Maulana Abul Kalam Azad University of Technology, West Bengal

Course: M.Sc. in Applied Chemistry

Duration: 2 Years; **Level**: Post graduation; **Type**: Degree

SEMESTER - I

Sl. No.	Paper code	Course name	Course type	Marks	Hours/credit			
					L	T	P	C
1.	MSAC-101	Biochemistry & Bioinorganic Chemistry	CF	100	3	0	0	3
2.	MSAC -102	Organic Chemistry I	CC	100	3	0	0	3
3.	MSAC -103	Statistical methods for Chemical and Biochemical Applications	DSE	50	2	0	0	2
4.	MSAC -104	Computer Aided Advanced Physical Chemistry	CC	100	3	0	0	3
5.	MSAC -105	Analytical Lab Techniques	CC	100	3	0	0	3
6.	MSAC-106	Research Methodology (From MOOC basket / 8-12 weeks)	VAC	100	2	0	0	2
7.	MSAC-191**(Lab)**	Lab techniques for quantitative and qualitative analysis	CC	100	0	0	6	3
8.	MSAC -192**(Lab)**	Introduction to programming and simulation applications for Physical/Chemical/Biological Problems	CC	100	0	0	6	3
9.	MSAC-193**(Lab)**	Computer Aided Determination of Stereo-chemical outcome of complex chemical reaction	CC	50	0	0	4	2
	Total			**800**	**24**			

SEMESTER - II

Sl. No.	Paper code	Course name	Course type	Marks	Credit			
					L	T	P	C
1.	MSAC -201	Quantum Chemistry	CC	100	3	0	0	3
2.	MSAC-202	Statistical Mechanics	CC	100	3	0	0	3
3.	MSAC -203	Organic Chemistry II	CC	100	3	0	0	3
4.	MSAC -204	Nano science and technology	DSE	100	3	0	0	3
5.	MSAC-205	Computational Methods	CC	100	3	0	0	3
6.	MSAC -206	Natural Products and Medicinal Chemistry	IDE	100	3	0	0	3
7.	MSAC -291 **(Lab)**	Computational methods in Chemistry	CC	100	0	0	6	3
8.	MSAC -292 **(Lab)**	Advanced Organic Chemistry Lab	CC	100	0	0	6	3
	Total			**800**	**24**			

SEMESTER - III

Sl. No.	Paper code	Course name	Course type	Marks	Credit			
					L	T	P	C
1.	MSAC -301	Bioorganic and Supramolecular Chemistry	CC	100	3	0	0	3
2.	MSAC -302	Industrial Chemistry	CF	100	3	0	0	3
3.	MSAC -303	Elective I	EF	100	3	0	0	3
4.	MSAC -304	Elective II	EF	100	3	0	0	3
5.	MSAC-391	Industrial Exposure	VAC	50	0	0	2	2
6.	MSAC-392	Mini Project and Seminar Presentation	SEC	50	0	0	2	2
7.	MSAC-393 **(Lab)**	Programming Lab - Python	SEC	100	0	0	4	2
8.	MSAC -394 **(Lab)**	Preparation of complex materials and their characterization by physiochemical techniques	CC	100	0	0	6	3
9.	MSAC -395 **(Lab)**	Spectroscopic Analysis Lab	CC	100	0	0	6	3
	Total			**800**	**24**			

SEMESTER - IV

Sl. No.	Paper code	Course name	Course type	Marks	Credit			
					L	T	P	C
1.	MSAC -401	Elective III	EF	100	3	0	0	3
2.	MSAC -491 **(Lab)**	Project Stage-I (Term paper focus on project & Seminar)	--	20	5			
3.	MSAC -492 **(Lab)**	Project Stage-II (Dissertation & Viva voce)	--	80	16			
	Total			**200**	**24**			

CC: Core Course, **VAC**: Value Added Course, **SEC:** Skill Enhancement Course, **IDE:** Interdisciplinary Course, **DSE:** Discipline Specific Course, **EF:** Elective Foundation, **CF:** Compulsory Foundation.

Electives:

1. Cheminformatics
2. Photochemistry and spectroscopy
3. Pharmaceutical Chemistry
4. Water and Wastewater Treatment
5. Solid Waste Management and Air Pollution
6. Industrial Catalysis
7. Industrial & Environmental Pollution Management and Industrial Process Safety
8. Alternative and green energy, solar cell and perovskite
9. Food Chemistry
10. Sensor Development
11. Semiconductor devices

Semester	Course Hours/week	Marks	Course credit
I	32	800	24
II	30	800	24
III	28	800	24
IV	45	200	24
	Total	**2600**	**96**

Maulana Abul Kalam Azad University of Technology, West Bengal

Course: M.Sc. in Applied Chemistry
Duration: 2 Years; **Level**: Post graduation; **Type**: Degree

SEMESTER-I

Biochemistry and Bioinorganic Chemistry

Paper code: MSAC-101
(3 Credit) (100 Marks)

Course Objectives (CO):

1. To gain knowledge on different interactions and energy change in cells can be understood. This will help in biochemical applications.
2. To gain knowledge on different methods of Preparation of organometallic compounds will be known and may be applied to industry.
3. T learn structure and bonding involved in supramolecules can be determined. These molecules are required in industry.
4. Transport of different elements and energy within cells can be determined which has applications in pharmaceutical field.

Module 1: Unit 1: Basics of Biochemistry (8L)
Principles of biophysical chemistry, Thermodynamics, Colligative properties, Stabilizing interactions: Van der Waals, Electrostatic, Hydrogen bonding, Hydrophobic interaction, etc.Composition, structure, function and metabolism of Carbohydrates, Lipids, Amino Acids and Nucleotides. Bioimaging.

Module 2: Unit 2: Organometallic Compounds (10L)
Metal carbonyls-synthesis, structure and bonding in mononuclear and polynuclear carbonyls with and without bridging, metal carbonyl hydrides and metal carbonyl clusters. Complexes with linear π donor ligands: olefins, acetylenes, dienes and allyl complexes. Catalysis by organometallic compounds-hydrogenation, hydroformylation and polymerisation reactions. (Wilkinson's catalyst, Ziegler-Natta catalyst & Synthetic gasoline should be included among various examples) and various others applications. Application of C-H, C-X activation and functionalization.

Module 3: Unit 3: Metal-Organic Framework and Covalent Organic Framework (8L)
Macrocycles and supramolecules non-covalent forces and interactions in supramolecules: crown ethers, cryptates, cryptands, carcerands, calixarenes, cyclodextrins, fullerenes, dendrimers, rotaxanes, self-assembly and preorganization, coordination driven self-assembly of supramolecular two and three dimensional architectures, host-guest chemistry, metal-organic frameworks, covalent-organic frameworks and their applications.

Module 4: Unit 4: Bioinorganic Chemistry (10L)

Principles of coordination chemistry related to bioinorganic chemistry, Essential and trace metal ions in biological systems, Porphyrin and related ligands, ATP as energy source, oxidative phosphorylation and phosphorylation of glucose. Transport and storage of dioxygen: Structure and function of hemoglobin, myoglobin, hemocyanin and hemerythrin. Synthetic oxygen carriers. Mechanism of gas transport (e.g.- NO_2, CO_2 etc).

Text Books:

1. F. A. Cotton, G. Wilkinson, C. A, Murillo, and M. Bochmann *Advanced Inorganic Chemistry*, 6th Edition Wiley-Interscience: New York, 1999.
2. D. F. Shriver, P. W. Atkins, C. H. Langford, *Inorganic Chemistry*, 3rd Ed. ELBS, 1999.

Reference texts:

1. J. W. Steed, J. L. Atwood, *Supramolecular Chemistry*, 2nd edition, John Wiley & Sons Ltd., (2009)
2. B. Douglas, D. McDaniel, J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3rd Ed., Wiley.
3. Berg, J.M., Tymoczko, J.L. and Stryer, L. (2010). *Biochemistry*. W.H. Freeman & Company. USA.
4. Brown, T.A. (2006). *Gene Cloning and DNA analysis: In Introduction*. Blackwell Publishing Professional. USA.
5. Haynie, D.T. (2007). *Biological thermodynamics*.Cambridge University. UK.
6. Mathews, C.K., Van Holde, K.E. and Ahern, K.G. (2000). *Biochemistry*. Oxford University Press Inc. New York.
7. J.E. Huheey, Ellen A. Keiter and Richard L. Keiter "*Inorganic Chemistry, Principles of structure and Reactivity*", 4th Ed., Harper Collin College Publishers, 1993

Sl.No	Content of the course	Module No.	%age of questions	Course Outcomes (CO)
1.	Basics of biochemistry	Module-1/ Unit-1	20%	1. Different interactions andenergy change in cells can be understood. This will help in biochemical applications.
2.	Organometallic compounds	Module-2/Unit-2	30%	2. Different methods of Preparation of organometallic compounds will be known and may be applied to industry.
3.	Metal-organic framework and covalent organic framework	Module-3/Unit-3	20%	3. Structure and bonding involved in supramolecules can be determined. These molecules are required in industry.
4.	Bioinorganic chemistry	Module-4/Unit-4	30%	4. Transport of different elements and energy within cells can be determined which has applications in pharmaceutical field.

Organic Chemistry-I

Paper code: MSAC-102
(3 Credit) (100 Marks)

Course Objectives (CO):

1. To write and assign reactive intermediates, stereochemistry of organic compounds.
2. To learn advanced knowledge of pericyclic and photochemical reactions.
3. To learn about the role and applications of oxidising and reducing agents in organic synthesis
4. To impart advanced knowledge regarding various rearrangement reactions for synthetic applications.

Module 1: Unit 1: Organic Reaction Mechanism and Introduction to Stereochemistry (8L)

Methods of determining reaction mechanisms (kinetic and non-kinetic methods): The Hammond postulate, reactivity vs selectivity principle, the Curtin-Hammett principle, microscopic reversibility, kinetic vs thermodynamic control. Isotope effects. Linear free energy relationships: Hammett and Taft parameters, Solvent effects, nucleophilicity and nucleofugality. Other Experimental techniques to determine reaction mechanisms: cross - over experiments, isotope scrambling. Concept of centre and plane of chirality, axial chirality and point groups.Winstein-Holness equation, Curtin-Hammett principle; Conformational analysis of cyclohexane, cyclohexene, cyclohexanone, alkyl ketone effect, 2- halo ketone effect, allylic strains ($A^{1,2}$ and $A^{1,3}$), decalin and their derivatives; perhydroanthracene, perhydrophenanthrene etc., Felkin-Anh, Cieplak Models; Addition Reactions to Carbonyl Compounds.

Module 2: Unit 2: Pericyclic reactions, Aromatcity, Polynuclear hydrocarbons and Application (10L)

Study of Frontier Molecular Orbital theory, aromatic transtionstate theory and the generalized Woodward – Hoffmann rule applied to cycloaddtions, electrocyclic reactions, sigmatropic rearrangements and chelotropic reactions– Stereochemistry and regiochemistry of cycloaddtions. Secondary orbital interactions in [4+2] cycloadditionsIntramolecular Diels–Alder reactions. 1,3-dipolar cycloaddition reactions. Photochromism and thermochromism, Cope rearrangement, Claisen rearrangement, and ene-reaction.

Aromatcity, Polynuclear hydrocarbons and their applications.

Module 3: Unit 3: Oxidising and reducing agents in organic synthesis (10L)

(a) Oxidation: metal-based oxidants (Cr, Mn, Os, Ag, Ru and Pb); non-metal-based oxidation: Swern oxidation, Moffat oxidation, Organic oxidants, Chemistry of hypervalent iodine based oxidants, CAN as oxidant.

(b) Reduction: metal hydrides (B-H, Al-H, Zn-H, Sn-H, Si-H based reagents); hydrogenation; dissolving metal reductions; samarium iodide, Organic reductants.

Module 4: Unit4: Rearrangements Reactions (8L)

General mechanistic considerations - nature of migration - migratory aptitude -nucleophilic, electrophilic and free radical rearrangements - Wagner-Meerwein,McLafferty, Demyanov, Benzil-benzilic acid, Favorskii, Fritsch-Buttenberg-Wiechell,Neber, Hofmann, Curtius, Beckmann, Schmidt, Lossen, Wolff, Baeyer-Villiger,Dienone-phenol, Pinacol, Stevens, Wittig, Chapman, Wallach, Orton, Bamberger, Pummerer and von Richter rearrangements.

Text Books:

1. March's *Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 7th ed. 2013, Wiley

2. F. A. Carey and R. J. Sundberg: *Advanced Organic Chemistry (parts A and B)*, 5th Edition2008, Springer.
3. J. Clayden, N. Green, S. Warren and P. Wothers: *Organic Chemistry*, 2nd Edition. 2012, Oxford University Press

Refrence texts:

1. T H.Lowry and K.S.Richardson: *Mechanism and Theory in Organic Chemistry*, 3rd ed. 1997, Benjamin-Cummings Publishing Company.
2.F. A. Carroll: *Perspectives on structure and mechanism in organic chemistry*, Wiley, 2011 edition.
3. *Organic Stereochemistry* by P.S. Kalsi.
4. I. Flemming: *Molecular orbitals and organic chemical reactions*, student edition, 2009, Wiley.
5. J. McMurry, *Organic Chemistry*, Fifth Edition, 2000, Brooks/Cole .

Sl.No	Content of the course	Module No.	%age of questions	Course Outcomes (CO)
1.	Organic reaction mechanism and introduction to stereochemistry	Module-1/ Unit-1	20%	1. Learn about reactive intermediates, stereochemistry of organic compounds
2.	Pericyclic reactions, aromatcity, polynuclear hydrocarbons and applications	Module-2/Unit-2	30%	2. To gain advanced knowledge of pericyclic and photochemical reactions
3.	Oxidising and reducing agents in organic synthesis	Module-3/Unit-3	30%	3. To learn about the role and applications of oxidising and reducing agents in organic synthesis
4.	Rearrangement reactions	Module-4/Unit-4	20%	4. To impart advanced knowledge regarding various areaarangement reaction for synthetic applications

Statistical methods for Chemical and Biochemical Applications

Paper code: MSAC-103

(2 Credit) (50 Marks)

Course Objectives (CO):

1. To know different statistical parameters and probability distribution can be learnt, these can be applied for data collection in different fields.
2. To learn various sampling techniques and their comparative studies can be known, which may be applied in different systems.

Module 1: Unit 1: Overview of Bio-Statistics (10L)

Overview of Biostatistics: Difference between parametric and non-parametric statistics, Univariant andmultivariant analysis, Confidence interval, Errors, Levels of significance, Hypothesis testing. Descriptive statistics: Measures of central tendency and dispersal, Histograms, Probability distributions (Binomial, Poisson and Normal), Sampling distribution, Kurtosis and Skewness.

Module 2: Unit 2: Experimental design and analysis of sampling techniques (10L)

Experimental design and analysis: Sampling techniques, Sampling theory, Various steps in sampling, collection of data-types and methods. Inferential Statistics: Student's t-test, Paired t-test, Mann-Whitney U-test, Wilcoxon signed-rank, One-way andtwo-way analysis of variance (ANOVA), Critical difference (CD), Least Significant Difference (LSD), Kruskal–Wallis one-way ANOVA by ranks, Friedman two-way ANOVA by ranks, $\chi 2$ test. Standard errors of regression coefficients, Comparing two regression lines, Pearson Product-Moment Correlation Coefficient, Spearman Rank Correlation Coefficient, Power and sampling size in correlation and regression.

Text books:

1. Norman, G. and Streiner, D. (2008). *Biostatistics: The Bare Essentials*. 3/e (with SPSS). Decker Inc. USA.
2. Sokal, R.R. and Rohlf, F.J. (1994). *Biometry: The Principles and Practices of Statistics in Biological Research*. W.H. Freeman publishers, USA.

Reference texts:

3. Gookin, D. (2007). *MS Word 2007 for Dummies*.Wiley, USA.
4. Johnson, S. (2009). *Windows 7 on demand. Perspiration* Inc. USA.

Sl. No	Content of the course	Module No.	%age of questions	Course Outcome
1	Overview of bio-statistics	Module 1/Unit 1	40%	1. Different statistical parameters and probability distribution will be learnt, these can be applied for data collection in different fields.
2	Experimental design and analysis of sampling techniques	Module 2/Unit 2	60%	2. Various sampling techniques and their comparative studies will be known, which may be applied in different systems.

Computer Aided Advanced Physical Chemistry

Paper code: MSAC-104
(3 Credit) (100 Marks)

Course Objectives (CO):

1. Effectively learn about quantum chemistry.
2. Effectively learn the grouptheory and its use for molecular term symbol.
3. Will be expertise to predict the reaction rate using computer softwere.
4. Will be able to treat ionic reaction probably.
5. Information regarding thermodynamic properties of different systems which may be applied to understand the equilibrium conditions of chemical reactions.

Module 1: Unit 1: Quantum Chemistry **(8L)**

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.

Module 2: Unit 2: Symmetry & Group Theory **(8L)**

Symmetry elements & operations; group, subgroup, class, point groups, group multiplication tables for cyclic and non-cyclic groups; matrix representations of symmetry operations and their characters,reducible representations, irreducible representations and great orthogonality theorem (no derivation), construction of character tables; application of group theory.

Module 3: Unit 3: Thermodynamics **(8L)**

Laws of Thermodynamics, General condition of Equilibrium, Entropy, Partial molar quantities, their significance. Thermodynamic properties of gases with special reference to real gas in pure state and in mixture. Thermodynamics of ideal and non ideal binary solutions. Gibbs Duhem equation, Duhem Margules equation. Different scales of activity coefficients for solutes and solvents.

Module 4: Unit 4: Kinetics **(8L)**

Brief review of collision theory & activated complex theory; ionic reaction, kinetic salt effect; steady state kinetics, kinetic & thermodynamic control of reactions; unimolecular reactions; chain reactions, fast reactions. Computational approach to understand the chemical kinetics of different ordered reactions.

Module 5: Unit 5: Electrochemistry **(8L)**

Activity and Activity coefficient of electrolytes, ionic strength, Debye Huckel theory of strong electrolytes. Debye Huckel limiting law, Mean ionic activity coefficient. Application of Debye Hückel theory to conductance bahaviour, Relaxation and electrophoretic effect, Debye-Hückel-Onsager equation and its derivation. Debye Falkenhagen effect. Wein effect.

Text books:

1. I. N. Levine , *Quantum Chemistry*, 6th Edn., Pearson Education, London, 2008
2. D. A. McQuarrie, *Quantum Chemistry*, 3rd Edn., Univ. Sci. Books, Mill Valley, California, 1983

Reference texts:

1. J. P. Lowe, *Quantum Chemistry* 3rd Edn., Academic Press, New York, 2008
2. D. D. Fitts, *Principles of Quantum Mechanics as Applied to Chemistry and Chemical Physics*, CUP, Cambridge, New York, 2002
3. M. Taketani, *The Formation and Logic of Quantum Mechanics*, Vol. I-III, World Scientific, New Jersey,2001

4. G. Esposito, G. Marmo and G. Sudarshan, *From Classical to Quantum Mechanics. An Introduction to the Formalism, Foundations and Applications*, Cambridge, 2004
5. L. Piela, *Ideas of Quantum Chemistry*, Elsevier, Amsterdam, 2007
6. P. W. Atkins, *Molecular Quantum Mechanics*, OUP, Oxford, 1983
7. P.W. Atkins, *Physical Chemistry*, 8th Edn., Wiley, New York, 2006
8. J. Bockris and A.K.N. Reddy, *Modern Electrochemistry*, 2B, 2nd Edn., Wiley, New York, 1998

Sl. No.	Content of the course	Module No.	%age of questions	Course outcome
1	Quantum chemistry	Module 1/Unit-1	20	1.Adequetly learn about quantum chemistry
2	Symmetry & group theory	Module 2/Unit-2	30	2.Effectively learn the group theory and its use for molecular term symbol.
3	Kinetics	Module 3/Uni-3	20	3.Will be expertise to predict the reaction rate using computer softwere.
4	Electrochemistry	Module 4/Unit-4	10	4.Will be able to treat ionic reaction probably.
5	Thermodynamics	Module 5/Unit-5	20	5.Information regarding thermodynamic properties of different systems which may be applied to understand the equilibrium conditions of chemical reactions

Theory for Analytical Techniques

Paper code: MSAC-105
(3 Credit) (100 Marks)

Course Objectives (CO):

1. To impart knowledge about spectroscopic techniques and solve structural problems based on UV-Vis, IR, ^{1}H-NMR, ^{13}C-NMR and mass spectral data.
2. Electron microscopy and mass spectroscopy will be learnt.
3. To impart knowledge about thermal analysis technique and associated methods
4. To learn separation techniques and data analysis using contemporary techniques

Module 1: Unit 1: Spectroscopy (12L)
Principles and applications of UV-Vis, Vibrational and Raman spectroscopy, Fluorescence and NMR spectroscopy in understanding chemical and biological interactions.

Module 2: Unit 2: Electron Microscopy and Mass spectroscopy (8L)
SEM, TEM, Tunnelling Electron Microscope. Instrumentation, Mass spectral fragmentation of organic compounds, McLafferty rearrangement, structure determination.

Module 3: Unit 3: Thermal Methods (6L)
Theory and application of TGA, DSC and DTA.

Module 4: Unit 4: Separation Techniques and Data Analysis (10L)
HPLC, GC, gel electrophoresis for biological samples. Uncertainties, errors, mean, standard deviation, least square fit, testing the fit (C2 test, residual etc.). Signal to noise ratio.

Text books:

1. *Spectroscopy of Organic Compounds* by P.S. Kalsi, New Age International
2. Kemp, W. *Organic Spectroscopy* 3rd Ed., W. H. Freeman & Co. (1991).

Reference texts:

1. Silverstein, R. M., Bassler, G. C. & Morrill, T. C. *Spectroscopic Identification of Organic* Compounds John Wiley & Sons (1981).
2. Pavia, D. L.; Lampmann, G. M.; Kriz, G. S.; Vyvyan, J. R. *Introduction to Spectroscopy* Cengage Learning (2014).
3. *Organic Structures from spectra*; L. D. Field, S. Sternhell and J R Kalman, John Wiley & Sons Ltd., 2007

Sl. No	Content of the course	Module No.	%age of questions	Course Outcomes
1.	Spectroscopy	Module 1/Unit 1	30	1. Knowledge about spectroscopic techniques and solve structural problems based on UV-Vis, IR, ^{1}H-NMR, ^{13}C-NMR and mass spectral data.
2.	Electron microscopy and mass spectroscopy	Module 2/Unit 2	20	2. Electron microscopy and mass spectroscopy will be learnt.
3.	Thermal methods	Module 3/Unit 3	20	3. To impart knowledge about thermal analysis technique and associated methods.
4.	Separation techniques and data analysis	Module 4/Unit 4	30	4. To learn separation techniques and data analysis using contemporary techniques.

Research Methodology

Paper code: MSAC-106
(2 Credit) (100 Marks)

One course from prescribed MOOC's basket on Research methodology of minimum 8 weeks based on following topics:

1. Review of literature
2. Reporting of experimental data.
3. Calculation of error.
4. Statistical data analysis.
5. Standard deviation of results.

Any course from MOOC's basket can be chosen having atleast 80% coverage of the above topics.

Lab Techniques for quantitative and qualitative analysis Paper code: MSAC-191

(3 Credit) (100 Marks)

(40 Hr)

Course Objectives (CO):

1. Characterization and analysis of organic compounds for identifying compounds.
2. To be able to synthesize organic compounds and separation of components in mixtures can be studied, which is of great use in different chemical fields.
3. To learn the techniques of purification of organic compounds from mixture.

Module 1: Unit 1: Identification of single organic compounds (solid/liquid) with one or more functional group(s) through preparation of derivatives.
Module 2: Unit 2: Organic preparations, including methods of purification (e.g., crystallization, steam distillation, vacuum distillation, sublimation, etc.).
Module 2: Unit 3: Chromatographic separation techniques to isolate single organic compound from mixture of compounds.

Reference texts:

1) *Vogel's textbook of practical organic chemistry* – Arthur Israel Vogel, B. S. Furniss
2) *Practical Organic Chemistry* - Frederick George Mann and Bernard Charles Saunders
3) *Advanced Practical Organic Chemistry* - N K Vishnoi
4) *Laboratory Manual of Organic Chemistry* - R. K. Bansal

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcomes
1.	Identification of functional groups in organic compounds	Module 1/Unit 1	30	1.Characterization and analysis of organic compounds for identifying functional groups can be learnt.
2.	Preparation of organic compounds	Module 2/Unit 2	30	2.Synthesis of organic compounds and separation of components in mixtures can be studied, which is of great use in different chemical fields.
3.	Purofication of organic compounds	Module 2/Unit 3	40	3.Purification of organic compounds from mixture.

Introduction programming and simulation applications for Physical/Chemical/Biological Problems

Paper code: MSAC-192
(3 Credit) (100 Marks)

Course Objectives (CO):

1. To know the basic operating systems of computer.
2. To know the basic structure and principles of computer programming.
3. To know how to use the computer softwere to solve chemical problems.
4. To learn computer programming.

Module 1: Unit-1: Computional Laboratory-I (20Hr)

Basic concepts of operating systems like MS DOS, MS WINDOW, UNIX, Algorithm & flow chart.

C Fundamentals: The C character set identifiers and keywords, data type & sizes, variable names, declaration, statements. Operators & Expressions:Arithmetic operators, relational and logical operators, type, conversion, increment and decrementoperators, bit wise operators, assignment operators and expressions, precedence and order of evaluation.Input and Output: Standard input and output, formatted output -- printf, formatted input scanf.

Flow of Control:Statement and blocks, if - else, switch, loops - while, for do while, break and continue, go to and labels.

C Programming Laboratory: Problems should cover basic features of the Language.

Fortran programming and application in computational chemistry.

Module 2: Unit-2: Computional Laboratory-II (10Hr)

Implementation of various Numerical problems using MATLAB/OCTAVE/C Programming and simulation applications in Physical/Inorganic and Organic Chemistry problems, Virtual nano Lab, MD Simulation, Quantum Wise, Atomic Scale Modeling. Hartree Fock, DFT theory Gaussian application.

Module 3: Unit-3: Computational Laboratory-III (10Hr)

Python and R: Modelling, simulation and analysis of materials. Define materials at the atomic level and calculate their physical, chemical and biological properties. New materials with best properties for new products or systems. Select and optimize materials in a product system.

Reference texts:

1. *Linux Command Line and Shell Scripting Bible*, 3rd Edition, Wiley
2. *Compueter programming in FORTRAN 77*, Y. Rajaramann
3. *Essentials of Computational Chemistry: Theories and Models*, 2nd Edition, Christopher J. Cramer

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcomes
1.	Computional Laboratory-I	Module 1/Unit 1	20	1. Will be familiar with different operating systems of computer.
2.	Computional Laboratory-I	Module 1/Unit 1	20	2.Will be able to write computer programme.
3.	Computional Laboratory-II	Module 2/Unit 2	30	3.Will be able to use computer softwere.
4.	Computional Laboratory-III	Module 3/Unit 3	30	4.Will be able to design new materials.

Computer aided Determination of Stereo-chemical Outcome of Complex Chemical Reaction

Paper code: MSAC-193

(2 Credit) (50 Marks)

(20 hr)

Course Objectives (CO):

1. To know how to draw chemical structures using computer.
2. To know how to compute basic chemical properties of a compound.

Module 1: **Unit-1**: Analysis of Stereochemistry of single organic molecule and stereochemicaloutcome of complex chemical reaction using computer as analytical tool.
Module 2: **Unit-2**: Use of ChemOffice (Chemdraw 14.0 suite and Chemdraw 3D ultra) in order to determine most stable conformation of certain chemical structure.

Reference texts:

1. *User manual of ChemDraw.*

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcomes
1.	Analysis of Stereochemistry	Module 1/Unit 1	20	1.Will be able to draw the structure of organic compounds.
2.	Use of ChemOffice	Module 2/Unit 2	20	2.Will be able to predict R, S nomencleature of an organic compound.

SEMESTER - II

Quantum Chemistry

Paper code: MSAC-201
(3 Credit) (100 Marks)

Course Objectives (CO):

1. To know the details of quantum numbers.
2. To know how to calculate different quantum numbers.
3. To know how to solve the wavefunction of a system by purterbation method.
4. To know different quantum numbers.
5. To know molecular structure theory.

Module 1: Unit 1: Recapitulations of the background (10L)

Wave function in spherical polar coordinates, Planar rotator, phi equation, wave functions in real forms, Polar diagrams, Nonplanar rotator, Theta equation and solutions Lagendre equation and Lagendre polynomials, Spherical harmonics, Angular momentum operator L^2 and Lz, Space quantization. Hydrogen atom, the R equation. Computational solutions to problems.

Module 2: Unit 2: Perturbation Theory (8L)

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

Module 3: Unit 3: Generalized Angular Momenta and Spin (8L)

Generalized angular momentum. Electron's magnetic Moment and Spin Angular Momentum. Gyromagnetic Ratio and Bohr Magneton and the g - factor. Energy associated with a magnetic dipole placed in magnetic field. Larmor's Theorem.Stern-Gerlach Experiment.Addition of angular momenta. Restriction of eigenvalues from $| j_1 - j_2|$ to $|j_1+j_2|$.

Module 4: Unit 4: Atomic and Molecular Structure (10L)

Many electron wave functions, Pauli exclusion principle, Helium atom, atomic term symbols. The self-consistent field method. Slater-type orbitals. Born-Oppenheimer approximation. Molecular orbital treatment for H2+. MO treatment of homo- and hetero nuclear diatomic molecules. Hückel MO treatment of simple and conjugated polyenes and alternate hydrocarbons.

Text books:

1. *Quantum Chemistry*, I.N. Levine, 5th edition, Pearson Educ., Inc. New Delhi (2000).
2. *Chemical Applications of Group Theory*, F. A. Cotton, John Wiley & Sons (2008).

Reference texts:

1. *Physical Chemistry: A Molecular Approach*, D. A. McQuarrie, and J. D. Simon, Viva Books (2011).
2. *Valence Theory*, J.N. Murrell, S.F.A. Kettle and J. M. Tedder, 2nd edition, John Wiley (1965).
3. *Introductory Quantum Chemistry*, A.K. Chandra, 4th Edition, Tata Mcgraw Hill (1994).
4. *Molecular Symmetry and Group Theory*, R. L. Carter, J. Wiley (1998).
5. *Group Theory and Chemistry*, D. M. Bishop, Dover Publications (1993).
6. *Quantum Chemistry*, J. P. Lowe, and Peterson, K., Academic Press (2005).

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcomes
1.	Recapitulations of the background	Module/Unit-1	10	1.Will be familiar with different quantum numbers.
2.	Recapitulations of the background	Module 1/Unit-1	15	2.Will be able to calculate the quntum number of an electron in a particular state.
3.	Perturbation Theory	Module 2/Unit-2	25	3.Will be able to findout the wave function of any chemical system.
4.	Generalized Angular Momenta and Spin	Module 3/Unit-3	25	4.Will be able to relate the spectra of a system with its electronic structure.
5.	Atomic and Molecular Structure	Module 4/Unit-4	25	5.Will be able to learn about the electronic structure of a molecule.

Statistical Mechanics

Paper code: MSAC-202
(3 Credit)(100 Marks)

Course Objectives (CO):

1. To gain concept of different ensembles and partition functions help in calculating specific heat of solids.
2. To impart knowledge on distribution and fluctuations of parameters in different systems can be learnt, which will help in understanding fluctuations in macroscopic observables
3. To impart knowledge on different thermodynamic properties in various systems can be known which have applications in real systems

Module 1: Unit 1: Review of Classical Mechanics And Partition Functions (10L)
Mathematical Review of Classical Mechanics: Lagrangian Formulation, Hamiltonian Formulation, Poisson Brackets and Canonical Transformations Classical approach to Ensembles: Ensembles and Phase Space, Liouville's Theorem, Equilibrium Statistical Mechanics and it's ensembles Partition Function: Review of rotational, vibrational and translational partition functions. Application of partition functions to specific heat of solids and chemical equilibrium. Real gases.

Module 2: Unit 2: Probability Theory And Distribution (10L)
Elementary Probability Theory. Distributions and Averages, Cumulants and Fluctuations, The Central Limit Theorem Distributions & Fluctuations:Theory of Ensembles, Classical and Quantum, Equivalence of Ensembles, Fluctuations of Macroscopic Observable.

Module 3: Unit 3: Basic Thermodynamics (8L)
Basic Thermodynamics: Review of Concepts, The Laws of Thermodynamics, Legendre Transforms, TheMaxwell Relations, The Gibbs-Duhem Equation and Extensive Functions, Intensive Function.

Module 3: Unit 4: Thermodynamic Properties (8L)
Bose-Einstein distribution: Einstein condensation. Thermodynamic properties of ideal BE gas. Fermi-Dirac distribution: Degenerate Fermi gas. Electron in metals. Magnetic susceptibility.

Text books

1. Kerson Haung, *Statistical Mechanics*, Wiley, 2nd Ed. (2008).
2. R. K. Pathria and P. D. Beale, *Statistical mechanics*, Elsevier, 3rd Ed (2011).

Reference texts:

1. D. A. Mcquarrie, *Statistical Mechanics*, University Science Books (2011).
2. D. Chandler, *Introduction to Statistical Mechanics*, Oxford University Press (1987).

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcomes
1.	Review of classical mechanics and partition functions	Module 1/Unit 1	30%	1. Concept of different ensembles and partition functions help in calculating specific heat of solids.
2.	Probability theory and distribution	Module 2/Unit 2	30%	2. Knowledge on distribution and fluctuations of parameters in different systems can be learnt, which will help in understanding fluctuations in macroscopic observables
3.	Basic Thermodynamics	Module	40%	3. Knowledge on different thermodynamic

	and thermodynamic properties	3/Units 3 and 4		properties in various systems can be known which have applications in real systems

Organic Chemistry-II

Paper code: MSAC-203
(3 Credit)(100 Marks)

Course Objectives (CO):

1. To gain knowledge on various metal-catalyzed coupling reactions, reducing agents, oxidizing agents, and their applications in organic synthesis
2. To acquire knowledge on organic spectroscopic techniques and solve problems and structural anylaysis
3. To impart knowledge on synthesis and utility of various heterocyclic compounds
4. To acquire knowledge of basic principles of photochemistry and advanced photochemical reactions

Module 1: Unit 1: Reagents in Organic Synthesis (10L)

Diborane - lithium aluminium hydride - sodium borohydride - selenium-di-oxide -osmium tetroxide - phenyl isothiocyanate - N-bromosuccinamide (NBS) – leadtetraacetate - dicyclohexylcarbodiimide (DCC) - pyridiniumcholorochromate (PCC) -Swern oxidation - p-toluenesulphonyl chloride - trifluoroacetic acid – lithiumdiisopropylamide (LDA) - 1,3-dithiane (reactive umpolung) - crown ethers - trimethylsilyl iodide - Gilman reagent - dichlorodicyanobenzoquinone (DDQ) – lithiumdimethylcuprate - tri-n-butyltin hydride - di-tert-butoxydicarbonate - dihydropyran -phase transfer catalysts - Wilkinson's catalysts - Peterson synthesis – and diethylaluminium cyanide- IBX and Swern oxidations.

Module 2: Unit 2: Organic Spectroscopy (10L)

Advanced Techniques and Applications of NMR: ^{1}H and ^{13}C NMR principles, rules for ^{13}C calculations, principles of decoupling, gated and inverse gated decoupling techniques, NOE, relaxation processes, population transfer, selective polarization transfer, NMR shift reagents and their applications, basic two-dimensional sequence.

Module 3: Unit 3: Heterocycles (10L)

Synthesis and reactivity of furan, thiophene, pyrrole, thiazole, pyridine, indole andtheir derivatives, quinoline, isoquinoline, pyrimidine, purine and flavone –Skraupsynthesis - Fischer indole synthesis and Pachmanncoumarin synthesis - alkaloids -sources and classification - structural elucidation by chemical degradation – totalsynthesis of quinine, morphine, reserpine, papaverine and nicotine (Any two).

Module 4: Unit 4: Photochemistry (10L)

Basic principles, Jablonski diagram, photochemistry of olefinic compounds, cis-trans isomeriation, Paterno-Buchi reaction, Norrish type I and II reactions, photoreduction of ketones, di-pi-methane, oxo di-pi methane and aza di-pi methane rearrangements,Barton reaction, Hofmann-Loefflar-Freytag reactions, photochemistry of arenes, SRN1 reaction, photooxidation, Photoreaction in solid state. Method of generation and detection of radicals (ESR), radical initiators, reactivity pattern of radicals, substitution and addition reactions involving radicals, synthetic applications: cyclisation of radicals including various ring expansion, ring contraction, remote functionalisation and radical fragmentation reaction. Photochemical reaction using UV, Sunlight and LED light etc.

Text books:

1. J. March, *Advanced Organic Chemistry*, 5th edition, Wiley-Intersciences, New York (2003).

2. F.A.Carey and R.J. Sundberg, *Advanced Organic Chemistry, Part A and Part B*, 5th edition, Plenum Press, New York (2005).

Reference texts:

1. T.H. Lowry and K.S. Richardson, *Mechanism and Theory in Organic Chemistry*, 2nd edition, Harper and Row Publishers (1981).
2. R.K. Mackie and D.M. Smith, *Guide book to Organic Synthesis*, 2nd edition, ELBS Publications, London (1998).
3. Horspool, W. M. *Aspects of Organic Photochemistry* Academic Press (1976).
4. *Heterocyclic Chemistry*: Joule, John A., Mills, Keith.
5. *Absorption spectroscopy of organic molecules*- V.M. Parikh
6. R.P.Wayne, "*Principles and Applications of Photochemistry*", Oxford University Press
7. C.H.Dupuoy, and O.L.Chapman, "*Molecular Reactions and Photochemistry*", Prentice Hall
8. *Essentials of molecular photochemistry*, A. Gilbert and J. Baggott. Blackwell Scientific Publication.
9. *Introductory photochemistry*. Cox and T. Camp Mc Graw –Hill
10. *Organic photochemistry* J. Coxon and B. Hallon Cambridge University press.

Sl. No	Content of the course	Module No.	%age of questions	Course Outcomes (CO)
1.	Reagents in organic synthesis	Module-1/ Unit-1	25%	1. Knowledge on various metal-catalyzed coupling reactions, reducing agents, oxidizing agents, and their applications in organic synthesis.
2.	Organic spectroscopy	Module-2/Unit-2	25%	2. Acquire knowledge on organic spectroscopic techniques and solve problems and structural anylaysis.
3.	Heterocycles	Module-3/Unit-3	25%	3. Learn about synthesis and utility of various heterocyclic compounds.
4.	Photochemistry	Module-4/Unit-4	25%	4. Knowledge of basic principles of photochemistry and advanced photochemical reactions.

Nano Science and Technology

Paper code: MSAC-204
(3 Credit)(100 Marks)

Course Objectives (CO):

1. To learn about synthesis of nano materials of various elements having different properties, which has diverse industrial applications.
2. To learn structure and characterization of nano materials and study for their applications in drug delivery processes.
3. To know symmetry in molecules and different properties of nano materials which help in applications in medical fields.

Module 1: Unit 1: Introduction to Nanoscience and Nanotechnology (10L)

Basic problems and limitations - opportunities of nano scale-evolution of band structures andFermi surface. Nanoparticles through homogeneous and heterogeneous nucleation-Growth controlled by surface and diffusion process- Oswald ripening process - influence of reducing agents-solid state phase segregation- grain growth and sintering precipitation in solid solutionhumerothery rule. Carbon Nanotubes (CNT) - Metals (Au, Ag, Pd, Cu) - Metal oxides (TiO2, CeO2, ZnO, MgO) -Semiconductors (Si, Ge, CdS, ZnSe). Classifications of nanomaterials-zero dimensional - one dimensional - two dimensional - three dimensional nanostructures - Quantum dots - Quantum wire, Quantum well-semiconductors and ceramics.

Module 2: Unit 2: Special nanomaterials (10L)

Carbon fullerenes-fullerene derived crystals-carbon nanotubes. Micro and Mesoporous material ordered mesoporous materials, Random mesoporous materials-crystalline microporous materials.Core/Shell structures, Metal oxide structures, Metal polymer structures, Intercalation compounds-nanograined materials. Nanomaterials in drug delivery.

Module 3: Unit 3: Materials Structure and Properties (10L)

Space lattice and unit cells, crystal system, Symmetry operation, Structures of common metallic, Semiconductor ceramic and superconductor materials, Miller Indices, Packing fractions, Formation of dangling bonds-atom like behavior of nanomaterials-physicochemical properties. Optical properties of nanomaterials-semiconductor-metal nanoparticles-Electrical and electronic properties, Thermal properties-Ferro electric properties-mechanical and magnetic properties.

Module 2: Unit 4: Organic Nanomaterials, nanoelectronics and engineering (8L)

Organic nanoelectronics. Advanced nanomaterials for applications. Nanosystems engineering to design, develop, and characterize materials on the nanoscale. Nanoparticles for Environment, Engineering, and Nanomedicine.

Text books:

1. *Introduction to Nanoscience and Nanotechnology*, By Gabor L. Hornyak, H.F. Tibbals, Joydeep Dutta, John J. Moore
2. *Nanostructures and Nanomaterials: Synthesis, Properties, and Applications*, By Guozhong Cao, Ying Wang.

Reference texts:

1. *Organic Nanomaterials: Synthesis, Characterization, and Device Applications*, By Tomas Torres, Giovanni Bottari
2. *Nanochemistry: A Chemical Approach to Nanomaterials*, By Geoffrey A. Ozin, André C. Arsenault, Ludovico Cademartiri
3. T. Pradeep, *Nano The Essentials: Understanding Nanoscience and Nanotechnology*.

Sl. No	Content of the course	Module No	%age of questions	Course Outcomes (CO)
1	Introduction to nanoscience and nanotechnology	Module 1/Unit 1	30%	1. Synthesis of nano materials of various elements having different properties can be learnt, which has diverse industrial applications
2.	Special nanomaterials, nanoelectronics and engineering	Module 2/Units 2 and 4	40%	2. Structure and characterization of Nano materials will be studied for application in drug delivery processes
3.	Material structures and properties	Module 3/Unit 3	30%	3. Symmetry in molecules and different properties of nano materials will be known which help in applications in medical fields

Computational Methods

Paper code-MSAC-205
(3 Credit)(100 Marks)

Course Objectives (CO):

1. To learn about the linear and non-linear equations.
2. To know how linear and non-linear equations may be solved.
3. To learn to handel the matrix and determinant for scientific problem solution using computer.
4. To learn numerical methods to solve the differential equation and integration.
5. To learn the method of error calculation.
6. To learn different methods of numerical problem solution.

Module 1: Unit 1: Linear and non-linear equations (10L)

Linear and Non –Linear equations:Solution of Algebra and transcendental equations, Bisection, Falsi position and Newton-Rhapson methods-Basicprinciples-Formulae-algorithms.
Simultaneous equations:Solutions of simultaneous linear equations-Guass elimination and Gauss Seidel iterative methods-Basic principles-Formulae-Algorithms, Pivotal Condensation.

Module 2: Unit 2: Matrix and Determinants (10L)

Matrix and Determinants:Matrix Inversion, Eigen-values, Eigen-vector, Diagonalization of Real Symmetric Matrix by Jacobi's Method. First Principle approach.

Module 3: Unit 3: Programme to solve differential equation and integration (10L)

Interpolations: Concept of linear interpolation-Finite differences-Newton's and Lagrange's interpolation formulae-principles and Algorithms Numerical differentiation and integration: Numerical differentiation-algorithm for evaluation of first order derivatives using formulae based on Taylor'sseries, Numerical integration-Trapezoidal Rule, Simpson's 1/3 Rule, Weddle's Rule, Gauss Quadrature Formulae-Algorithms. Error in numerical Integration. Curve Fit: least square, straight line and polynomial fits.

Module 4: Unit 4: Numerical Solution of differential equations (10L)

Numerical Solution of differential Equations: Picards Method, Taylor's Series Method, Euler's Method, Modified Euler's Method, Runge-Kutta Method, Predictor-Corrector Method.

Text books:

1. V. Rajaraman, *Computer Oriented Numerical Methods*, PHI, 1993.
2. E. Balaguruswamy, *Numerical Methods*, Tata McGraw Hill, 2017.

Reference texts:

1. F. Acton, *Numerical Methods that Work*, Harper and Row, 1997.
2. S. D. Conte and C.D.Boor, *Elementary Numerical Analysis*, McGraw Hill, 2005.
3. S. S. Shastri, *Introductory Methods of Numerical Analysis*, PHI, 2012.

Sl. No	Content of the course	Module No	%age of questions	Course Outcomes (CO)
1	Linear and non-linear equations	Module 1/Unit-1	20	1.Will be able to handle linear and non-linear equations.
2.	Linear and non-linear equations	Module 1/Unit-1	20	2.Will be able to solve linear and non-linear equations.

3.	Matrix and Determinants	Module 2/Unit-2	10	3.Will be able to handle matrix and determinant using computer.
4.	Programme to solve differential equation and integration	Module 3/Unit-3	10	4.Will be able to write computer programme to solve differential equation and integration.
5.	Programme to solve differential equation and integration	Module 3/Unit-3	20	5.Will be able to calculate error of experimental results.
6.	Numerical Solution of differential Equations	Module 4/Unit-4	20	6.Will be able to use proper method for any kind of problem solution using numerical methods.

Natural Products and Medicinal Chemistry

Paper code: MSAC-206
(3 Credit)(100 Marks)

Course Objectives (CO):

1. To acquire knowledge on structure and synthesis of amino acids, peptides and nucleic acids
2. To acquire knowledge on basic concepts and application of natural products and synthetic molecules in medicinal chemistry
3. To learn basics of lead drugs and to describe the biosynthetic studies of different classes of drugs

Module 1: Unit 1: Proteins and Nucleic Acids (10L)

Classification - structure and synthesis of amino acids – peptides – Merrifield solidphase peptide synthesis - structure determination - peptide sequence and synthesisof - primary, secondary, tertiary and quaternary structures- Merrifield solid phasepeptide synthesis - nucleic acids - structure and synthesis of DNA - structure andsynthesis of RNA-WC Model.

Module 2: Unit 2: Introduction to Medicinal Chemistry (10L)

Antibiotics – Penicillins, Cephalosporins, tetracyclins, newer generation of antibiotics.

Vitamins - Definition of vitamins and coenzymes, classification of vitamins, mechanism of function with synthesis of vitamin A, B1, B6 and folic acid, etc.

Drugs - Introduction and classification of drugs, brief discussion on drug targets. Sulphur drugs, anti tubercular drugs, anti diabetic drugs and newer generation of antacids.

Module 2: Unit 3: Advanced Medicinal Chemistry (10L)

Drug design and synthesis, Molecular and quantum mechanics; Drawing chemical structures, equations, and diagrams; 3D structures; Molecular modelling and Energy Minimization; Molecular properties, Conformational analysis, Docking Procedures, *De novo* design, Molecular Recognition, Receptor Based Molecular Modeling, QSAR studies, Antineoplastic agents, cardiovascular drugs, Local anti-infective drugs, Antimalarial, Anticholenergic and CNS-active drugs.

Module 3: Unit 4: Lead Drugs (10L)

Introduction, isoprene rule, general methods of isolation, structure elucidation and synthesis of some representative members of mono and sesquiterpenes. Biogenesis and biosynthesis of mono-, sesqui- and di-terpenoids.

Definition and classification, general methods of isolation and structure elucidation, structure and synthesis of ephedrine, piperine, nicotine and papaverine. Biosynthesis of ephedrine and nicotine.

Text books:

1. Gringauz, A. *Introduction to Medicinal Chemistry: How Drugs Act and Why?* John Wiley & Sons (1997).
2. Patrick, G. L. *Introduction to Medicinal Chemistry,* Oxford University Press (2001).

Reference texts:

1. Lemke, T. L. & William , D. A., Foye's *Principles of Medicinal Chemistry*, 5th Ed., USA, (2002).
2. D. Sriram , P. Yogeswari, *Medicinal Chemistry*, Pearson Education India, 2010.
3. C.O. Wilson, J.M. Beale, J.H. Block, *Textbook of Organic Medicinal and Pharmaceutical Chemistry*, 12th Edn., Lippincott Williams and Wilkins, 2010
4. S. S. Kadam, *Principles of Medicinal Chemistry*, Vol. I & II, Pragati Books, 2008

Sl. No	Content of the course	Module No	%age of questions	Course Outcomes (CO)
1	Proteins and nucleic acids	Module 1/Unit 1	25	1. To acquire knowledge on structure and synthesis of amino acids, peptides and nucleic acids
2.	Introduction and advanced medicinal chemistry	Module 2/Units 2 and 3	50	2. To acquire knowledge on basic concepts and application of natural products and synthetic molecules in medicinal chemistry
3.	Lead Drugs	Module 3/Unit 4	25	3. To learn basics of lead drugs and to describe the biosynthetic studies of different classes of drugs

Computational methods in Chemistry (Lab)

Paper code: MSAC-291
(3 Credit)(100 Marks)

Course Objectives (CO):

1. To familiar with the geometry optimization.
2. To know how to use computational tool to compute the properties of a compound.
3. To know how we could handel the data to analyse using computer.

Module 1: Unit-1: Computational Lab **(20hr)**
Simulation and structures and geometry optimisation with the commercial programs like "Materials Studio" (Forcite, Force Field: COMPASS), Gaussian.

Module 2: Unit-2: Computational Lab **(10hr)**
Computational studies on opto-electronic and charge transport properties in conjugated systems. Other computational application introducing "ChemCraft", "Gaussian", "SCM ADF" softwares GAMMES.

Module 3: Unit-3: Computational Lab **(10hr)**
Plotting, analysis and interpretation of data from UV-Vis or Fluorescence spectrophotometry using Origin.

Reference texts:

1. *User guide of Gaussian*.
2. *Molecular Dynamics Simulation: Fundamentals and Applications*, Kun Zhou and Bo Liu, Academic Press Inc (1 November 2020)

Sl. No	Content of the course	Module No	%age of questions	Course Outcomes (CO)
1	Computational Lab	Module 1/Unit 1	20	1.Will be able to draw structure and optimize it using DFT.
2.	Computational Lab	Module 2/Unit 2	40	2.Will be able to compute physical and chemical properties of a compound.
3.	Computational Lab	Module 3/Unit 3	40	3.Will be able to plot and analyse data with the help of computer.

Advanced Organic Chemistry Lab

Paper code: MSAC-292
(3 Credit)(100 Marks)

Course Objectives (CO):

1. To acquire knowledge of laboratory techniques for organic synthesis and characterization.
2. To learn synthetic procedures: aqueous workup, distillation, reflux, separation, isolation, and crystallization.
3. To gain knowledge about starting materials, functional groups, mechanism, and typical reaction conditions.

Module 1: **Unit-1: Some important techniques in practical organic chemistry**: **(8hr)**
Recrystallization, mixed melting point, drying of solvents and steam distillation.

Unit-2: Preparation of **(16hr)**
i) Methyl orange ii) Coumarin iii) Pyrazolone iv) Azalactone

Unit-3: Preparation of **(16hr)**
i) Benzanilide by Beckmann's rearrangement:
(a) Preparation of benzophenone oxime
(b) Beckmann's rearrangement to benzanilide
ii) Benzilic acid from benzoin:
(a) Benzil from benzoin
(b) Benzilic acid from benzyl
iii) Anthranilic acid from phthalic anhydride:
(a) Phthalimide from Phthalic anhydride
(b) Hoffmann's rearrangement to anthranilic acid
iv) m-Nitroaniline from Nitrobenzene:
(a) m-Dinitrobenzene from Nitrobenzene
(b) m-Nitroaniline from m-Dinitrobenzene

Reference texts:
1) *Vogel's textbook of practical organic chemistry* – Arthur Israel Vogel, B. S. Furniss
2) *Practical Organic Chemistry* - Frederick George Mann and Bernard Charles Saunders
3) *Advanced Practical Organic Chemistry* - N K Vishnoi
4) *Laboratory Manual of Organic Chemistry* - R. K. Bansal

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcomes
1.	Some important techniques in practical organic chemistry	Module 1/Unit 1	20%	1. Will learn laboratory techniques for organic synthesis and characterization.
2.	Preparation of organic compounds	Module 1/Unit 2	40%	2. Learn synthetic procedures: aqueous workup, distillation, reflux, separation, isolation, and crystallization.
3.	Preparation of organic compounds via multistep synthesis	Module 1/Unit 3	40%	3. Gain knowledge about starting materials, functional groups, mechanism, and typical reaction conditions.

SEMESTER - III

Bioorganic and Supramolecular Chemistry

Paper code: MSAC – 301
(3 Credit)(100 Marks)

Course Objectives (CO):

1. Concept of Supra Molecules and their interactions.
2. Concept of Bio-Organic molecules and their applications.

Module 1: Unit -1: Supramolecular Chemistry (20L)

Basic concepts of supramolecular chemistry, different noncovalent forces (e.g. H-bonding, cation-π, anion-π, π-stacking, hydrophobic, hydrophilic interactions etc.) leading to strong bonding of guest molecules to the hosts, thermodynamics of host-guest complexation, solvent effects and salt effects in complexation, design principle of host molecules, experimental techniques for characterization of host – guest complexation, examples of different design-based receptor molecules for cation, anion and neutral molecules binding, chiral recognition with examples, supramolecular devices (optical and electrochemical) and molecular switches, self-organization process-template association and supramolecular synthesis, self-replication and autocatalysis, supramolecular reactivity and catalysis, transport processes and carrier design, supramolecular gel, cyclodextrins, catenanes and rotaxanes.

Module 2: Unit -2: Bioorganic Chemistry (16L)

Structure and utility of natural and unnatural compounds, carbohydrates, biopolymers, nucleic acids, amino acids, peptides, drug molecules. Drug – Receptor binding and Bioorganic compounds for drug delivery and bio-signalling.

Text books:

1. Steed, J. W.; Turner, D., R.; Wallace, K. J., *Core Concepts in Supramolecular Chemistry and Nanochemistry*, John Wiley & Sons, West Sussex (2007).
2. Steed, J. W.; Atwood, J. L., *Supramolecular Chemistry*, 2nd Ed., John Wiley & Sons, West Sussex (2009).

Reference texts:

1. Cotton, F. A.; Bochmann, M.; Murillo, C. A.; Wilkinson, G., *Advanced Inorganic Chemistry*, 6th Ed., Wiley India, New Delhi (2007).
2. Ariga, K.; Kunitake, T., *Supramolecular Chemistry: Fundamentals and Applications*, Springer, Heidelberg (2006).
3. Lehn, J.-M., *Supramolecular Chemistry: Concepts and Perspectives*, Wiley India, New Delhi (2014).

Sl. No	Content of the course	Module No.	%age of questions	Course Outcome
1.	Supramolecular chemistry	Module 1/Unit 1	50%	1. To gain knowledge in bonding in supra molecules and their formations will help in understanding supra molecular devices and molecular switches
2.	Bio-organic Chemistry	Module 2/Unit 2	50%	2. To learn structure and utility of natural and unnatural organic compounds which will help in understanding drug-receptor binding for applications in drug delivery processes

Industrial Chemistry

Paper code: MSAC-302
(3 Credit)(100 Marks)

Course Objectives (CO):

1. Basic principles of different separation processes.
2. Preparation of gases and chemicals for industrial use.
3. Manufacture of chemicals of industrial importance.
4. Metallurgy and Ceramics

Module 1: Unit -1: Chemical Technology (10L)

Basic principles of distillation, solvent extraction, solid-liquid leaching and liquid-liquid extraction, separation by absorption and adsorption. An introduction into the scope of different types of equipment needed in chemical technology, including reactors, distillation columns, extruders, pumps, mills, emulgators. Scaling up operations in chemical industry. Introduction to clean technology.

Module 2: Unit -2: Industrial Gases and Inorganic Chemicals (10L)

Industrial Gases: Large scale production, uses, storage and hazards in handling of the following gases: oxygen, nitrogen, argon, neon, helium, hydrogen, acetylene, carbon monoxide, chlorine, fluorine, sulphur dioxide and phosgene. Oils and waxes. Polymer – plastic, rubber.

Module 3: Unit -3: Inorganic Chemicals (10L)

Inorganic Chemicals: Manufacture, application, analysis and hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, common salt, borax, bleaching powder, sodium thiosulphate, hydrogen peroxide, potash alum, chrome alum, potassium dichromate and potassium permanganate. Soap and detergent. Fertilizer. Glasses. Cement.

Module 4: Unit -4: Industrial Metallurgy and Ceramics (10L)

Preparation of metals (ferrous and non-ferrous) and ultra-pure metals for semiconductor technology. Crystalline ceramics and Noncrystalline ceramics and their electrical and optical properties.

Text books:

1. ULLMANN's Encyclipedia of Industrial Chemistry
2. Industrial chemistry: Part 1 & part 2: by R. K. das

Refernce texts:

1. Dryden's outlines of Chemical Technology for 21st Century by Kirk-Othmer.
2. Industrial Inorganic chemistry by Mark Anthony Benvenuto.

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcome
1	Chemical technology	Module 1/Unit 1	25%	1. Separation of components from a mixture will be learnt, for scaling up operations in chemical industries
2	Industrial gases and inorganic chemicals	Module 2/Unit 2	25%	2. To acquire knowledge in large-scale production of industrial gases for application in Industry
3	Inorganic chemicals	Module 3/Unit 3	25%	3. To gain knowledge about different chemical manufacturing for use as raw material in industrial processes
4	Industrial metallurgy and ceramics	Module 4/Unit 4	25%	4. To learn extraction of metals and preparation of pure metals of use in semi-conductor and ceramic technology

Photochemistry & Spectroscopy

Paper code: MSAC- 303: (Elective I)
(3 Credit) (100 Marks)

Course Objectives (CO):

1. To learn changes in energy levels of a molecule after absorption of radiation to understand the effect of sunlight on living systems.
2. To gain knowledge about manufacture of laser for use in different field.
3. To know life time in the excited states of molecules which helps in predicting the reactions at excited state.
4. To learn characterization of the molecules and their applications for use in different field.

Module 1: Unit 1: Photophysical processes in molecules (8L)

Jablonski diagram, Fluorescence and Phosphorescence, Kasha's rule, Delayed fluorescence, Quantum yield, Mechanism and decay kinetics of photophysical processes. Fluorescence Quenching (dynamic and static), Stern Volmer equation. Energy transfer, Electron transfer phenomenon (Marcus theory, Rehm Weller theory), Proton transfer phenomenon, complex formation phenomenon (excimer, exciplex).

Module 2: Unit 1: Interaction of electromagnetic radiation with matter (8L)

Interaction of electromagnetic radiation with matter, Transition probabilities, Transition moment integral and its applications. Selection rules, Franck Condon principle, Oscillator strength, Nature of transitions, solvent effect on absorption and emission spectra, Stokes shift. Laser, different types and applications.

Module 3: Unit 3: Properties of electronically excited molecules and different non radiative electronic transition (8L)

Properties of electronically excited molecules: Life time,redox potential,dipole moment, pK values. Potential energy diagram for donor acceptor system, polarized luminescence.

Nonradiative intramolecular electronic transition; internal conversion, intersystem crossing, crossing of potential energy surface.

Module 4: Unit 3: Raman, Mossbauer, NQR and Photoelectron spectroscopy and applications (16L)

Raman Spectroscopy: Classical and quantum mechanical treatment of rotational and vibrational Raman spectra, Polarization and depolarization of Raman lines.Resonance Raman spectroscopy.

Mossbauer spectroscopy; Principles,technique,chemical shift,quadrupole effect,effects of magnetic field, applications. NQR spectroscopy: Principle, technique,coupling in atom, applications.

Photoelectron spectroscopy: principles and applications.

Text Books:

1. Lampman, G. M.; Pavia, D. L.; Kriz, G. S.; Vyvyan, J.R., *Introduction to Spectroscopy*, 5th Ed., Cengage Learning India, New Delhi (2015).
2. *An introduction to Photochemistry* by K.K.Rohatgi-Mukherjee.

Reference texts:

1. *Photochemistry* by Wayne and Wayne.
2. *Photochemistry* by J.A. Barltrop and J.D.Coyle
3. *Spectroscopy* by Raymond Chang
4. *Fundamentals of Molecular Spectroscopy* by C. N. Banwell
5. *Spectroscopy* by Barrow.
6. *Molecular Structure and Spectroscopy* by G.Aruldhas.
7. W. Kemp, *NMR in chemistry-A Multinuclear Introduction*, McMillan, 1986.

Sl.No.	Content of the course	Module No.	%age of questions	Course Outcome
1	Photophysical processes in molecules	Module 1/Unit 1	20%	1. Changes in energy levels of a molecule after absorption of radiation can be learnt to understand the effect of sunlight on living systems.
2	Interaction of electromagnetic radiation with matter	Module 2/Unit 2	20%	2. Manufacture of laser can be learnt for use in different field.
3.	Properties of electronically excited molecules and different non radiative electronic transition	Module 3/Unit 3	20%	3. Life time in the excited states of molecules are known which helps in predicting the reactions at excited state.
4	Raman, Mossbauer, NQR and photoelectron spectroscopy and applications	Module 4/Unit 4	40%	4. Characterization of the molecules and their applications can be learnt for use in different field.

Pharmaceutical Chemistry

Paper code: MSAC- 304: (Elective II)
(3 Credit) (100 Marks)

Course Objectives (CO):

1. To handle doctor's prescription.
2. To know about how to prepare different medical solutions.
3. To know about different types of powder used in medicinal techniques.
4. To know how drugs act in our body.
5. To know how the dose of a drug is considered.
6. To know what is the process after the action of a drug.

Module 1: Unit-1: Pharmaceutics basics (15L)

a. ***Prescription:*** Parts of prescription, handling of prescription, Posology.
b. ***Solution:*** Formulation, aqueous and non-aqueous vehicles, factors affecting rate of solubilization and solubility, methods to improve aqueous solubility, formulation additives; Elixirs; Linctus; Mouthwashes and Gargles; Nasal and Ear drops; Lotions; Stability of solution; Syrups.
c. ***Powder:*** Classification, advantages of powder formulation, milling, mixing and dividing of powders, factors influencing blending of powders, powders containing liquids, eutaxia.
d. Pharmaceutical calculations Labelling of Pharmaceutical products

Module 2: Unit -2: Basics of Drug Action (25L)

a. ***Interactions:*** Inter- and intramolecular interactions. Weak interactions in drug molecules. Chirality and drug action. Covalent, ion-ion, ion-dipole, Hydrogen bonding, C-H hydrogen bonding, dihydrogen bonding, Van der Waals interactions and the associated energies
b. ***Receptorology:*** Drug-receptor interactions, Receptor theories and drug action: Occupancy Theory, Rate Theory, Induced Fit Theory, Macromolecular perturbation theory, ActivationAggregation theory. Topological and stereochemical consideration.
c. ***Enzyme Kinetics:*** enzyme kinetics in drug action. Do all molecules of an enzyme have same kinetics? Mechanisms of enzyme catalysis, Electrostatic catalysis and desolvation. Covalent catalysis, Acid-base catalysis, Strain / distortion in enzyme catalysis. Coenzyme catalysis.
d. ***Enzyme Inhibition***: Drug action through enzyme inhibition. Examples based on PDE4, GSK3, etc. Theories of enzyme inhibition and inactivation. Enzyme activation of drugs prodrugs.
e. ***Nucleic acids& drug research:*** NA as targets for drug action. NA-interactive agents. Classes of drugs that interact with nucleic acids. Intercalation, NA-alkylation, NA-strand breaking and their importance in drug action.
f. ***Drug likeness:*** Drug like molecules and theories associated with the recognition of drug like properties. Physical organic chemistry of Drug metabolism, drug deactivation and elimination.
g. ***Drug action after Metabolism:*** Phase I and Phase II transform.Concept of hard and soft drugs. Chemistry of ADME and Toxicity properties of drugs.

Text books:

1. C.O. Wilson, J.M. Beale, J.H. Block, *Textbook of Organic Medicinal and Pharmaceutical Chemistry*, 12th Edn., Lippincott Williams and Wilkins, 2010.
2. J. P. Remington, *Remington's Pharmaceutical Sciences*, Vol.13, 19th Edn., Mack, 1990.

Reference texts:

1. *Pharmaceutical Chemistry – I*, Dr. A. V. Kasture, Dr Sg Wadodkar, Pragati Books Pvt. Ltd., 2015
2. *Essentials of Pharmaceutical Chemistry*, Cairns, Donald, Fourth edition, 2012
3. *A Textbook of Pharmaceutical Chemistry*, Jayashree Ghosh, S. Chand Publishing, 2010.

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcome
1.	Pharmaceutics basics	Module 1/Unit-1	5	1.Will be able to explain the prescription of a doctor.
2.	Pharmaceutics basics	Module 1/Unit-1	15	2.Will be able to learn the variation of solutions used in medicine.
3.	Pharmaceutics basics	Module 1/Unit-1	15	3.Will be able to prepare and identify different types of powder used to prepare medicine.
4.	Basics of Drug Action	Module 2/Unit-2	15	4.Will be able to know how drugs works in our body.
5.	Basics of Drug Action	Module 2/Unit-2	25	5.Will be able to know about the importance and measurement methods of IC_{50} of a drug.
6.	Basics of Drug Action	Module 2/Unit-2	25	6.Will be able to know different process of the metabolism of a drug.

Industrial Exposure

Paper Code: MSAC-391
(2 Credit)(50 Marks)

To visit industry facility and subsequent submission of a report to the department from individual student. This is a value added course for students. Credits may be transferred after submission of report.
For industrial exposure, any industry should be chosen for the visit to observe their work and the experience in report form shall have to be submitted to the department.

Mini Project and Seminar Presentation

Paper Code: MSAC-392
(2 Credit)(50 Marks)

Students will have to pursue literature survey under the guidance of faculty on scientific cutting edge progress related to the course curriculum. Then after, they have to make presentation followed by viva-voce.
For project report submission: 25 marks
For presentation and viva-voce: 25 marks

Python programming (Lab)

Paper Code: MSAC-393
(2 Credit)(50 Marks)

(20hr)

Course Objectives (CO):

1. To know different commands and environment of Python programming.
2. To use python programming for the solution of simple mathematical equations.

Module 1: Unit-1: Basics of Python programming, Object and data structure, Comparison operator, Python statement, methods and functions, object oriented programming, modules and packages, errors and expectation calculation.

References Texts:

1. *Python Programming Language: A Complete Guide For Beginners To Master And Become An Expert In Python Programming Language*, Brian Draper, 12 October 2016.
2. *Core Python Programming*, R. Nageswara Rao, 1 January 2018.

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcome
1	Python programming	Module 1/Unit-1	25	1.Will be able to write a python program
2	Python programming	Module 1/Unit-1	25	2.Will be able to solve simple equations using python

Preparation of complex materials and their characterization by physiochemical techniques(Lab)

Paper code: MSAC-394
(3 Credit) (100 Marks)

(40hr)

Course Objectives (CO):

1. To determine relative average molecular mass of a polymer by viscosity method.
2. To determine thermodynamic solubility product of a sparingly soluble salt in aqueous medium.
3. To perform conductometric titration of a mixture of HCl and CH_3COOH with NaOH.
4. To determine CMC of surfactants from interfacial tension measurements.
5. To determine rate constant of acid catalysed inversion of canesugar by polarimetric method.
4. To determine second order rate constant of alkaline hydrolysis of ester by conductometric method.
5. To perform potentiometric titration of Ferrous ion by dichromate and evaluation of the formal potential of Fe^{3+}/Fe^{2+}.
6. To determine the redox potential E^0 of the quinhydrone electrode by potentiometric method and pH of buffer solution.

Module 1: Unit 1:

1. Determination of relative average molecular mass of a polymer by viscosity method.
2. Determination of thermodynamic solubility product of a sparingly soluble salt in aqueous medium.

Module 2: Unit 2:

1. Conductometric titration of a mixture of HCl and CH_3COOH with NaOH.
2. Determination of CMC of surfactants from interfacial tension measurements.

Module 3: Unit 3:

1. Determination of rate constant of acid catalysed inversion of canesugar by polarimetric method.
2. Determination of second order rate constant of alkaline hydrolysis of ester by conductometric method.

Module 4: Unit 4:

1. Potentiometric titration of Ferrous ion by dichromate and evaluation of the formal potential of Fe^{3+}/Fe^{2+}.
2. Determination of the redox potential E^0 of the quinhydrone electrode by potentiometric method and pH of buffer solution.

Reference texts:

1. *Practical Physical Chemistry* by S.R.Palit and A.K.De.
2. *Experimental Physical Chemistry* by V.D.Athawale and Parul Mathur.

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcome
1	Determination of relative average molecular mass of a polymer by viscosity method. Determination of thermodynamic solubility product of a sparingly soluble salt in aqueous medium	Module-1	25	Characterization of molecules can be done for their applications
2	Conductometric titration of a mixture of HCl and CH_3COOH with NaOH. Determination of CMC of surfactants from interfacial tension measurements.	Module-2	25	Estimation of the components amount in a mixture.
3	Determination of rate constant of acid catalysed inversion of canesugar by polarimetric method. Determination of second order rate constant of alkaline hydrolysis of ester by conductometric method.	Module-3	25	Rate of reactions are known for applications.
4	Potentiometric titration of Ferrous ion by dichromate and evaluation of the formal potential of Fe^{3+}/Fe^{2+}. Determination of the redox potential E_0 of the quinhydrone electrode by potentiometric method and pH of buffer solution.	Module-4	25	Characterization of electrodes are done.

Spectrpscopic Analysis Lab (LAB)

Paper code: MSAC-395
(3 Credit)(100 Marks)

Spectroscopic Analysis: (40hr)

1. Determination of bonding in a molecule by using Fourier Transform Infrared (FTIR) spectroscopy.
2. Characterization of an compound by Attenuated Total Reflection Infra-Red Spectroscopy (ATR-FTIR, MID-IR).
3. Study of a charge-transfer complex between iodine and tritron-X 100 using UV-visible Spectroscopy (UV-Vis).
4. Determination of bond length of a diatomic molecule by Far-Infra-Red and Near Infra-Red spectroscopy.
5. Study of protein folding and defolding by Circular Dichroism (CD), and ORD.
6. Estimation of quenching constant of fluorescence quenching of a fluorescent molecule by Fluorescence spectrophotometer.
7. Quenching of fluorescence of a fluorescent molecule will be studied by time resolve fluorescence spectrophotometer.
8. Analysis and interpretation of sample data of given chemicals or compounds using Origin/ ChemOffice softwares.

SEMESTER - IV

Cheminformatics **Paper code: MSAC-401: (Elective III)**
(3 Credit) (100 Marks)

Course Objectives (CO):

1. To know how the information of a compound is stored in computer.
2. To find out a compound from a database using computer techniques.
3. To know the available softwere to draw chemical structure of compounds.
4. To know the important properties of a compound to be a drug.
5. To know different methods to design a drug.

Module 1: Unit-1: In-silico Representation of Chemical Information (10L)

a. CIF IUCr Crystallographic Information Framework
b. CML Chemical Markup Language
c. SMILES -- Simplified Molecular Input Line Entry Specification
d. Graph theory and its application
e. InChi -- IUPAC International Chemical Identifier
f. Other representations

Module 2: Unit-2: Chemical Databases and Data Mining (10L)

a. Cambridge Structural Database CCDC CSD
b. Crystallographic Open Database COD
c. Protein Data Bank PDB Ligand Explorer
d. Chemspider
e. Other Data Bases

Module 3: Unit-3: Molecular Drawing and Interactive Visualization (10L)

a. ChemDraw
b. Marvin Sketch
c. ORTEP
d. Chimera, RasMol, PyMol
e. Quantumwise

Module 4: Unit-4: Computer-Aided Drug Design Tools (10L)

a. Molecular Modelling Tools
b. Structural Homology Modelling Tools
c. Docking Tools and Screening Tools
d. Methods for computation of IC_{50}, LogP, toxicity etc.

Text books:

1. *Chemoinformatics: A Textbook*, Johann Gasteiger (Editor), Thomas Engel (Editor), November 2003, Wiley.
2. *Chemoinformatics in Drug Discovery*, Tudor I. Oprea (Editor), Raimund Mannhold (Series Editor), Hugo Kubinyi (Series Editor), Gerd Folkers (Series Editor), March 2006, Wiley.

Reference texts:

1. *Chemoinformatics in Drug Discovery*, Prof. Dr. Tudor I. Oprea, 26 January, 2005. Wiley online library.

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcome
1.	In-silico Representation of Chemical Information	Module 1/Unit 1	10	1.Will be able to identify a compound written in different format.
2.	Chemical Databases and Data Mining	Module 2/Unit 2	20	2.Will be able to search drug like compounds from a data base to test new compounds as a drug.
3.	Molecular Drawing and Interactive Visualization	Module 3/Unit 3	10	3.Will be able to draw and store a compound in computer.
4.	Computer-Aided Drug Design Tools	Module 4/Unit 4	30	4.Will be familiar with the different properties of a drug.
5.	Computer-Aided Drug Design Tools	Module 4/Unit 4	30	5.Will be able to desing a drug and predict its drug efficacy.

Project Stage-I (Term paper focus on project & Seminar)

Paper code: MSAC-491
(5 Credit) (20 Marks)

1.Review of literature and submission of report on a project based on an experiment using a sophisticated equipment and the duration of work is four weeks. The project report has to be submitted and will be evaluated by a committee consisting of faculties of the department and one from allied department, through seminar presentation on the report.

Project Stage-II (Dissertation & Viva-voce)

Paper code: MSAC-492
(16 Credit) (80 Marks)

1. Review of literature, project work and submission of dissertation.
2. Viva-voce on submitted work.

Laboratory work on any topic which will be useful for further studies, to be performed in-house or in any institute. After completion of work of minimum 12 weeks duration the project report shall be submitted in dissertation form and that will be evaluated through presentation on submitted work followed by viva-voce in presence of a committee constituted by an external expert and internal teachers.