University of Pune
Department of Chemistry
Syllabus for M.Sc. (Medicinal Chemistry)

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

•CD 100 Chemical Mathematics and Chemical Bonding (5 credits) 60L

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 8L

2) Differential Equations

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

7L

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. 4L

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. 5L

5) The principles of quantum mechanics, Wave particle duality, Uncertainty principle, Schrodinger equation, Simple systems- free particle, particle in a box, Harmonic oscillator, hydrogen-like Atoms (no derivation), Legendre and Hermite polynomials, Atomic orbital

10L

6) The variational method, Many electron atoms, Orbital angular momentum Electron spin, Wave functions of many electron atoms, The Pauli exclusion principle, Spin-orbit interaction, Fine structure, The vector atom model, Spectral terms 8L

7) Molecular Orbital theory of diatomic molecules, Born Oppenheimer approximation, H2 molecule and related system, Homo- and hetero nuclear diatomic molecules, Correlation diagrams 6L

8) Valence Bond theory of simple molecules, quantitative treatment of hydrogen molecule and related systems, Orbital Hybridization, Comparison of VB and MO Theories 6L

9) Pi electron systems, Huckel Treatment for conjugated hydrocarbons, Electron densities, Bond orders and free valence indices, Illustrations, Cyclic conjugated systems, Application of the Huckel method to linear and cyclic polyenes. 6L

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, Stereochemistry and Mechanism (6 credits) 72L

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*

Mechanism and Stereochemistry

42L

a) Inductive and Resonance efforts, acidity and basicity, aromaticity

6L

b) Nucleophilic substitution reactions

10L

c) Aromatic electrophilic and nucleophilic substitution

6L

c) Stereochemistry

18L

Reference Books:

1.Advanced Organic Chemistry, J. March, 4th edition. Wiley-Interscience publication, 1999

2. Advanced Organic Chemistry, F A Carey and R J Sundberg, Part A, Plenum press (for autonomous centers).

3. Stereochemistry of carbon compounds, E L Eliel, 4th edition Tata McGraw Hill edn.

4. Mechanism and structure in organic chemistry, E S Gould, Holt, Rinehart and Winston

(to be used for problem solving of topics a-c).

CD 102 Main Group Chemistry and Basic Biochemistry I (5 Credits)

A. Main Group Chemistry : (2 credits) 24L

Chemistry of s & p block elements. 16L

Hydrogen, s & p block metals, boron and carbon groups, nitrogen and oxygen groups, halogen and nobel gases.

Main group organometallic chemistry. 8L

Classification, nomenclature and structure, electron deficient compounds, electron precise compounds, electron rich compound.

B. Basic Biochemistry I: (3 credits) 30L

1. **Introduction of Biochemistry:** Scope of the subject in Pharmaceutical Sciences, Biochemical reactions, highlights of prokaryotic and Eukaryotic cell metabolism. 3L
2. **The molecular logic of life:** The chemical unity of diverse living organisms, composition of living matter. Macromolecules and their monomeric subunits. 3L
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. 5L
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. 10L

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. 5L
6. **Vitamins and Co-enzymes:** Classification, water-soluble and fat-soluble vitamins. Structure, dietary requirements, deficiency conditions, coenzyme forms. 4L

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.

Semester II

CD 200 Molecular Spectroscopy and its Applications (5 credits)

60L

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) Moessabauer 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)*

CD 210

Chemical Kinetics, Thermodynamics and Coordination Chemistry (5 credits)

60L

Chemical Kinetics

20L

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. 4L
2) Techniques and Methods, Fast reactions, flow techniques, relaxation methods, flash photolysis, Kinetic isotopic effect 3L
3) Reactions in gas phase, Collision theory, unimolecular reactions, Lindemann mechanism, potential energy surface, Transition state theory, Free radical and chain reactions, explosive reactions 9L
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 4L

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.

Coordination Chemistry

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 pairedequilibria

6L

CD 230 Biomolecules II and Bioinorganic Chemistry (5 credits) 60L

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 – hamoglobin.
   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 rena -turation 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

Overviews of Bioinorganic Chemistry. 2L

1. Principles of coordination Chemistry related to Bioinorganic–Proteins, nucleic acids

and other metal binding biomolecules. 6L

2. Choice, uptake and assembly of metal containing units in Biology 4L.

3. Control and utilization of metal ion concentration in cells. 4L

4. Metal ion folding and cross –linking of biomolecules. 4L

5. Binding of metal ions and complexes to biomolecular active centers 4L

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 ,2nd edn (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)*

CD 250 Synthetic Organic Chemistry (5 credits) 60L

Synthetic Organic Chemistry

a) Oxidation and reduction 12L

b) Addition and Elimination reactions 8L

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 6L

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.*

Practicals

CD 120 Physical Chemsitry: (5 credits)

Conductometry:

(1) Hydrolysis of NH_4Cl or H_3COONa or aniline hydrochloride

(2) Solubility of a sparingly soluble salt.

(3) Hydrolysis of ethyl acetate by NaOH.

(4) Determination of ΔG, ΔH, and ΔS of Silver Benzoate by conductometry.

Potentiometry:

(1) Stability constant of a complex ion.

(2) Solubility of a sparingly soluble salt.

(3) Determination of dissociation constant of acetic acid.

(4) Estimation of halide in mixture.

pH metry:

(1) Hydrolysis of aniline hydrochloride

(2) Determination of the acid and base dissociation constants of an amino acid and hence the isoelectric point of the acid.

Polarography:

(1) Determination of half wave potential E ½ and unknown concentration of an ion.

(2) Amperometric titration of $Pb(NO_3)_2$ with $K_2Cr_2O_7$.

Colorimetry:

(1) Analysis of a binary mixture.

(2) Copper EDTA photometric titration.

(3) Determination of stability constant of ferrisalicylate complex by colorimetric measurements.

Radioactivity:

(1) Estimation of Mn in tea leaves by NAA.

(2) Half-life of a radioactive nuclide.

(3) Determination of E_{max} of beta radiation and absorption coefficients in Al.

(4) Counting errors.

Chemical kinetics:

(1) Kinetic decomposition of diacetone alcohol by dilatometry.

(2) Determination of an order of a reaction.

(3) Bronsted primary salt effect.

Non-Instrumental:

(1) Freundlich and Langmuir isotherms for adsorption of acetic acid on active charcoal.

(2) Statistical treatment of experimental data.

(3) Molecular weight by steam distillation.

(4) Glycerol radius by viscosity.

(5) Partial Molar Volume (Pykenometry) Determination of the densities of a series of solutions and to calculate the molar volumes of the components.

Each candidate should perform a minimum of 20 experiments with at least two experiments from each technique.

Text Books

(1) Practical Physical Chemsitry, A.Finday, 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).

CD-260 Organic Chemistry Practicals: (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 → quinone → 1,2,4-triacetoxybenzene

5. Three stage preparations (minimum one preparation)
   1. *p*-Nitro toluene → *p*-nitro benzene → ethyl-*p*-nitrobenzoate → *p*-aminobenzen
   2. Pthalic acid → pthalic anhydride → phthalimide → anthranilic acid

CD 140: Inorganic Chemistry: (5 credits)

2) Ore Analysis: At lest two of the following:

a). Determination of silica and manganese in pyrolusite.

b). Determination of copper and iron from chalcopyrite.

c). Determination of iron from heamatite.

3) Alloy analysis (At least two of the following)

a). Determination of tin & lead from solder.

b). Determination of iron & Chromium from mild steel.

c). Determination of copper and nickel from cupranickel.

4) Inorganic Synthesis and purity determination (any five)

a) Cis-trans potassium di-aquo di-oxalato chromate (III)

b) Chloro penta-ammino cobalt (III) chloride

c) Nitro penta-ammino cobalt (III) chloride

d) Nitrito penta-ammino cobalt (III) chloride

e) Bis,2-4 pentanedionato cobalt (II) and cobalt (III)

f) Potassium tri-oxalato aluminate

g) Reineckes: salt

5) Chelation in Nickel complexes: Preparation of Ni(II) ethylenediamine complexes and studying their absorption spectra.

6) Instrumental methods of analysis.

a). Colorimetry .

7) Simultaneous determination of Cr & Mn.

ii) Determination of K_{eq} of M-L Systems such as ,

Fe(III)- Salisylicylic acid

Fe(III)-Sulphosalicylic acid

Fe(III)- □ -resorcilicic acid by Jobs's & Mole- ratio method.

iii) Determination of iron by solvent extraction technique in a mixture of Fe^{+3} + Al^{+3} & Fe^{+3} + Ni^{+2} using 8- hydroxyquinoline reagent.

b) Thermochemistry

i) Lattice energy of binary salt by heat of dissolution, systems such as $CaCl_2$, NaCl, KCl.

ii) Determination of heat of neutralization of strong base and strong acid

c) Conductometry

Verification of Debye Hückle theory of ionic conductance for strong Electrolytes KCl, BaCl2.K2SO4, $K_3[Fe(CN)_6]$

d) Table work: (any one)

i. Analysis of Electronic spectra of transition metal complexes at least for one system (d^n Oh or Td) and calculation of Crystal Field parameters, inter electronic repulsion parameter and bonding parameter.

i. Data analysis, error analysis, least squares method. Plot of Born Maeyer to determine for 1:1 type molecule to determine internuclear separation. Characterization of metal ligand bonding using IR spectroscopy.

References

1) Text book of Quantitative Analysis, A.I.Vogel. 4th edn (1992).

2) Electronic Spectroscopy by A.B.P. Lever.

3) Inorganic Synthesis (Vol. Series)

4) Practical Manual made By Department of Chemistry, University of Pune

Syllabus for II year M.Sc (Medicinal Chemistry) under Credit System

Total: **50 credits**

For practical: **15 credits**

CD-377: 4 credits Isolation of natural products and Preparations

CD-477: 4 credits Instrumental Analysis

CD-478:7 credits Projects

Credits for Theory courses:

Semester III: 4 courses = **19 credits.**

CD-350: Organic Reaction Mechanism: 4 credits

Carbanions : formation and stability,mechanism of important reactions (12)

Neighbouring Group Participation (10)

Formation and hydrolysis of esters,amides etc. (8)

Linear free energy relationships :Hammett equation and its modifications, Taft equation, applications of these in determining mechanism and drug actions (12)

Enamines in organic synthesis (4)

Aromaticity (2)

CD-351: Advanced analytical Techniques 5 credits

Carbon magnetic resonance spectroscopy elementary and advanced ideas (16)

Mass theory, instrumentation, principle, fragmentations etc. (12)

Problems based on joint applications of UV, IR, PMR CMR and mass spectroscopy (12)

2D NMR elementary ideas and applications (4)

Separation techniques: Fundamental principles, Theory, instrumentation and application of GLC, HPLC, GC-MS, HPTLC. (16)

CD-352: Stereochemistry: 5 credits 60L

Acyclic stereochemistry (6)

Stereochemistry of six membered rings relation to physical properties, conformation and chemical reactivity, conformational effects in six membered rings containing unsaturation. (8)

The shapes of rings other than six membered rings: five membered, medium rings, transannular effects, concept of I strain (4)

Fused rings and bridged rings (14)

Stereochemistry of natural products menthol, strychnine, podophyllotixin (3)

Resolution methods (2)

Stereoselective synthesis and Assymetric Synthesis (15)

ORD and CD (8)

CD 371: Medical Biochemistry and Immunology (5 Credits) 60L

Medical Biochemistry

1. Mechanism of action at molecular level of selected antibiotics, antimetaboilites, analgesics, hallucinogens and other drugs, mechanism of resistance to antibiotics and other drugs.
2. Lysosomes and their physiological role.
3. Cerebrospinal fluid, composition in health and disease.

   i) Blood coagulation, clotting factors, mechanism of coagulation, fibrinolysis, abnormal haemoglobins, fibronectins. Diseases of cardiovascular system.

   ii) Cancer causative agents and control theories of cancer and carcinogenesis, viral etiology, control of cancer and carcinogenesis, viral etiology, control of cancer –basic approaches.

   iii) Biochemical basis of infective diseases

   iv) Genetic diseases and genetic counseling, teratogenesis.

Reference Books

1) Biochemistry of antimicrobial action (4th ed) TJ Franklin, Chapman hall (1989)
2) Mecahnism of microbial diseases, M Schaechter et al,Williams and Wilkino Int. Ed.(1989)
3) General Microbiology, Pelczar, Rard and Chan (1987)
4) Biochemistry, L Stryer,(3rd ed), Freeman and Co.

5) Biochemistry, L Stryer,(3rd ed), Freeman and Co.
6) Textbook of Biochemistry with clinical correlations, Thomas Devlin,(2nd ed),John Wiley and sons
7) Biochemical aspects of human diseases (1983), RL E lkeles, Slackwell scientific publishers, Oxford
8) Analogues of nucleic acids, Ray Berman (1970), Spring velrag.

Immunology

1. Cellular basis of immunity: immunological memory, specificity, diversity, discrimination between self and non self, primary and secondary lymphoid organs, cell mediated and humoral immune responses, T and B lymphocytes, autoimmune reactions.
2. Antigen and antibody: antigen, antigenic determinant, immunopotency, structure of antibody, constant and variable regions, Fab, F(ab2) and Fc fragments, different classes of antibodies and their functions, fine structures of antibodies, X ray diffraction studies, isotypes, allotypes and idiotypes,
3. Measurement of antigenantibody interaction, diffusion, immunodiffusion, immunoelectro- phoresis, radioimmunoassay, immunoflorescence, ELISA, western blotting
4. Clonal selection theory of antibody production, monoclonal and polyclonal antibodies
5. Complement system: classical and alternate pathway
6. T lymphocytes and cell mediated immunity, T cell sub populations, immune response genes, MHC gene complex, polymorphism, graft rejection, graft versus host response
7. Hypersensitivity, immunodeficiency diseases
8. Vaccines, interferon, AIDS
9. Blood antigens: blood group substances and Rh factor

Reference books

1. Molecular biology of the cell –Garland publishing Inc.,NY,London
2. Immunology 3rd ed Janis Kubay
3. Essentials of immunology (5th ed) Roit, Blackwell scientific publishing, London
4. Cellular and Molecular Immunology, 3rd ed, Abbas

CD-377 Practicals : 4 credits

1. Isolation of natural products: Tea, Coffee, Clove oil, Cinnamon oil, Eucalyptus oil
2. Representative Synthesis of drug molecules:
    - i) β-Binaphthol
    - ii) Ethyl(+)-(S)-3-hydroxybutyrate using Baker's yeast
    - iii) 3-Methyl 2-butenoic acid methyl ester
    - iv) 2- Methyl 3-buten-1-ol using LAH
    - v) 1,2,3,4-tetrahydrocabazole be Fischer Indole synthesis
    - vi) N-Benzoyl-α-phenylglycine
    - vii) Methyl 2,3,6 tri-o-benzoyl α-D-galactopyranoside
    - viii) Paracetomol, ibuprofen, methyl salicylate, Dicyclofenac
    - ix) Sulfadrugs
2. Instrumental Analysis of Drug molcules
    - i) Gas Chromatography, Infra-Red Spectroscopy, Nuclear Magnetic Resonance Spectroscopy, Mass Spectrometry and High Performance Liquid Chromatography
    - ii) Biochemistry practicals
    - iii) Microbiology practicals
    - iv) Pharmacology practicals

Semester IV 3 Courses = 16 credits

CD – 450: Chemistry of Heterocycles and Biologically active compounds (4Credits)

Transition metal complexes in organic synthesis (12)

Heterocyclic chemistry, (10)

Furan, thiophene, pyrrole, indole, pyridine, quinoline, isoquinoline,

imidazole, oxazole, thiazole,

Purines, pyrimidines

Umpolung in organic synthesis (4)

Designing Organic Synthesis (4)

Protecting groups for hydroxy,amino,carboxyl and aldehyde functions as illustrated in synthesis of polypeptide and polynucleotides (4)

Supra molecular Chemistry (2)

Combinatorial Chemistry (2)

Structure determination and synthesis of natural products like taxol, epothiolones and (24)

Metallo proteins and Medicines (4)

References:

Chemobiodynamics and drug design, F. W. Schueler

Bacterial resistance and sesceptilabilty to chemotherapeutic agents, L. E. Bryan

Priniples of medicinal chemistry, W. O. Foyetllimke and D, A, Williams

CD – 451: Organic Chemistry and Drug Design: 6 credits

Membranes and Receptors: Drug transport mechanism and absorption processes, (15)
Pharmacodynamic and Pharmacokinetic aspects, Prodrugs and Bioactivation,
Receptor theories and Receptor models, drug receptor interactions

Drug design, physiochemical principles and basis of drug design, quantitative description (15)
Physicochemical approach of drug molecules. Different methods of drug design,
Free Wilson method and its application to extrathermodynamic approach.

Biomimetic Synthesis (4)

Commercial synthesis and mode of action of vitamins, hormones and antibiotics (12)

Patents and drug laws

References:

Modern synthetic reactions, H. O. House (1972)

Designing organic synthesis, S. Warren (1978)

CD- 452: **Design, development and mechanism of action of drugs: 6 credits**

Antimicrobial, anticancer, antidiabetic, antiinflammatory and antitubercular drugs and (18)
their mechanism of action.

Cardiovascular drugs: Cardiotonic, Antihypertensive, Antirhythmic and Lipotropic drugs (14)

Metals in Drug design: Historical development and advantages (6)

Immunopharmacology and drug development (6)

Toxicology: Principles and methods of determination, short term and long term toxicity (12)

Biological evaluation of new drugs, immuno assay, enzyme assay, Microbial assay, Clinical trials, bioavailability (12)

Computer aided drug designing QSAR, Molecular modeling (4)

References:

1 Medicinal Chemistry for the 21st Century. Ed. C. G. Wermuth, Blackwell, Oxford, 1992, ISBN 0632034084.

2 Drug Metabolism: Databases and High Throughput Testing During Drug Design and Development. Ed. P. W. Erhardt, Blackwell, Oxford, 1999. ISBN 0632054329.

3 Pharmaceutical Salts: Properties, Selection, and Use–A Handbook, C.G. Wermuth and P.H. Stahl, Wiley, 2002 ISBN 3-906390-26-8

3. Principles of Drug Action- Goldstein