M.Sc. Medicinal Chemistry Part- I

The following will be the structure for Medicinal Chemistry Syllabus from June 2013 for Semester I and Semester II

Semester – I	**No. of Credits**	**No. of Lectures + Tutorial/Seminar**
CHM – 100 Chemical Mathematics and Biostatistics	4 Credits	48+ 12
CHM – 101 Symmetry, Group theory and Chemical Bonding	4 Credits	48+ 12
CHM – 102 Stereochemistry and Mechanism	4 Credits	48+ 12
CHM – 140 Kinetics and Thermodynamics in Chemistry	4 Credits	48+ 12
Semester – II		
CHM – 200 Molecular Spectroscopy and its Applications in Organic Physical, Inorganic and Biomolecules	5 Credits	60+ 15
CHM – 201 Synthetic Organic Chemistry	5 Credits	60+ 15
CHM – 220 Basic Biochemistry, Biomolecules and Bioinorganic Chemistry	5 Credits	60+ 15
Optional Courses (any two)		
CHM – 204a Coordination Chemistry	2 Credits	24+ 06
CHM – 204b Principles of Medicinal Chemistry	2 Credits	24+ 06
CHM – 204c Biophysical Techniques	2 Credits	24+ 06

CHM – 110 Organic Chemistry practical (Departmental Course)	4 Credits
CHM – 120 Biochemistry practical (Departmental Course)	4 Credits
CHM – 130 Physical Chemistry Practical (Departmental Course)	4 Credits
CHM- 140 Computer applications in medicinal chemistry and Instrumentation	3 Credits

Tentative Structure of Medicinal Chemistry

M.Sc. Part – II

SEMESTER : - III –

1. CHM – 301 Medical Biochemistry and Immunology	5 Credits	60+ 15
2. CHM – 302 Advanced Analytical Techniques	6 Credits	72+ 18
3. CHM – 303 Advanced Organic and Inorganic hemistry and Drug Discovery Principles.	6 Credits	72+ 18

Practical Courses

4. CHM – 310 Organic Chemistry	4 Credits	
5. CHM – 320 Medicinal Chemistry	4 Credits	

SEMESTER :- IV

1. CHM – 401 Medicinal Chemistry of Natural Products.	5 Credits	60+ 15
2. CHM – 402 Chemistry of Drug Action	5 Credits	60+ 15
3. CHM – 403Pharmacological screening assays and Pharmacodynamics	5 Credits	60+ 15
4. CHM – 404 Drug Design and Development.	3 Credits	36+ 08
5.. CHM – 410 Project	7 Credits	

Syllabus for M.Sc. (Medicinal Chemistry) course would be of total 100 credits.

First year M.Sc. 50 Credits
Second year M.Sc. 50 Credits

Semester – I

SEMESTER - I

CHM 100 Chemical Mathematics (2 credits) 30L

1) Functions, Differential and Integral calculus

Functions, Limits, Derivative, physical significance, basic rules of differentiation, Maxima and Minima, Applications in Chemistry, Exact and inexact differential, Taylor and McLaurin series, Curve sketching.

Partial differentiation, maxima and minima of functions of several variables, chemical applications.

Rules of Integration, definite and indefinite integrals, geometrical meaning of integration, Applications in Chemistry

2) Differential Equations

Separation of variables, homogeneous, exact, linear equations, Equations of Second order,Series solution method

3) Probability and Theory of Errors

Permutations and Combinations, probability and probability theorems,Probability curves, Errors and Deviations, thermodynamic probability. Methods of Averages and Least Squares. 4) Vectors, Matrices and Determinants

Vectors, dot, cross and triple products.

Introduction to Matrix Algebra, Addition and Multiplication of Matrices, inverse, adjoint and transpose of matrices, unit, diagonal matrices, matrix eigenvalues and eigenvectors, diagonalization, determinants and their evaluation.

Biostatistics (2 Credit) 30L

1. Statistics: Introduction, its role and uses. Collection; Organization; Graphics and pictorial representation of data; Measures of central tendencies and dispersion. Coefficient of variation.
2. Probability: Basic concepts; Common probability distributions and probability distributions related to normal distribution.
3. Sampling: Simple random and other sampling procedures. Distribution of sample mean and proportion.
4. Estimation and hypothesis testing: Point and interval estimation including fiducial limits. Concepts of hypothesis testing and types of errors. Student- t and Chi square tests. Sample size and power.

5. Experimental design and analysis of variance: Completely randomized, randomized blocks. Latin square and factorial designs. Post- hoc procedures.
6. Correlation and regression: Graphical presentation of two continuous variables; Pearson's product moment correlation coefficient, its statistical significance. Multiple and partial correlations. Linear regression; Regression line, coefficient of determination, interval estimation and hypothesis testing for population slope. Introduction to multiple linear regression model. Probit and logit transformations.
7. Non-parametric tests: Sign; Mann-Whitney U; Wilcoxon matched pair; Kruskal wallis and Friedman two way ANOVA tests. Spearman rank correlation.
8. Statistical techniques in Pharmaceutics: Experimental design in clinical trials; Parallel and crossover designs. Statistical test for bioequivalence. Dose response studies; Statistical quality control.

Text Books

1) The Chemical Maths Book, E. Steiner (Oxford University Press) 1996

2) Quantum Chemistry, I. Levine, Fifth Edition, Prentice Hall 1999

Reference Books

1) Valence, C. A. Coulson, ELBS (1974)

2) Introduction to Quantum Mechanics- with Applications to Quantum Chemistry, L. Pauling and E. Bright Wilson, Dover Publishers, NY (1999)

3) Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill, NY (1972)

CD 101 Symmetry, Group Theory and Chemical Bonding (4 credits) 60L

Symmetry and Group theory

1) Definitions and theorems of group theory, subgroups, classes. 2L

2) Molecular symmetry and symmetry groups - symmetry elements and operations,. Symmetry planes, reflections, inversion center, proper / improper axes and rotations, products of symmetry operations, equivalent symmetry elements and atoms, symmetry elements and optical isomerism, symmetry point groups, classes of symmetry operations, classification of molecular point groups. 4L

3) Representations of groups. Great orthogonality theorem, character tables, properties of characters of representations. 4L

4) Group theory and quantum mechanics. Wave function as bases for irreducible representation 2L

5) Symmetry Adapted Linear Combinations -(SALC) - projection operators and their

use to construct SALC. 4L

6) Molecular Orbital Theory -

a) Principle, Symmetry factoring of secular equation, Carbocyclic systems, LCAO-MO π bonding, Worked example-Naphthalene, Three center bonding, symmetry based "selection rules " for cyclization .

b) Transformation properties of atomic orbital, MO's for Sigma bonding AB_n molecules, tetrahedral AB_4case, Hybrid orbital, MO's for pi bonding in AB molecules, cage and cluster compounds, MO's for metal sandwiched compounds 6L

7) Mechanism of metal complexes.

Ligand substitution reactions, substitution of square - planar complexes, substitution in octahedral complexes, redox reactions and photochemical reactions. 8L

Text Books:-

1. *Chemical applications and group theory: F.A.Cotton, 3rd edition (1999) chapters 1 to 8.*
2. *Inorganic chemistry: Shriver and Atkins, 3rd edn (1999) Oxford, chapter 8-12,14-15.*
3. *Group theory and its chemical applications: P.K Bhattacharya, 2nd edn (1989) Himalaya publ.*
4. *Molecular symmetry and group theory -A.Vincent.*
5. *Symmetry in Chemistry: H.Jaffe' and M.Orchin.*
6. *Symmetry in Inorganic Chemistry: J.P Fackler*

Chemical Bonding (2 Credits)

1. Recapitualtion, quantization, Postulates of Quantum mechanics, Schrödinger equation, particle in a box, particle in 3-D box, degeneracy, hydrogen like atoms (no derivation) atomic orbitals 12L

2. Variation method, many electron atoms, orbital angular momentum, electron spin, wave function of many electrons, Pauli exclusion principle, spin-orbit interaction, fine structure, vector atom model spectral terms 5L

3. Molecular Orbital theory, Born-Oppenheimer approximation, H_2 molecule, homo and hetero-nuclear diatomic molecules, MO diagrams of simple triatomic molecules. 5L

4. Valence bond theory of simple biomolecules, quantitative treatment of hydrogen molecule and related systems, hybridization, comparison of VBT and MOT 4L

5. Hückel theory of conjugated hydrocarbons, Electron densities, Bond orders and free valence indices, Illustrations 6L

Text books

1. Quantum Chemistry, I. Levine, 5th Edition, Prentice Hall (1999)

Reference Books:

1. Valence, C.A. Coulson, ELBS (1974)
2. Introduction to Quantum Mechanics-with applications to Quantum Chemistry, L.Pauling and E.B.Wilson, Dover Publishers (1999)
3. Orbitals in Chemistry, V. Gil, Cambridge University Press (2000).

CHM – 120 Stereochemistry and Mechanism 4 Credits 60L

Organic Reaction Mechanism

a) Acidity and basicity, Structure reactivity relationship –Introduction to aromaticity in Benzenoid and non – Benzenoid compounds, Inductive, Mesomeric, and steric effect, hyperconjugation, tautomerism and other effects and their influence on the physical and chemical properties of organic compounds 8L

b) Nucleophilic Substitution Reactions at saturated carbon 2L

The S_N2, S_N1, mixed S_N1 and S_N2 and SET mechanism. The neighboring group mechanism, The Neighboring group participation by π & σ bonds, anchimeric assistance, classical and non classical carbocations, phenonium ions, norbornyl system, carbocation rearrangements in neighboring group participation. The S_Ni, ion pair mechanism, Nucleophilic substitution at an allylic, aliphatic trigonal and vinylic carbon. Reactivity effects of structure, attacking nucleophile, leaving group and reaction mechanism, solvent effect, phase transfer catalyst, ambident nucleophile and regioselectivity.

c) Aromatic electrophilic and nucleophlic substitution Reactions 11L

Arenium ion mechanism, orientation and reactivity, energy profile diagram, calculation of partial rate factor, the ortho/ para ratio ipso attack, orientation in other ring systems such as Naphthalene, Anthracene, Six and five membered heterocycles, Diazonium coupling Vilsmeier reaction, Gattermann – Koch reaction, and other named reactions of carbocyclic rings. The ArS_N1, Benzyne and SNR1, Mechanisms, Reactivity effect of substrate structure, leaving group and attacking nucleophile.

Ref. 1 (page no. 539 to 594)

Books –

Texts –

1. F. A. Carey and R. J. Sundberg. (Ed. IV), Part A and part B – Adv. Organic Chemistry, Kluwer Academic pub.

2. J. March, (Ed IV), Adv. Organic Chemistry.
3. R.O.C. Norman, Organic Chemistry.
4. R. T. Morrison and R. N. Boyd, Organic Chemistry

References –

1. J. Clayden, N. Greeves. et. al Organic Chemistry , Oxford Univ. Press, 2001.
2. Gould E.S., Mechanism and Structure in Organic Chemistry.
3. H.O. House, Synthetic Organic Chemistry.

2. Stereochemistry of Organic Compounds 15L

a) Symmetry properties of organic compounds, Chirality of organic compounds, chiral centre, configuration of chiral centre, enantiomerism, diastereomerism, pseudoasymmetric carbon
b) Homotopic and heterotopic ligands and faces, Prochirality of center and faces,
c) Stereochemistry of Natural products as exemplified by the study of stereochemistry of menthol
d) Conformational concepts, conformations of acyclic molecules, cyclohexane and mono, di-substituted cyclohexane, Conformational effect on physical properties of the molecules

Books –

1. F. A. Carey and R. J. Sundberg. (Ed. IV), Part A – Adv. Organic Chemistry, Kluwer Academic pub., 2001.
2. E. L. Eliel, Stereochemistry of carbon compounds.

CHM – 140 Kinetics and Thermodynamics in Chemistry 4 Credits 60L

Kinetics

1) Recapitulation, First, Second, Third and n^{th} order reactions, reactions of fractional order, complex reactions, parallel and consecutive reactions, reversible reactions, autocatalysis, oscillatory reactions.
2) Techniques and Methods, Fast reactions, flow techniques, relaxation methods, flash photolysis, Kinetic isotopic effect
3) Reactions in gas phase, Collision theory, unimolecular reactions, Lindemann mechanism, potential energy surface, Transition state theory, Free radical and chain reactions, explosive reactions
4) Reactions in solutions, effect of solvation, ionic strength on rates, Linear free energy relationships, correlation of rate with solubility parameters, Enzyme catalysis, Michaleis and Menton analysis

Text Books

i) Principle of Chemical Kinetics, J. C. House, Wm C Brown Publishers, (1997)

ii) Chemical Kinetics, K. J. Laidler, Mc Graw Hill, Third Edition (1987).

Thermodynamics:

1. Recapitulation of fundamental concepts in Thermodynamics 2L

Work, Heat, Temperature, Mechanical Equivalent of Heat, Heat Capacities (C_p & C_v), Ideal Gas, Equation of State, Thermodynamic Equilibrium, Different types of Thermodynamic Processes-(Reversible, Irreversible, Adiabatic, Isothermal, Isobaric, etc.) Reservoir, Molecular Energies, State Functions and Path Functions, Exact & Inexact Differentials, Condition for Exact Differentials.

2. Laws of Thermodynamics and Thermodynamics Functions 6L

Zeroth-, First-, Second- and Third Laws -Conceptual Development & Implications. Internal Energy (U), Enthalpy (H), Entropy (S), Helmholtz and Gibb's Free Energies (A & G), Absolute Entropy, Work under various conditions. Maxwell's Equations and their application, Various relationships for (C_p -Cv) & Cp/Cv, Conditions for Equilibrium and Spontaneity, Relationship between Free Energy change (ΔG) and Equilibrium Constant (K), Concept of Partial Molar Quantities -Chemical Potential *(μ).*

3. Applications 7L

Heat Engine, Refrigeration, Joule-Thompson effect, Liquefaction of Gases. Flame Temperatures, Explosion Temperature and Pressure. Phase Equilibria (melting, vaporisation, sublimation, crystal modifications). Calculation of , ΔH , ΔS, ΔG & K and effect of Temperature & Pressure thereon for various types of Chemical Reactions -(Combustion, Hydrogenations, Bond Dissociation, Hydration/(Solvation), Ionisation, Isomerisation, Decomposition, Reduction of Metal Oxides, Ammonia synthesis, etc.). Electrochemical Cells- Electrode Potentials and Cell E.M.F., Determination of ΔG from cell E.M.F. Ideal & Non-ideal Solutions.

4. Statistical Thermodynamics 5L

Microscopic point of view. Thermodynamic Probability (W)- Distinguishable and Indistinguishable Particles, Different ways of Arrangements and Maximisation ofW, Maxwell-Boltzmann Distribution Law, Partition Function (Q), Fermi-Dirac and Bose-Einstein Statistics.

Books & References*:*

(1). Physical Chemistry -RA.Alberty & R.J.Silby, 1st ed. (1995), John Wiley.

(2). Physical Chemistry -G.B.Castellan, 3rd ed.(1986), Narosa Publishers, Mumbai.

(3). Physical Chemistry -G.M.Barrow, 5th ed. (1988), Tata McGraw Hill.

(4). Physical Chemistry -P.W.Atkins, 4th ed. ( ), E.L.B.S.

Semester II

CD 200 Molecular Spectroscopy and its Applications in Organic, Physical Inorganic and Biomolecules (5 credits) 75 L

1) Recapitulation, The width and intensity of spectral transitions, Fourier Transformation microwave spectroscopy, rotation of molecules, rotational spectra of di- and poly- atomic molecules, Stark effect 5L

2) Infrared Spectra: The vibrating diatomic molecule, the diatomic vibrating rotator, Interaction of rotations and vibration, vibrations of polyatomic molecules, The influence of Rotation on the spectra of polyatomic molecules 4L

3) Symmetry and Normal Vibrations, Potential energy distribution (PED), force constants, selection rules, group frequencies, factors affecting band positions and intensities metal-ligand vibration, Normal coordinate Analysis. 5L

Interpretation of spectra, Applications to Structural problems in organic chemistry. 6L

Applications of spectroscopy to Inorganic Chemistry. 3L

4) Raman Spectroscopy: Introduction, Rotational Raman spectra, vibrational Raman spectra, Polarization of light and the Raman effect, Structure elucidation from the combined Raman and Infrared spectroscopy 4L

Applications of Raman spectroscopy in Inorganic Chemistry 2L

5) Electronic Spectroscopy: Electronic spectra of diatomic molecules, vibrational coarse structure, progressions, intensity of vibrational-electronic spectra: the Franck-Condon Principle, oscillator strengths, spectroscopic and equilibrium dissociation energies, rotational fine structure of electronic-vibration Transitions, fortrat parabola, predissociation. 5L

Interpretation of Spectra, solvent effects, chromophores and auxochromes, effect of conjugation, Woodward Rules for dienes, unsaturated ketones and aldehydes, aromatic compounds, applications to structural problems 4L

6) Spin resonance Spectroscopy: Basic Concepts, Nuclear spin states, mechanism of absorption, population densities of nuclear spin states, NMR Spectrometer. 2L

7) NMR Chemical shifts, integration, coupling constants, rate processes, spin spin splitting multiplicity, diamagnetic anisotropic effects, First order analysis, Applications to aliphatic and aromatic compounds, . 10L

Application of spin resonance spectroscopy to inorganic systems. 2L

8) Electron Paramagnetic Resonance: Underlying principle, presentation of spectra, instrumentation, hyperfine splitting (applications to radicals) 4L

9) Mosbauer Spectroscopy: Basic principles, spectral parameter Applications – oxidation states of iron compounds 4L

Text Books

1) *Fundamentals of Molecular Spectroscopy, C. M. Banwell and E. McCash, Tata McGraw Hill, Fourth Edition (1994)*
2) *Spectroscopic Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley, Fifth Edition (1991)*
3) *Spectroscopy of Organic Compounds, P. S. Kalsi, New Age International, Fourth Edition (1999)*
4) *The Infrared Spectra of Complex Molecules, L. J. Bellamy, Chapman and Hall, NY, Third Edition (1975)*
5) *Physical Methods in Chemistry, R. S. Drago, Saunders (1977).*
6) *Infrared and Raman Spectra of Inorganic and Co-ordination Compounds, Part A and Part B, K. Nakamoto, John Wiley, Fifth Edition (1997)*

CHM 201 Synthetic Organic Chemistry (5 credits) 75L

Synthetic Organic Chemistry

a) Oxidation and reduction 12L

b) Addition and Elimination reactions 12L

c) 1. Rearrangements: 10L

Beckmann, Hofmann, Lossen, Curtis

Schmidt, Wolf, Loftman

Baeyer – Villiger

Stevens, Wittig, Sommelet, Favorskii

Pinacole – Pinacolone, Benzil – Benzilic acid

Claisen and Cope rearrangement

2.Reactive intermediates 2L

Carbene, nitrene and free- radicals – structure, generation and their stabilities

3. Pericyclic reactions 2L

d) Organometallics

Non- transtion metals

Mg, Li, B, P, 8L

Zn, Cu, Sn, Al, Si 5L

Ylides 4L

Ester Hydrolysis 5L

References:

1. *Advanced Organic Chemistry, F A Carey and R J Sundberg, Part B (for autonomous centers).*
2. *Basic principles of organic chemistry, J D Roberts and M C. Caseiro Benjamin (1964).*
3. *Advanced organic chemistry, J. March 4th edition. Wiley-Interscience publication 1999.*
4. *Mechanism and structure in organic chemistry, E S Gould, Holt, Rinehart and Winston.*

CHM – 220 Basic Biochemistry, Biomolecules, Bioinorganic Chemistry 5 Credits 75L

Biomolecules II, Proteins and Nucleic Acids

1. Amino acids: Classification, Properties, reactions, rare amino acids, separation techniques.
2. Protein classification: Reactions, functions, properties peptide synthesis. Solid phase synthesis.
3. Structure:
   a) Peptide bond, end group analysis, sequencing.
   b) Secondary: alpha-helix beta- structure, 310 helix, super secondary structure.
   c) Tertiary Structure: Forces Stabilizing, unfolding / refolding expt. Prediction of tertiary Structure.
   d) Quaternary structure – haemoglobin.
   e) Ramachandran plot.
   f) Helix coil transitions, Van der Waals, electrostatic, Hydrogen bonding, and hydrophobic interactions.
   g) Energy terms in Biopolymer conformational calculation.
4. Molecules of Heredity: Structure of DNA and RNA, DNA as genetic material, Double helix. Denaturation and renaturation A, B, and Z forms of DNA.

Reference Books:

1 Principle of Biochemistry, Lehinger D.L. Nelson and M.M. Cox. Macmillan Worth Publishers.

2 Biochemistry, L. Stryer, W.H. Freeman, San Francisco.

3 Schaum's Outline Steries of Theory and Problems of Biochemistry, Philip W. Kuchel and G.B. Ralston. Int. Ed., McGraw-Hill Book Co.

Problem Approaches in Biochemistry. Wood and Hood

Bioinorganic Chemistry

1. Principles of coordination Chemistry related to Bioinorganic–Proteins, nucleic acids and other metal binding biomolecules.
2. Choice, uptake and assembly of metal containing units in Biology
3. Control and utilization of metal ion concentration in cells.
4. Metal ion folding and cross –linking of biomolecules.

5. Binding of metal ions and complexes to biomolecular active centers

Text Books:

1. Ligand field theory & its application: B.N.Figgis & M.A.Hitchman (2000) Wiely VCH publ. Chapters 5,6,8,9,11.
2. Principles of Bioinorganic Chemistry: S.J.Lippard & J.M Berg (1994), University science books, Mill Valley, California Chapters- 1,2,3,5,6,7,8.
3. Inorganic Chemistry: Shriver & Atkins (1999) Oxford.
4. Inorganic Electronic spectroscopy: A.B.P.Lever ,2^{nd} ed^{n} (1984), Elsevier Science Publishers, New York.
5. Biological Chemistry of the Elements: R.J.P.Williams & F.R.deSalvia, Oxford University Press-(1991)
6. Bioinorganic Chemistry : Inorganic elements in the Chemistry of life: An introduction & guide : W.Kaim,B.Schwederski, VCH,(1991)

Basic Biochemistry

1. **Introduction of Biochemistry:** Scope of the subject in Pharmaceutical Sciences, Biochemical reactions, highlights of prokaryotic and Eukaryotic cell metabolism.
2. **The molecular logic of life:** The chemical unity of diverse living organisms, composition of living matter. Macromolecules and their monomeric subunits.
3. **Properties of Water:** With interactions in aqueous systems. Ionization of water, weak acids and weak base. The pH scale, measurement of pH, pH metry, Acid base titration curves. Buffers, biological buffer systems.
4. **Carbohydrates:** Classification, basic chemical structure, monosaccharides, aldoses, and ketoses, cyclic structure of monosaccharides, stereoisomerisms, anomers and epimers. Sugar derivatives, deoxy sugars, amino sugars, and sugar acids. Reducing properties of monosaccharides, Disaccharides, oiligosaccharides, polysaccharides, structural studies methylation and periodate oxidation. Polysaccharides-structure and function of complex. Carbohydrates, proteoglycans, glycoproteins, glycolipids, mucopolysaccharides.
5. **Lipids:** Classification, structure and function of major lipid subclasses-acylglycerols, circulating lipids: Lipoproteins, chylomicrons, LDL, HDL, and VLDL. Pathalogical changes in lipid levels. Formation of micelles, monolayers, bilayter, liposomes.
6. **Vitamins and Co-enzymes:** Classification, water-soluble and fat-soluble vitamins. Structure, dietary requirements, deficiency conditions, coenzyme forms.
7. **Amino acids**: Classification, Properties, reactions, rare amino acids, separation techniques.
8. **Protein classification**: Reactions, functions, properties peptide synthesis. Solid phase synthesis.
9. Structure:
    h) Peptide bond, end group analysis, sequencing.

i) Secondary: alpha-helix beta- structure, 310 helix, super secondary structure.

Covalent bonds , Ionic bonds, Hydrogen bonds, Van der Waals bonds, Repulsive forces

Relative importance of binding forces

j) Tertiary Structure: Forces Stabilizing, unfolding / refolding expt. Prediction of tertiary Structure.

k) Quaternary structure – haemoglobin.

l) Ramachandran plot.

m) Helix coil transitions, Van der Waals, electrostatic, Hydrogen bonding, and hydrophobic interactions.

n) Energy terms in Biopolymer conformational calculation.

10. **Nucleic acids**

a) Molecules of Heredity: Structure of DNA and RNA, DNA as genetic material, Double helix. Denaturation and renaturation A, B, and Z forms of DNA.

b) The primary, secondary and tertiary structure of DNA

c) Drugs acting on DNA

d) Intercalating agents

e) Alkylating agents

f) Drugs acting by chain 'cutting*

g) Ribonucleic acid

Reference Books:

1 Principle of Biochemistry, Lehinger D.L. Nelson and M.M. Cox. Macmillan Worth Publishers.

2 Biochemistry, L. Stryer, W.H. Freeman, San Francisco.

3 Schaum's Outline Steries of Theory and Problems of Biochemistry, Philip W. Kuchel and G.B. Ralston. Int. Ed., McGraw-Hill Book Co.

4 Problem Approaches in Biochemistry. Wood and Hood.

CHM – 110 Organic Chemistry practical (Departmental Course) 5 Credits

1. **Techniques:** Crystallization, fractional crystallization, fractional distillation, sublimation, steam distillation, column chromatography and thin layer chromatography.
2. **Derivatives** of functional groups such as acetyl, 2,4-DNP, anilide, amide and aryloxy acetic acid
3. **Single stage preparations (minimum** 4 preparations)

Preparation of *p*-nitro acetanilide from acetanilide

Preparation of *p*-bromo acetanilide from acetanilide

Diels-Alder reaction of sulpholane and maleic anhydride

Sandmeyer reaction

Conversion of *t*-butanol to *t*-butylchloride

4. **Two stage preparations** (minimum 4 preparations)

Benzoin → Benzil → benzilic acid

↓

quinoxaline

Acetophenone → oxime → acetanilide

Phthalic anhydride → *o*-benzoyl benzoic acid → anthraquinone

Acetophenone → benzalacetophenone → epoxide

Hydroquinone → uinine → 1,2,4-triacetoxybenzene

5. Three stage preparations (minimum one preparation)

1. *p*-Nitro toluene → *p*-nitro benzene → ethyl-*p*-nitrobenzoate → *p*-aminobenzene

2. Pthalic acid → pthalic anhydride → phthalimide → anthranilic acid

4. Computer applications: (1) Conformational energetics of simple organic molecules through molecular mechanics force fields.

(2) Insights for reaction mechanisms of simple SN^1 and SN^2 reactions.

Reference Books. Vogel's Text book of Practical Organic Chemistry,5th Edition

CHM – 120 Biochemistry Practical (Departmental Course) 5 Credits

1) Estimation of carbohydrates
2) Estimation of proteins
3) Molar extinction coefficient of molecules
4) Extraction and estimation of lipids
5) Direct microscopic counts
6) Total viable counts
7) Control of microbial growth
8) Determination of MIC (plate method)
9) Isolation of Bacterial, animal, plant and plasmid DNA
10) Agarose gel electrophoresis of DNA

Reference Book:

1. Biochemical Methods by Dr. S. Sadasivam and Dr. A. Manikam, 3rd Edition New Age International, 2006.
2. Practical Biochemistry, Principles and Techniques (1995). Ed. Kelth Wilson and John Walker.
3. Introductory Practical Biochemistry (2001). Ed. S.K. Sawhny and Randhir Singh.

CHM – 130 :- Physical Chemistry Practicals (5 Credits)

A) Conductometry:

i) Hydrolysis of NH4Cl or CH3COONa or aniline. hydrochloride.

ii) Determination of λ0 or λα and dissociation constant of acetic acid.

iii) Hydrolysis of ethylacetate by NaoH.

iv) Determination of ..G, ..H, and .. S of Silver Benzoate by conductometry.

B) Poetentiomerty:-

1. Stability Constant of a complex ion.
2. Solubility of a sparingly soluble salt.
3. To determine the ionic product of H2O
4. Estimation of halide in mixure.

C) pH metry:-

1. Determination of the acid and base dissociation constant of an amino acid and hence the isoelectric point of the acid.

D) Polarography

1. Determination of half wave potential E 1/2 and unknown concentration of an ion.
2. Amperometric titration of Pb(NO3)2 with K2Cr2 O7

E) Colorimetric :-

1. Analysis of a binary mixture.
2. Copper EDTA photometric titration.

F) Radioactivity:-

1. Estimation of Mn in tea leaves by NAA
2. Half – life of a radioactive nuclide and Counting errors.
3. Determination of Emax of beta radiation and absorption coefficients in Al.

G) Chemical Kinetics:

1. Kinetic decomposition of diacetone alcohol by dilatometry.

2. Determination of an order of a reaction.

3. Bronsted primary salt effect.

H) Non- Instrumental :-

1) Freundlich and Longmuir isotherms for adsorption of acetic acid on active charcoal

2) Statistical treatment of experiemntal data

3) Molecular weight by steam distillation.

4) Glycerol radius by viscosity.

5) Partial Molar Volume (Polynometry) Determination of the densities of a series of soltions and to calculate the molar volumes of the components. Each candidate should perform a minimum of 18 experiments with at least one experiment form each techniques.

I) Surface area analysis by BET method e.g. industrial pigment

References:-

1. Practical physical chemistry, A. Findary, T.A. kitchner (Longmans, Green and Co.)

2. Experiments in Physical Chemistry, J.M. Wilson, K.J. Newcombe, A.r. Denko. R.M.W. richett (Pergamon Press)

3. Senior Practical Physical Chemistry, B.D. Khosla and V.S. Garg (R. Chand and Co., Delhi.)

Optional Courses (any two)

CHM -204a Coordination Chemistry (2 Credits) 30L

1.Concept & Scope of ligand Fields. 2L

2. Energy levels of transition metal ions, Free ion terms, term wave functions, spin –orbit coupling 8L

3. Effect of ligand fields on energy levels of transition ions, weak cubic ligand field effect on Russell-Saunders terms, strong field effect, correlation diagrams,Tanabe-Sugano diagrams, Spin-pairing energies. 10L

4. Electronic spectra of complexes band intensities, band energies, band width & shapes, spectra of 1^{st},2^{nd}& 3^{rd} row ion and rare earth ion complexes, spectrochemical & Nephelauxetic series, charge transfer & luminescence spectra, calculations of Dq,B, □ parameters. 10L

5. Magnetic properties of complexes paramagnetism,1st & 2nd ordered Zeeman effect, quenching of orbital angular momentum by Ligand fields, Magnetic properties of A,E,T ground terms in complexes ,spin free–spin paired equilibria 6L

CHM – 204b Principles of Medicinal Chemistry. 2 Credits 30L

1. Molecular Recognition in Drug-Receptor Binding
    a. Molecular forces
    b. Binding energetics
2. Enzyme Inhibitors
    a. Modes of inhibition
    b. General approaches
3. Case studies

a. Antibacterial Drugs
    i. Major drug classes
    ii. Drug resistance

b. Antiviral Drugs
    i. Description of viruses
    ii. Major drug classes
    iii. Drug resistance

c. Anticancer Drugs
    i. Major cancer drug targets
    ii.MOA of anticancer drugs
    iii.Drug resistance

d. Analgesic Drugs

e. anesthetics (general, local)

f. Neurotransmitters (adrenergic, cholinergic effects; psychopharmacology)

g. CNS depressants (sedative/hypnotic, major/minor tranquilizers)

h. CNS stimulants

i. Steroids

4. Drug Metabolism
    a. Phase I metabolism
    b. Phase II metabolism
5. Prodrug Design
    a. Bioprecursor prodrugs
    b. Carrier-linked prodrugs
6. Case Studies

CHM – 204c Biophysical Techniques **2 Credits** **30L**

1. Calorimetry – Isothermal Titration Calorimetry (ITC) 4L
2. Chromatography – various techniques from this field are used for the purification and analysis of biological molecules 12L
3. Circular Dichroism – 1L
4. Electron microscopy (SEM & TEM)– used to gain high-resolution images of subcellular structures 5L
5. Fluorescence spectroscopy – for detecting structural rearrangements, as well as interactions of biomolecules. 2L
6. Gel electrophoresis – determines the mass, the charge and the interactions of biological molecules 2L
7. Imaging – scientific imaging of biological materials, usually by some form of microscopy, or sometimes indirectly such as in x-ray crystallography or by computer imaging; at a wide range of magnifications to see macromolecules, cells, tissues, or organisms. 1L
8. Microscopy – used in many ways, for example, to enabled the use of laser instruments for scanning and transmission.. Atomic force microscopy – 1L
9. Ultracentrifugation – gives information on the shape and mass of molecules 1L
10. X-ray crystallography – method to determine the exact structure of molecules with atomic resolution 1L

Reference Books:

1. Advanced Techniques in Biophysics Series: Springer Series in Biophysics, Vol. 10
Arrondo, José Luis R.; Alonso, Alicia (Eds.) 2006, XIV

2. Methods in Modern Biophysics by Bengt Nölting Springer Verlag Berlin Heidelberg 2009. ISBN 975-3-642-03022-2.

3. Introduction to Biophysical Methods for Protein and Nucleic Acid Research *by*
Jay A. Glasel, Murray P. Deutscher and Murray P. Deutscher Copyright © 1995 Elsevier Inc. All rights reserved ISBN: 978-0-12-286230-4

Reference Books

11. An Introduction to Medicinal Chemisty by Graham L Patrick, 4th Edition, 2009, ISBN 978-0-19-923447. Oxford University Press
12. Fundamentals of Medicinal Chemistry by Gareth Thomas, 1st Edition, December 2003. ISBN 0-470-84307-1. John Wiley & Sons Inc.
13. Molecules and Medicines E.J.Corey, Laszlo Kurti, Barbara Czako 1st Edition, 2007 ISBN 3-13558-406-6.

CHM-140 Computer Applications in Medicinal Chemistry & Instrumentation **3 credits**

1. Molecular Modeling: Energy minimization, geometry optimization, conformational analysis, global conformational minima determination; Approaches and problems; Bioactive vs. global minimum conformations; Automated methods of conformational search; Advantages and limitations of available software; Molecular graphics; Computer methodologies behind molecular modeling including artificial intelligence methods.
2. QSAR: Electronic effects; Hammett equation, Lipophilicity effects; Hansch equation, Steric Effects; Taft Equation; Experimental and theoretical approaches for the determination of physico-chemical parameters, parameter inter-dependence; Case studies; Regression analysis, extrapolation versus interpolation, linearity versus non-linearity; The importance of biological data in the correct form;
3. Molecular docking and dynamics: Rigid docking, flexible docking, manual docking;
4. Pharmacophore: Concept, pharmacophore mapping, methods of conformational search used in pharmacophore mapping;

Instrumentation:

1. HPTLC analysis of medicinal plants.
2. HPLC analysis of lipids and sugars
3. GC-MS of fatty acid esters
4. IR & NMR of simple organic compound synthesized in the lab.
5. Fluorescence interaction of drug with BSA.