6.	CMC.597-Seminar-III	Seminar	FC	-	-	-	2	-	-	-	-	50
Opt any one course from following elective												
7	CMC.556	Bioinorganic and Biophysical Chemistry	EC	4	1	-	4	25	25	25	25	100
	CMC.557	Current Trends in Organic Synthesis										
	CMC.558	Nuclear Chemistry										
	Total			**20**	**5**	**4**	**24**					**600**

FC: Foundation Course, **CC**: Core Course, **EC**: Elective Course

A: Surprise Tests (Based on Objective Type Tests), and internal assessment including term paper and assignments.

B: Mid-Semester Test – I: Based on Subjective Type Test

C: Mid-Semester Test – II: Based on Subjective Type Test

D: End-Term Exam (Final): Online Objective Type Test

E: Total Marks **L: Lectures T: Tutorial P: Practical Cr: Credits**

SEMESTER 4

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	Weightage (%)				E
								A	B	C	D	
1	CMC.571	Organic Chemistry - IV	EC	4	1	-	4	25	25	25	25	100
2	CMC.599	Project Work	CC	-	-	-	20	-	-	-	-	-
		Total		**4**	**1**	**-**	**24**					

CC: Core Course, **E**C: Elective Course

A: Surprise Tests (Based on Objective Type Tests), and internal assessment including term paper and assignments.

B: Mid-Semester Test – I: Based on Subjective Type Test

C: Mid-Semester Test – II: Based on Subjective Type Test

D: End-Term Exam (Final): Online Objective Type Test

E: Total Marks

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

Semester 1

Course Title: Computer Applications
Paper Code: CMC.501

L	T	P	Credits	Marks
2	1		2	50

Unit I **18 hours**

Fundamentals of Computers: Parts of computers, Hardware, BIOS, Operating systems, Binary system, Logic gates and Boolean Algebra. Introduction to computer network and World Wide Web, Storage space, CPU and Memory. MS Word (Word Processing, Creating and Saving Documents, Text Formatting, Tables, Document Review Option, Inserting Table of Contents), Power point, Excel sheet.

Unit II **18 hours**

Scientific information retrieval and web browsing: Introduction to various search engines such as Protein Data Bank, PubMed, NISCAIR, ACS, RSC, Elsevier, SciFinder, Google Scholar, Google patent, Espacenet, Beilstein databases, etc. Bibliography management and research paper formatting using reference software EndNote and reference manager. Sketching of molecules using ChemBio Draw, ChemSketch, etc.

Suggested Readings

1. Gookin, D. 2007. MS Word for Dummies. Wiley.
2. Harvey, G. 2007. MS Excel for Dummies. Wiley
3. Sinha, P.K. Computer Fundamentals. BPB Publications.
4. Bott, E. 2009. Windows 7 Inside Out. Microsoft Press.
5. Goel, A., Ray, S. K. 2012. Computers: Basics and Applications. Pearson Education India.

Course Title: Organic Chemistry-I

Paper Code: CMC.506

L	T	P	Credits	Marks
4	1	0	4	100

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

- Understand the stereochemistry, spatial arrangement of atoms/groups and apply it on the course of reactions and mechanism prediction.
- The basics of organic chemistry will enable understand students to build knowledge in drug synthesis and their interaction with receptors

Unit 1 **22 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 2 **18 hours**

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

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

Aromatic electrophilic substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams, *ortho/para* ratio, ipso attack, orientation in other ring

systems, quantitative treatment of reactivity in substrates and electrophiles, Diazonium coupling, Vilsmeier–Haack reaction.

Unit 3 **16 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 4 **16 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, 2nd edition
2. Finar, I.L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, 6th edition, UK.
3. Mc Murry J., *Organic Chemistry***,** Asian Book Pvt. Ltd, 8th edition, 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., 4th edition, New Delhi-110002.
6. Bansal, R. K., (2010). *A text book of Organic Chemistry*,New Age Inrternational (P) Ltd., 5th edition, 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., 3rd edition, 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., 3rd edition, New York.

11. Morrison, R.T., Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of India, 6th edition, New Delhi.
12. Mukherjee, S.M. Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry.* Macmillan India Ltd., 3rd edition, New Delhi.
13. Robert and Casereo, (1977). *Basic principle of Organic Chemistry***,** Addison-Wesley, 2nd edition.
14. Solomn, C.W.G, Fryble, C.B. (2009). *Organic Chemistry*. John Wiley and Sons, Inc., 10th edition.
15. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, 6th edition.
16. Eliel, E. L., & Wilen, S. H. (2008). *Stereochemistry of organic compounds*. John Wiley & Sons.

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

L	T	P	Credits	Marks
-	-	4	2	50

1. Demonstration of Stereochemical aspects of the compounds through molecular models.
2. Awareness to various glasswares and plasticwares used in the organic synthesis.
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 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

Course Title: Modern Spectral & Chromatographic Techniques

Paper Code: CMC.508

L	T	P	Credits	Marks
4	1	-	4	50

Learning Outcomes

- Explain the general principle and theory of spectroscopy
- Describe the concept and instrumentation of UV-Vis, IR, NMR, Mass and Chromatographic techniques
- To study the spectra of the compounds and propose structure of the compounds
- Separation and identification of constituents of mixture by chromatographic techniques

Unit 1 **14 hours**

UV-Visible spectroscopy: Principle of UV-Visible Spectroscopy, Role of solvents, Chromophores and their interaction with UV-visible radiation and their utilization in structural, qualitative and quantitative analysis of drug molecules. Woodward-Fieser rules, stereochemical aspects.

Infrared Spectroscopy: Infrared radiation and its interaction with organic molecules, vibrational mode of bonds, instrumentation and FT-IR, applications, effect of hydrogen bonding and conjugation on absorption bands, interpretation of IR spectra

Unit 2 **16 hours**

Nuclear magnetic resonance spectroscopy: Magnetic properties of nuclei, Field and precession, Chemical shift concept, Isotopic nuclei, Reference standards and solvents. ^{1}H-NMR spectra, Relaxation processes, Chemical shifts, Spin spin coupling, Coupling constants, Integration of signals, Interpretation of spectra, Decoupling, double resonance and shift reagent methods, Long range coupling, Resonance of other nuclei e.g. ^{19}F, ^{15}N, ^{31}P

Unit 3 **16 hours**

Principles of FT-NMR with reference to ^{13}C NMR, Free induction decay, Average time domain and frequency domain signals, Spin-spin and spin-lattice relaxation phenomenon, Nuclear Overhauser enhancement (NOE), ^{13}C NMR spectra, their interpretation and application. DEPT techniques, Principle of 2-D NMR, Correlation spectroscopy (COSY) Homo COSY (^{1}H-^{1}H COSY), Hetro COSY (^{1}H-^{13}C COSY, HMQC), long range ^{1}H-^{13}C COSY (HMBC), NOESY

Unit 4 **16 hours**

Mass spectrometry: Basic principles and brief outline of instrumentation, Ion formation, molecular ion, metastable ion, Mc Lafferty rearrangement, Nitrogen rule, fragmentation process in relation to molecular structure and functional groups. Relative abundance of

isotopes, chemical ionization, FAB, ESI, MALDI and other recent advances in mass spectrometry

Unit 5 **12 hours**

Chromatographic techniques: Principle andClassification of chromatography, Criteria for selection of stationary and mobile phase, Nature and types of mobile phases, Normal and reversed phase, Separation mechanism, Applications of Chromatography in different fields of Sciences, Column chromatography, TLC, LC, GC, HPTLC.

Suggested Readings:

1. Banwell, C.N.; McCash, E. M. (2000). *Fundamentals of Molecular Spectroscopy*, Tata McGraw-Hill, New Delhi.
2. Dyer, J.R. (2009). *Application of Absorption Spectroscopy of Organic Compounds*, Publisher: Phi Learning.
3. Kalsi, P.S. (2004). *Spectroscopy of Organic Compounds*, New Age International Ltd.
4. Kemp, W. (Latest edition). *Organic spectroscopy*, ELBS London.
5. Khopkar, S.M. (2007). *Basic Concepts of Analytical Chemistry***,** New Age International Pvt. Ltd.
6. Melinda J.D., (2010). *Introduction to Solid NMR Spectroscopy*,Wiley India Pvt. Ltd.
7. Mendham, J.; Denney, R.C.; Barnes, J. D.; Thomas, M. J. K. (2003). *Vogel's Textbook of Quantitative Chemical Analysis***,** Pearson Education Pvt. Ltd., New Delhi.
8. Pavia, D.L.; Lampman, G. M. (2010). *Introduction to Spectroscopy***,** G. S. Kriz, Harcourt College, NY.
9. Popov, A.I.; Halenga, K. (1991). *Modern NMR Techniques dnd Their Applications***,** Marcel Deckker.
10. Silverstein, R. M., Webster, F. X., Kiemle, D., & Bryce, D. L. (2014). *Spectrometric Identification of Organic Compounds*. John Wiley & Sons.
11. Skoog, D.A.; West, D.M.; Holler, F.J.; Crouch, S.R. (2004). *Fundamental of Analytical Chemistry*, Saunders College Publishing, New York.
12. Williams, D.H.; Fleming, I. (2004). *Spectroscopy Methods in Organic Chemistry*, Tata McGraw-Hill Publishing Co. Ltd., New Delhi.
13. Sethi, P. D.; Sethi, R. (2007). *HPLC: High Performance Of Liquid Chromatography*, Vol 2, CBS
14. Willard, H.H.; Merrit, L.L.; Dean, J.A.; Settle, F.A. (2001). *Instrumental Methods of Analysis*, CBS Publishers and Distributors.

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

L	T	P	Credits	Marks
-	-	4	2	50

1) Exercises of structure elucidation of unknown compounds *via* spectral interpretation of ^{1}H, ^{13}C NMR, IR, UV and Mass.
2) Hands on experience with various analytical instruments such as FT-IR, UV-vis spectrophotomer, GC-MS, and HPLC.

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

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

L	T	P	Credits	Marks
4	1	0	4	100

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

- Understand basics concepts of drugs, their effects and screening.
- Know how drugs interact with various types of enzymes and receptors
- Know the process of drug discovery and its progress.

Unit 1 **10 hours**

History of drug discovery: Introduction, Drug discoveries, Recent trends in drug discovery.

Unit 2 **20 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 3 **22 hours**

Molecular drug targets: Introduction, Enzymes as drug targets, Membrane transporters as drug targets, Voltage-gated ion channels as drug targets, 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 4 **20 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. (2008). *Principles of Medicinal Chemistry*, Publisher: Lea and Febiger, Philadelphia.
3. King, F. D. (2006). *Medicinal Chemistry Principles and Practice*, Royal Society of Chemistry, Second Edition.
4. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press, Third Edition.
5. Patrick, G.L. (2009). *An Introduction to Medicinal Chemistry*, Publisher: I.K. International Pvt. Ltd.

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, Fourth Edition.
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.

Course Title: Seminar

Paper Code: CMC-597-Seminar-I

L	T	P	Credits	Marks
-	-	4	2	50

Semester –2

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

L	T	P	Credits	Marks
4	1	0	4	100

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

- Understand the disconnection approaches apply it on synthetic strategies and mechanism prediction.
- understand the basics of photochemical reactions that will enable understand students to build knowledge in drug synthesis

Unit 1 **14 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, neighbouring group participation.
Aromaticity: Benzenoid and non-benzenoid compounds – generation and reactions.

Unit 2 **20 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 3 **16 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 4 **22 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. Acheson, R.M. (1976). *An introduction to the Chemistry of heterocyclic compounds*, Wiley India Pvt. Ltd., 3rd edition.
2. Clayden, J., Greeves, N., Warren, S., Wothers, P. (2012). *Organic chemistryOrganic Chemistry*Oxford press, 2nd edition
3. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*,Narosa Publishing House (P) Ltd., 4th edition, India.
4. Bansal, R. K., (2012). *Organic Reaction Mechanism*, New Age International (P) Ltd., 4th edition, New Delhi.
5. Bansal, R. K., (2007). *A text book of Organic Chemistry*,New Age Inrternational (P) Ltd., 5th edition, New Delhi.
6. Bansal, R.K. (2010). *Hetrocyclic Chemistry*, New Age Inrternational (P) Ltd., 5th edition, New Delhi.
7. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B, Springer, 5th edition*.
8. Finar, I. L., (2012). *Organic Chemistry Vol. 1,* Pearson Education, 6th edition, UK.
9. Gilchrist, T.L. (1997). *Heterocyclic Chemistry*, Longman, Prentice Hall, 3rd edition, 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, 5th edition, New York.
12. Kalsi P. S., (2010). *Organic Reactions and Their Mechanisms*, New Age International Publication, 3rd edition, New Delhi.
13. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, 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 Chemistr*y Elsevier, 3rd edition, 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, *The Logic of Chemical Synthesis*, Pubs: John Wiley & Sons, (1989).

Course Title: Organic Synthesis-II (Practical)

Paper Code: CMC.522

L	T	P	Credits	Marks
-	-	4	2	50

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 alcoholcs 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.

Course Title: Medicinal Chemistry-II
Paper Code: CMC.523

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 18 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 2 18 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 3 **18 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 4 **18 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. (2008). *Principles of Medicinal Chemistry*, Publisher: Lea & Febiger, Philadelphia.
3. King, F. D. (2006). *Medicinal Chemistry Principles and Practice*, Royale Society of Chemistry, 2nd edition, London.
4. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press, 3rd edition, UK.
5. Patrick, G.L. (2009). *An Introduction to Medicinal Chemistry*, Oxford University Press, 4th edition, US.
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, 4th edition.
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, 7th edition, New York.

Course Title: Basics of Drug Design and Drug Actions

Paper Code: CMC.524

L	T	P	Credits	Marks
4	1	0	4	100

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

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

Unit 1 **14 hours**

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

Theoretical Aspects of Drug Action: Drug distribution, Active transport, Passive transport, The Ferguson Principle Physicochemical Parameters and Pharmacological Activity-Solubility, Partition Coefficient, Surface Activity, pKa, Ionisation, Stereochemical Factors, Bio-isosterism.

Unit 2 **14 hours**

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

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

Unit 3 **24 hours**

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

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

Unit 4 **20 hours**

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

Suggested Readings:

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

Course Title: Computer Aided Drug Design (Practical)

Paper Code: CMC.525

L	T	P	Credits	Marks
-	-	4	2	50

Following practicals utilizing the available softwares such as ChemBio Draw, Autodock, Schrodinger, etc. need to be conducted.

1) Determination of logP, MR, HBD and HBA of selected drugs
2) Calculation of ADMET properties of drugs molecules and their analysis
3) Homology Modelling based experiments.
4) Practical based on 2D and 3D-QSAR of drug molecules.
5) Docking and virtual screening based experiments.

Course Title: Seminar

Paper Code: CMC.597-Seminar-II

L	T	P	Credits	Marks
-	-	4	2	50

Elective courses

Course Title: Chemistry of Natural Products

Paper Code: CMC.526

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **18 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 2 **18 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: Forskolin, Rohitukine (Flavopiridol) and Morphine.

Unit 3 **18 hours**

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

Unit 4 **9 hours**

Plant pigments: Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of anthocyanins and flavonoids.

Unit 5 **9 hours**

Carbohydrates: Introduction of sugars, structures of triose, tetrose, pentose, hexose, stereochemistry and reactions of Glucose, conformation and anomeric effects in hexoses, oligosaccharides/polysaccharides.

Suggested Readings:

1. Bhat, S.V., Nagasampagi, B.A., Meenakshi, S. (2009). *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, 2nd edition, US.
5. Dewick, P.M. (2009). *Medicinal Natural Products: A Biosynthetic Approach*. Willey & Sons, 3nd edition, UK.
6. Finar, I.L. (2006). *Organic Chemistry: Stereochemistry and the Chemistry of Natural Products.* Dorling Kindersley Pvt. Ltd., 6th edition, India.
7. Peterson, F., Amstutz, R. (2008). *Natural Compounds as drugs.* Birkhauser Verlay.
8. Thomson, R.H. (2008). *The Chemistry of Natural Products*, Springer, 1st edition.

Course Title: Quantum Chemistry
Paper Code: CMC.527

L	T	P	Credits	Marks
4	1	0	4	100

Course objective: To acquire knowledge of the quantum chemical description of chemical bonding, reactivity and their applications in molecular spectroscopy and inorganic chemistry.

Unit 1 **18 Hrs**

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 2 **18 Hrs**

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

Unit 3 **18 Hrs**

Angular Momentum: Ordinary angular momentum, Eigen functions and Eigen values for angular momentum, Addition of angular momenta, Spin, Antisymmetry 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 4 **18 Hr**

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.

Course Outcome: The students will acquire knowledge of

1. Schrodinger equation for a particle in a box and quantum chemical description.
2. Electronic and Hamiltonian operators for molecules.
3. Quantum chemical description of angular momentum and term symbols for a one and many-electron systems.
4. Born-Oppenheimer approximation, the Pauli principle, Hund's rules, Hückel theory and the variation principle.

SUGGESTED READINGS

1. Levine, I.N. Quantum Chemistry, 5th edition, 2000, Pearson Educ., Inc. New Delhi.
2. Chandra, A.K. Introductory Quantum Chemistry, 4th Edition, 1994, Tata Mcgraw Hill.
3. Prasad, R.K., Quantum Chemistry, 4th Edition, 2009, New Age Science.

4. McQuarrie, D. A. and Simon, J. D. Physical Chemistry: A Molecular Approach, 1st edition, 1998, Viva Books.
5. Murrell, J.N. Kettle S.F.A. and Tedder, J. M. Valence Theory, 2nd edition, 1965, John Wiley.
6. Lowe, J. P. and Peterson, K. Quantum Chemistry, 3rd Edition, 2006, Academic Press.

Semester –3

Course Title: Organic Chemistry-III

Paper Code: CMC.551

L	T	P	Credits	Marks
4	1	0	4	100

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

- Propose and determine the mechanism and feasibility of a chemical reaction
- Apply principle of photochemistry in various chemical transformations
- Explore various metal and non-metal reagents towards oxidation and reduction reactions
- Name different fused and bridged heterocyclic compounds and perform their synthesis through different methods

Unit 1 **16 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 2 **16 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 3 **18 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 4 **22 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., 3rd edition.
2. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*,Narosa Publishing House (P) Ltd., 4th edition, India.
3. Bansal, R. K., (2012). *Organic Reaction Mechanism*, New Age International (P) Ltd., 4th edition, New Delhi.
4. Bansal, R. K., (2007). *A text book of Organic Chemistry*,New Age Inrternational (P) Ltd., 5th edition, New Delhi.
5. Bansal, R.K. (2010). *Hetrocyclic Chemistry*, New Age Inrternational (P) Ltd., 5th edition, New Delhi.
6. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B, Springer, 5th edition*.
7. Finar, I. L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, 6th edition, UK.
8. Gilchrist, T.L. (1997). *Heterocyclic Chemistry*, Longman, Prentice Hall, 3rd edition, 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, 5th edition, New York.
11. Kalsi, P. S., (2008). *Stereochemistry: Conformation and Mechanism*, New Age International (P) Ltd., 7th edition, India.
12. Kalsi P. S., (2014). *Organic Reactions and Their Mechanisms*, New Age International Publication, 3rd edition, New Delhi.
13. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, 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, 3rd edition, 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., 7th edition, India.
19. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, 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.

Course Title: Medicinal Chemistry-III

Paper Code: CMC.552

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **18 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 2 **18 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 3 **18 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 4 **18 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., 7th edition, Philadelphia.
2. Foye, W. O. (2008). *Principles of Medicinal Chemistry*, Publisher: Lea and Febiger, 6th edition, Philadelphia.
3. King, F. D. (2003). *Medicinal Chemistry Principles and Practice*, Royale Society of Chemistry, 2nd Edition, London.
4. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press, 3rd edition, New York.
5. Patrick, G.L. (2009). *An Introduction to Medicinal Chemistry*, Oxford University Press, 4th edition. 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, 4th edition, UK.
8. Wermuth, C.G. (2009). *The Practice of Medicinal Chemistry*, Academic Press (Elsevier), 3rd edition.
9. Wolff, M E, Ed., (2010). *Burger's Medicinal Chemistry and Drug Discovery*, John Wiley and Sons, New York.

Course Title: Organic Chemistry-III (Practical)
Paper Code: CMC.553

L	T	P	Credits	Marks
-	-	4	2	50

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 of ^{1}H, ^{13}C NMR, IR, UV and Mass.

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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

Course Title: Green Chemistry

Paper Code: CMC.554

L	T	P	Credits	Marks
4	1	0	4	100

Learning outcome:

Students who successfully complete this course will be able to

- Understand various aspects of green chemistry for sustainable development
- Utilize ionic liquids and soild supported reaction conditions to reduce or eliminate use of volatile organic solvents
- Use water as solvent in chemical transformations
- Utilize MW and sonicator in organic synthesis

Unit 1 **22 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, 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 2 **20 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. Ionic liquids as green solvents.

Unit 3 **18 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.

Unit 4 **12 hours**

Organic synthesis in aqueous phase and in solid state: Aqueous reactions. Solid state reactions (i) Solid phase synthesis without using any solvent (ii) Solid supported synthesis.

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.

Course Title: Bioorganic Chemistry

Paper Code: CMC.555

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **15 Hrs**

Carbohydrates and Lipids

Classification of carbohydrates, reducing and non-reducing sugars, General Properties of Glucose and Fructose, their open and closed chain structures. Epimers, mutarotation and anomers. Determination of configuration of Glucose (Fischer proof). Linkage between monosaccharides, structure of disaccharides (sucrose, maltose, lactose) and polysaccharides (starch and cellulose) excluding their structure elucidation.

Structural polysaccharides-starch and glycogen. Carbohydrate metabolism-Kreb's cycle, glycolysis, glycogenesis and glycogenolysis, gluconeogenesis.

Fatty acids: essential fatty acids, structure and function of triacylglycerols, glycerophospholipids, sphingolipids, cholesterol, bile acids, lipoproteins-composition and function, role in atherosclerosis. Properties of lipid aggregates-micelles, bilayers, liposomes and their possible biological functions. Biological membranes. Fluid mosaic model of membrane structure.

Unit 2 **14 Hrs**

Amino acids, Peptides, Proteins and Nucleic Acids

Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing.

Secondary structure of proteins, forces responsible for holding of secondary structures. α–helix, β-sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein- folding and domain structure. Quaternary structure. Amino acid metabolism-degradation and biosynthesis of amino acids, sequence determination: chemical/enzymatic/mass spectral, recemization/detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH).

RNA and DNA Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis for heredity, an overview of replication of DNA, transcription, translation and genetic code.

Unit 3 **13 Hrs**

Enzyme and Co-enzyme Chemistry

Inroduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic powder, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by use of inhibitors, affinity labeling and enzyme modification by site directed mutagenesis. reversible and irreversible inhibition.

Transition-state, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortation. Examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A. Cofactors as derived from vitamins, coenzymes, prothetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD+, NADP+, FMN, FAD, lipoic acid, vitamin B12. Mechanisms of reactions catalyzed by the above cofactors.

Unit 4 **12 Hrs**

Organic Macromolecules

Rise of the concept of polymers, general method of preparation, polymerization techniques, mechanistic understanding Polymer geometry, structural unit variety, and structural unit orientation.

Synthesis and modifications of Macromolecules: Polylolefins, polystyrene and styrene copolymers poly vinyl chloride and related polymers, poly vinyl acetate. Acrylic fluoro polymers. Aliphatic polyethers. Polyamides, polyimides, polyesters, phenolformaldehyde polymers. Amino-polymers Polyurethanes, oxides. Polydienes rubbers. Modification in natural polymers such as cellulose and proteins.

Suggested Books

1. Principles of Biochemistry, A. L. Lehninger, Worth Publishers., Latest edition
2. Biochemistry, L. Stryer, W. H. Freeman, Latest edition
3. Outlines of Biochemistry, E. E. Conn and P. K. Stumpf, John Wiley, Latest edition
4. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer Verlag, Latest edition
5. Understanding Enzymes, Trevor Palmer, Prentice Hall, Latest edition
6. Enzyme Chemistry: Impact and Applications, Ed. Collin J. Suckling, Chapman and Hall, Latest edition
7. Enzyme Mechanisms Ed, M. I. Page and A. Williams, Royal Society of Chemistry.
8. Saunders K.J., Organic Polymer Chemistry, 2nd Edn; Pubs: Chapman and Hall, London (1988), Latest edition
9. Creighton T.E., Proteins: Structure and Molecular Properties, Pubs: W.H. Freeman and Co., N.Y., Latest edition

Course Title: Seminar
Paper Code: CMC. 597-Seminar-III

L	T	P	Credits	Marks
-	-	4	2	50

Course objective: The course would develop scientific aptitude, critical thinking, research writing and research presentation.

The seminar must include discussion on topics such as awareness about weapons of mass destruction (chemical, biological, radiological, and nuclear weapons), disarmament, peaceful uses of chemistry, International Regulation of Biological and Chemical or Weapons of Mass Destruction.

Course outcome: The student would be able to

1. Investigate various aspects related to the chemistry problem.
2. Appreciate the literature and its relevance to his topic of interest
3. Technical write and presentation the chemical problem in hand.
4. Generate interest in current topics of research and commercial worth of chemistry.

Elective courses

Course Title: Bioinorganic Chemistry and Biophysical Chemistry

Paper Code: CMC.556

L	T	P	Credits	Marks
4	1	0	4	100

Learning outcome:

Students who successfully complete this course will be able to

- Understand various aspects of electronic distribution in different energy levels
- Students will understand stereo-chemical aspects of metal complexes and their application in medicinal chemistry
- Understand the phenomenon of reaction kinetics and their applications in medicinal chemistry
- Understand partition coefficient of solutes in different solvent, phenomenon of adsorption and electrochemistry

Unit 1 **15 Hrs**

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 2 **15 Hrs**

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 3 **14 Hrs**

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 4 **13 Hrs**

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.

Unit 5 **15 Hrs**

Electrochemistry: Nernst equation, redox systems, electrochemical cells; electrolytic conductance–Kohlrausch's law and its applications; Fugacity and activity; Activity-coefficients, mean activity coefficients; Debye-Huckel theory (point ion size and finite ion size model); Excess functions; Conductometric and potentiometric titrations.

Nuclear Chemistry: Classification of nuclides, Nuclear stability, Atomic energy, Types of nuclear reactions-fission and fusion, Conservation in nuclear reactions-linear momentum and mass-energy, Reaction cross-section, Bohr's compound nucleus theory of nuclear reaction.

Suggested Books

1. Drago, Russell S. *Physical Methods for Chemists*, 2nd edition, Saunders College Publishing, 1992.
2. Ebsworth, E.A.V.; Rankin, D.W.H.; Cracock, S. *Structural Methods in Inorganic Chemistry*, 1st edition, ELBS, 1987.
3. Cotton, F.A.; Lippard, S.J. *Progress in Inorganic Chemistry,* Vol. 8, Vol. 15, Wiley Internationals.
4. Huheey, James E. *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th edition, Harper Collins College Publishers, 1993
5. Physical Chemistry, G. M. Barrow, TATA MCGRAW-HILL, 2007.
6. Text Book of Physical Chemistry, K. L. Kapoor, MACMILLAN, 2006.
7. Physical Chemistry, A. W. Atkins, W. H. Freeman, and Company, 1997.
8. Physical Chemistry: A Molecular Approach, D. A. McQuarrie, and J. D. Simon,Viva Books, 2011.
9. Kinetics and Mechanism, J. W. Moore, and R. G. Pearson, John Wiley and Sons, 1981.
10. Physical Chemistry, R. J. Silbey, R. A. Alberty, and M. G. Bawendi, Wiley-Interscience Publication, 2013.
11. Physical Chemistry, T. Engel, and P. Reid, Prentice-Hall, 2012.

Course Title: Current Trends in Organic Synthesis
Paper Code: CMC.557

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **18 Hrs**

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 2 **18 Hrs**

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 3 **18 Hrs**

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

Unit 4 **18 Hrs**

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.

ESSENTIAL BOOKS:

1. Finar, I.L., (2012). *Organic Chemistry Vol. 1***,** Pearson Education, 6th edition, UK.
2. Finar, I.L., (2012). *Organic Chemsitry Vol. 2*: *Stereochemistry and The Chemistry of Natural Products,* Pearson Education, 6th edition, 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., 3rd edition, 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., 8th edition, New York.
15. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, 6th edition, US.
16. W. Carruthers, (2004). *Some Modern Methods of Organic Synthesis***,** Cambridge Uni. Press, 4th edition, UK.

Course Title: Nuclear Chemistry
Paper Code: CMC.558

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **16 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 2 **20 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 3 **20 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 4 **16 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

ESSENTIAL BOOKS:

1. Friedlander, Kennedy and Miller, Nuclear and Radio Chemistry: John Wiley
2. B.G. Harvey, Nuclear Chemistry
3. Hassinsky: Translated by D.G. Tuck, Nuclear Chemistry and its application: Addison Wiley
4. B.G. Harvey, Introduction to Nuclear Physics and Chemistry

5. Maeclefort: Nuclear Chemistry: D.Van Nostrand
6. An N.Nesmeyannoy: Radiochemistry: Mir
7. Jacobs et al: Basic Principles of nuclear Science and Reactors, V.Nost & EWAP
8. N. Jay: Nuclear Power Today Tomorrow: ELBS
9. Kenneth: Nuclear Power Today, Tomorrow: ELBS
10. Essentials of Nuclear Chemistry, H.J. Arnikar, John Wiley
11. Nuclear and Radiation Chemistry: B.K. Sharma, Krishna Publication
12. A Introduction to Nuclear Physics: R. Babber and Puri

Semester-4

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

L	T	P	Credits	Marks
4	1	0	4	100

Learning Outcomes:

Students who successfully complete this course will be able to:

- Understand the asymmetric synthesis, chiral resolution and apply it on the resolution of chiral drugs.
- The basics of organic chemistry will enable understand students to build knowledge in drug synthesis and their interaction with receptors

Unit 1 **14 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 2 **18 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 3 **20 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 4 **20 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,Crownethers, 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.

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*, *Vol 1-26.* Wiley Interscience, 3rd edition.
3. Finar, I.L., (2012). *Organic Chemistry*, Pearson Education, 6th edition, UK.
4. Li, J.J., (2009). *Name Reactions: A Collection of Detailed Reaction Mechanism*, Springer, 4th edition.
5. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
6. Reich, H.J., Rigby, M., (1999). *Handbook of Reagents for Organic Synthesis Acidic and Basic Reagents VoI. IV*Wiely-Interscience
7. Warren, S., (2010). *Organic synthesis: The Synthon Approach*. John wiley& Sons, New York,
8. Warren, S., (2010). *Designing organic synthesis: A Disconnection Approach*. John Wiley & Sons, New York.
9. Corey E.J., Cheng Xue-Min, The Logic of Chemical Synthesis, Pubs: John Wiley & Sons, (1989).
10. FuhrhopJurgen, Penzlin Gustav, Organic Synthesis: Concepts methods, Starting Materials, Pubs: Verlagchemie, (1994).
11. Stuart Warren, Organic Synthesis: The Disconnection Approach, Pubs: John Wiley & sons (1982).
12. Devies Stephen G., Organotransition Metal Chemistry: Application to Organic Synthesis, Pubs: Pergamon Press (1994).
13. Morrison J. D. (eds) Asymmetric Synthesis, Vol. 1 to 5, Pubs:Academic Press.(1992).
14. Aitken R.A. and Kilenyi S.N., Asymmetric Synthesis, Pubs:Academic Press. (1994).
15. Proctor Garry, Asymmetric Synthesis, Pubs:Academic Press (1996)

Course Title: Project Work
Paper Code: CMC.599

L	T	P	Credits	Marks
-	-	-	20	-