SADAKATHULLAH APPA COLLEGE
(AUTONOMOUS)

(Reaccredited by NAAC with 'A' GRADE and ISO 9001: 2008 certified)

Rahmath Nagar, Tirunelveli – 627 011

M.Sc. (M.M.D.D.)

UNITIZED SYLLABUS (CBCS)

FOR

(2011 - 2014)

(Applicable for students admitted in June 2011 and onwards)

(Updated as per the resolutions passed in the Academic Council Meeting held on 14-03-2013)

Department of MMDD (2011 – 2014)

M.Sc. Molecular Modeling and Drug Design (MMDD)

Course structure (CBCS)							
	Course	**H/W**	**C**		**Course**	**H/W**	**C**
I Semester	Core 1	5	5	**II Semester**	Core 4	5	5
	Core 2	5	5		Core 5	5	5
	Core 3	5	5		Core 6	5	5
	Elective – 1 (A/B)	5	4		Elective – 2 (A/B)	5	4
	Core Practical – I*	5	-		Core Practical – I*	5	4
	Elective Practical I	5	-		Elective Practical I	5	3
Total		**30**	**19**		**Total**	**30**	**26**
	Course	**H/W**	**C**		**Course**	**H/W**	**C**
III Semester	Core 7	5	5	**IV Semester**	Core 10	5	5
	Core 8	5	5		Core 11	5	5
	Core 9	5	5		Project	5	5
	Elective – 3 (A/B)	5	4		Elective – 4 (A/B)	5	4
	Core Practical – II*	5	-		Core Practical – II*	5	4
	Elective Practical 2	5	-		Elective Practical 2	5	3
Total		**30**	**19**	**Total**		**30**	**26**
* → Practical Exam – End of Even Semester							

Department of Molecular Modeling and Drug Design								
CBCS Syllabus – M.Sc., M.M.D.D (2011 – 2014)								
Sem	**P**	**Title of the Paper**	**Sub. Code**	**H / W**	**C**	**Marks**		
						I	**E**	**T**
I	C1	Organic synthesis	11PCMD11	5	5	25	75	100
	C2	Introduction to Molecular modeling	11PCMD12	5	5	25	75	100
	C3	Numerical Methods & Computer programming	11PCMD13	5	5	25	75	100
	E1A	Structural biochemistry **OR**	11PEMD1A	5	4	25	75	100
	E1B	Metabolic concept of Energetics	11PEMD1B					
	CP1	Drug synthesis, Natural product extraction and evaluation of activities of drugs	-	5	-	Exam – II Sem		
	EP1	Linux, Perl Program and Quantum Mechanical Calculation	-	5	-	Exam – II Sem		
II	C4	Drug synthesis	11PCMD21	5	5	25	75	100
	C5	Computational chemistry	11PCMD22	5	5	25	75	100
	C6	Bioinformatics and Cheminformatics	11PCMD23	5	5	25	75	100
	E2A	Molecular biology **OR**	11PEMD2A	5	4	25	75	100
	E2B	Enzyme technology	11PEMD2B					
	CP1	Drug synthesis, natural product extraction and evaluation of activities of drugs	11PCMDP1	5	4	40	60	100
	EP1	Linux, Perl Program and Quantum Mechanical Calculation	11PEMDP1	5	3	40	60	100
III	C7	Drug design and Development	11PCMD31	5	5	25	75	100
	C8	Molecular Modeling	11PCMD32	5	5	25	75	100
	C9	Genomics and Proteomics	11PCMD33	5	5	25	75	100
	E3A	Chromatography and Spectroscopy **OR**	11PEMD3A	5	4	25	75	100
	E3B	Structural Genomics	11PEMD3B					
	CP2	Rational, Pharmacophore and Ligand Based Drug Design	-	5	-	Exam – IV Sem		
	EP2	Chromatography and Bioinformatics	-	5	-	Exam – IV Sem		

Department of Molecular Modeling and Drug Design								
CBCS Syllabus – M.Sc., M.M.D.D (2011 – 2014)								
Sem	**P**	**Title of the Paper**	**Sub. Code**	**H / W**	**C**	**Marks**		
						I	**E**	**T**
IV	C10	Advanced Topic in Drug Design	11PCMD41	5	5	25	75	100
	C11	Advanced Topic in Molecular Modeling	11PCMD42	5	5	25	75	100
	C12	Project work	11PCMD43	5	5	0	100	100
	E4A	Advanced Computational Chemistry & Clinical Studies **OR**	11PEMD4A	5	4	25	75	100
	E4B	Medical Instrumentation and Clinical Chemistry	11PEMD4B					
	CP2	Rational, Pharmacophore and Ligand Based Drug Design	11PCMDP2	5	4	40	60	100
	EP2	Chromatography and Bioinformatics	11PEMDP2	5	3	40	60	100
			Total	**120**	**90**	**535**	**1465**	**2000**

I Semester / Paper - 1			
C 1	**Organic Synthesis**		**11PCMD11**
Hrs / Week : 5	**Hrs / Sem. : 75**	**Hrs / Unit : 15**	**Credit : 5**

UNIT –I: Reaction Intermediates, Ylides and Enamines:

Objective: *To understand the concept of reaction intermediates*

Reaction intermediates:

Carbocation: Structure and stability of carbo-cations, Classical and non-classical carbocations, Neighbouring group participation and rearrangements including Wagner-Meerwein, Pinacol-pinacolone, semi-pinacol rearrangement, Oxymercuration, halo-lactonisation**.**

Carbenes and Nitrenes:Structure, generation of carbenes, addition and insertion reactions of carbenes, rearrangement reactions of carbenes - Wolff rearrangement, generation and reactions of ylides, Structure, generation and reactions of nitrene, Curtius, Hoffmann, Schmidt, and Beckmann rearrangements.

Enamines : Generation and reactions, metalloenamines.

Unit –II:Reagents in organic synthesis

Objective: *To study the use of various reagents in organic synthesis*

Reagents in Organic Synthesis:

Use of following reagents in Organic Synthesis and functional group transformations: Complex metal hydrides, Gilman's reagent, Lithium diisopropylamide (LDA), dicyclohexylcarbodiimide, Umpolung of reactivity (dipole inversions), tri-*n*-butyltinhydride, Woodward and Prevost hydroxylation, Osmium tetraoxide, Selenium dioxide, Phase transfer catalysis, Crown ethers, Merrifield resin, Peterson's synthesis, Wilkinson's catalyst and Baker's Yeast.

Unit – III: Organic Synthesis – I

Objective: *To study the oxidation products of some compounds, reducing agents and the formation of carbon –carbon single bond.*

Oxidation of alcohols to carbonyl. Phenols to quinones, conversion of alkene to epoxides and diols, Oxidative bond cleavages, Oxidation of Sulfur, Selenium & Nitrogen. Reduction with metal hydrides, Alkoxyaluminates, alkoxy– and alkyl-Borohydrides, Stereoselectivity in hydride reduction. Catalytic hydrogenation and dissolving metal reductions.

Ketone enolates, O Vs C alkylation, Enamine and related reactions, Thio and Selenocarbanions, Aldol condensation, Allylic alkylations of alkenes. Coupling reactions - Organocopper, Organopalladium and Organonickel complexes.

Unit – IV: Organic Synthesis - II

Objective: *To study about reactions involved in the formation of carbon-carbon double bonds:* Elimination reactions, Pyrolytic syn eliminations, fragmentation reactions, Alkenes from hydrazones, 1,2-diols, alkynes, sulfones – titanium, chromium reagents - Alkene metathesis reactions and Wittig related reactions

Unit – V:Some Classics in Organic Synthesis

Objective: *To understand about the synthetic methodologies followed for some important compounds*

Corey synthesis of prostaglandins (PGF2 and PGE2) - Woodward synthesis of Strychnine, Reserpine, Cholesterol - W.S. Johnson synthesis of Progesterone - Harries synthesis of Biotin - K.C. Nicolau synthesis of Hirustene and 9 (12)-Capnellene, Taxol - Danishefsky synthesis of Indolizomycin.

REFERENCES:

1. Organic reaction Mechanisms, Fourth edition V.K. Ahluwalia, Rakesh Kumar Parashar, **2011**, Narosa Publishing House.

2. Modern methods of Organic Synthesis, Fourth Edition, W. Carruthers and Lain Coldham, **2004**,Cambridge University Press.

3. Organic Synthesis M.B. Smith, **1994**, McGraw International Edition.

4. The Logic of Organic Synthesis E.J. Corey and X.M. Cheng, **1989**, John Wiley and Sons.

5. Modern Synthetic Reactions Herbert O.House, Second Edition, **1972**, W.A. Benjamin Inc.

7. Comprehensive Organic Synthesis Vol. 5 ed. L A Paquette, **1991**, Oxford, Pergamon.

8. Classics in Total synthesis, by K.C. Nicolau and E.J. Sorensen, **1996**, VCH.

9. Cyclo Additions in Organic Synthesis, W. Carruthers, **1990**, Pergamon Press.

10. Pericyclic reactions by Ian Fleming, **1999**, Oxford Science Publications.

I Semester / Paper – 2			
C 2	**Introduction to Molecular Modeling**		**11PCMD12**
Hrs / Week : 5	**Hrs / Sem. : 75**	**Hrs / Unit : 15**	**Credit : 5**

Unit - I- Basic Concepts of Mechanics:

***Objective*:** To understand the various equations of motion and wave function.

Derivation of motion – Newton's equation, Lagrange's equation and Hamiltonion equation – Poison bracket - Classical wave theory- black body radiation – Planck's quantum hypothesis – Photoelectric effect – Compton effect – Wave – particle duality – de Broglie wave equation – Uncertainty principle – Expression, Experimental proof, outcomes, limitation and Application – Bohr's correspondence principle – Schrodinger wave equation – Interpretation and properties of the wave function – significance, orthogonality and nomenclature of the wave function.

Unit – II: Molecular mechanics

Objective: *To have an idea about the important concepts in molecular mechanics*

Force field – general features– Bond stretching, angle bending, Torsional terms, Improper torsions, out of Cross terms and non-bonded interactions – Electrostatic interactions, van der Waal's interactions – Many body effects in empirical potential – Effective pair potential – Hydrogen bonding in molecular mechanics – Force field parameterization –Differences in force field – Validation of force fields – MM2, MM3, MM4, AMBER, CHARMM, Merck Force Field, Consistent Force Field - Advantages and Limitations of force field methods.

Unit - III: Molecular coordinates, Symmetry and visualization tools

Objective: *To understand the basic concept of molecular coordinates, group theory and visualization tools of molecules.*

Coordinate systems – Crystal coordinates – Cartesian coordinates – Internal coordinates – bond length, bond angle and torsional angle –Line notations – SMILES construction – Wiswesser Line notation – Sybyl Line notation – Group theory – Symmetry elements – symmetry operations – Postulates of Group-Point groups – C_p, C_{2v}, C_{3v}, C_{2h}, D_2, D_6, D_{2d}, D_{2h} – Determination of Point groups – Representation of molecular point groups – reducible representation and irreducible representation– Great orthoganality theorem (GOT) – Use of GOT to construct character tables – character tables for point groups – C_{2v}, C_{3v} – Visualizations – Ball and Stick model – CPK model – 3D structure from X-ray crystallography data.

Unit - IV: Statistical Mechanics

Objective*: To have an idea about the statistical mechanics and thermodynamic properties of gaseous molecules:*

Degrees of freedom – translational, rotational and vibrational degrees of freedom – Phase space - Unit cells – Microstate – Macrostate – systems (open, closed, isolated) – Assembly – Ensembles - types of ensembles - ensemble average – Statistical equilibrium.

Thermodynamic probability – Stirling's theorem- Molecular Basis of residual entropy – Boltzmann distribution law- Bose-Einstein statistics – Fermi-Dirac statistics – comparison – Partition function – Evaluation of Translational, Rotational, Vibrational and Electronic partition function –Relation between partition function and Enthalpy, C_v, C_p, Entropy, Helmholtz free energy, Pressure, Gibb's free energy, enthalpy and chemical potential – Thermodynamic properties of an ideal monoatomic and diatomic gas.

Unit – V: Quantum Chemistry I

Objective: *To have an understanding about the basics of quantum chemistry.*

Operators – Vector- Laplacian – Hermitian – Unity – Projection parity - Ladder operator and density operator – Postulates of Quantum mechanics – Applications of quantum mechanics to the following 1D, 3D box – degeneracy, tunneling, one dimensional Simple Harmonic Oscillator, Rigid rotor and Hydrogen atom – Radial distribution function – Angular part of the wave function – Electron spin – Quantum numbers.

REFERENCES:

1. Quantum Chemistry, Donald A. Mcquire, **2011**, Viva Books.
2. Quantum Chemistry, A.B. Samigrahi, **2010**, Books and Allied PVT Ltd.
3. Introductory Quantum Chemistry, A.K. Chandra, Edition IV, **2001**, Tata McGraw Hill.
4. Quantum Chemistry – IRA N. Levin, Edition VI, **2009**, PHI Learning PVT Ltd., New Delhi.
5. Molecular Quantum Mechanics, Atkins P W and R S Friedman, Edition III, **1996**, Oxford University Press.
6. *Ab initio* Molecular Orbital Theory, Hehre W J, L Random, P V R Schleyer and J A Pople, **1986**, John Wiley & Sons, New York.
7. Applications of Electronic Structure Theory, Schaeffer H F, Edition III, **1977**, Plenum Press, New York.
8. Methods of Electronic Structure Theory, Schaeffer H F , Edition III, **1977**, Plenum Press, New York.
9. Modern Quantum Chemistry. Introduction to Advanced Electronic Structure Theory, Szabo A and N S Ostuld, **1982**, Tata McGraw Hill, New York.
10. Molecular Modeling, Principles and Applications, Second Edition, Andrew R Leech, **2001**, Prentice Hall, NY.
11. Guide Book on molecular modeling in Drug Design, N.Claude Cohen, I Edition, **1996**, Academic Press.
12. Chemometric methods in Molecular design, Water beamed H Van De Weinheim, **1995**, VCH publishers.
13. Principles of Physical Chemistry, Puri, Sharma and Pathania, **2008** Vishal Publications.

I Semester / Paper - 3			
C 3	Numerical Methods & Computer programming		11PCMD13
Hrs / Week : 5	Hrs / Sem. : 75	Hrs / Unit : 15	Credit : 5

Unit – I: Mathematical Concepts:

Objectives: To study about the fundamental of mathematical concepts related to molecular modeling.

Mathematical concepts – Series expansion - Taylor's – Vectors – Cross product, dot product – Matrices – properties of determinants – Eigen Vectors – Eigen Value – Jacobis' method - Complex numbers – Differentiation-product rule, quotient rule – Integration-Chain rule – Differential equation – Solution for linear second order equations – Polar coordinates (elementary ideas only) – Lagrange Multiples – Multiple Integral – Fourier Series – Fourier Transform and Fast Fourier Progress.

Unit – II: Numerical Methods-I

Objectives: *To study the various equations involved in numerical methods applied for mechanics*

Algebraic and Transcendental equations – Bisection method - Regular Falsi Method and Newton-Raphson method. Simultaneous equations - Gauss elimination method, Gauss Jordan elimination method, Gauss Jacobi iteration method and Gauss - Siedel iteration method – Interpolation – Newtons' forward interpolation, Newtons' backwards interpolation, Central difference interpolation – Gauss forward, Gauss backward and Sterling's method – Lagrange's interpolation formulae – Hermitte's interpolation formulae.

Unit – III: Algorithms and Graphs:

Objectives:*To have a basic idea about the algorithms and graphs*

Algorithm – Definition – Pseudo code - Deterministic and non-deterministic Algorithms – Heuristic Algorithms –Differences between Algorithms and computer programming – Analysis of algorithms – iterative algorithm – recursive algorithm – Tower of Hanoi problem – Exhaustive search – Branch and bond algorithm – travelling salesman problem – divide and conquer algorithim – merge and quick sort - greedy algorithm.

Graph – different types of graphs – Kongsherg bridge problem, Euclerian cycle problem – shortest path problem – DiKjistra's algorithm – Minimum cost spinning tree - Prim's algorithm and Kriskal's algorithm.

Shortgun sequencing method – Shortest superstring problem – sequencing by hybrisiation - Hamiltonian and Euclidian path problem.

Unit - IV: Perl programming

Objective: *To have some basic idea about Perl Programming*

Data Structure: Scalar Variables, Scalar Operations and Functions, Array, Variables, Literal Representation of Array, Array Operations and Functions, Scalar and List Context, Hash Variables, Literal Representation of a Hash, Hash Functions, Using Hashes for the Genetic Code, Gene Expression Data Using Hashes.

Modular Programming: Basics of Subroutines, Modules and Libraries of Subroutines, Concept about File handle, Opening and Closing a File handle, Opening and Closing a Directory Handle, Reading a Directory Handle, File and Directory Manipulation.

Unit V:BioPerl programming

Objective: *To study the concepts, principles, features of BioPerl Program*

BioPerl:

Introduction to Bioperl, Installing procedures, Architectures, General BioPerl Classes, Sequences (Bio::Seq Class, Sequence Manipulation), Features and Location Classes (Extracting CDS), Alignments (AlignIO), Analysis (Blast, Genscan), Databases (Database Classes, Accessing a local database), Implementing REBASE.

REFERENCES

1. Numerical Methods, S. Arumugam, A. Thangapandi Isaac, A. Somasundaram, **2007**, Scitech Publication s (India) Pvt. Ltd.
2. Numerical Analysis and Computational Procedures, S.A. Mollah, Edition V, **2012**, Allied (P) Ltd, Kolkata.
3. Applied Numerical Analysis, Patrick O. Wheatley, Edition VII, **2012**, Pearson Edition (India) for Dorling Kinderesly (P) Ltd, South Asia.
4. Schaum's Outlines Numerical Analysis, Francis Scheid, Edition II, **2009**, Tata McGraw–Hill (P) Ltd, New Delhi,
5. Applied Numerical Analysis using MATLAB, Laurene V. Fauseff, Edition VII, **2009**, Pearson Edition (India) for Dorling Kinderesly (P) Ltd, South Asia.
6. Introduction to Numerical Analysis, S.A. Mollah, Edition III, **2012**, Books and Allied (P) Ltd, Kolkata,
7. Numerical methods, Babu Ram, Edition VII, **2012**, Pearson Edition (India) for Dorling Kinderesly (P) Ltd, South Asia,
8. Programming Perl, Larry Wall, Tom Christiansen and Jon Orwant Third Edition, **2000**, O'Reilly.
9. Bioinformatics by A. John De Britto, **2012**, John Wiley and Sons.
10. Perl Programming for Bioinformatics by Harshawardan P Bal, **2006**, Tata McGraw Hill

I Semester / Elective Paper – 1			
E 1 A	**Structural Biochemistry**		**11PEMD1A**
Hrs / Week : 5	**Hrs / Sem : 75**	**Hrs / Unit : 15**	**Credit : 4**

UNIT –I: CARBOHYDRATE & LIPIDS

Objective: *To study about the structure, significance and functions of carbohydrates, Lipids and their derivatives*

Carbohydrate – classification – Structure of glucose, fructose, galactose maltose, lactose, sucrose – Deoxy sugars – Deoxy ribose, D ribose, starch, cellulose, glycogen, inuline, pectin, chitin – Glycosides – physiological significance – amino sugars –importance — Carbohydrate metabolism – Citric acid cycle – Embden-Meyerhof pathway.

Classification of lipids – Structure and Function of phospholipids – complex lipids – Sphingolipids – sphingomycin, cerebroside, gangolioside and Cholesterol.

UNIT –II: **AMINO ACIDS AND PROTEINS**

Objective : *To study the important ideas about the structure, functions of amino acids and proteins*

Structure and Classification – abbreviated names (1 letter and 3 letter) – Physical properties of amino acids – chemical properties – codons – Structure and importance of glutathione, Carnosine, anserine, vasopressin – gramicidine, bacitracine and actinomycin D - Peptide synthesis – Acid chloride method – DCC method – Determination of primary structure of peptide – Identification of N-terminal amino acid –Barger's method – DNP method – identification of C-terminal amino acid – Hierarchial representation of protein Primary, Secondary, tertiary and quaternary structures – structural classification of protein – fibrous - globular and membrane protein – amino acid metabolism – urea cycle.

UNIT –III:PURINE, PYRIMIDINE AND NUCLEIC ACIDS

Objective : *To study about the structure, functions and types of RNA*

Structure of Purines, Pyrimidines – Nucleoside, ribonucleoside, deoxyribonucleosides, nucleotides, ribonucleotides, deoxyribonucleotides – Structure and functions of DNA - Watson and Crick model – Types of DNA (α-DNA, β-DNA, Z-DNA) – RNA structure of different types: m-RNA, t-RNA and r-RNA – structure and function of DNase, RNase – polynucleotides, cAMP, cGMP nucleoprotein – Ramachandran plot.

UNIT –IV: ENZYMES

Objective : *To understand the functions, action and applications of enzymes*

Enzymes – Classification–factors affecting enzyme reaction – Michaelis – Menten equation and its applications – Enzymes specificity – Inhibition of enzyme action– competitive inhibition – non–competitive inhibition – uncompetitive inhibition – structure and mechanism of irreversible coenzyme (PLP, FAD, NAD^+, TPP) – immobilization of enzymes – industrial and medical application of enzymes– enzyme patterns in diseases.

UNIT –V: BIOINORGANIC CHEMISTRY

Objective: *To understand the role of inorganic chemistry in enzymatic reactions*

Metalloproteins – structure and function of Hemaglobin, Myoglobin, – Cytochrome – metal storage protein - ferritin,transferins, ceruloplasmin - Iron storage – transport – biomineralisation and siderphores – Structure and function of superoxide dismutase – cytochrome oxidase – coenzymes – molybdenum enzyme – Xanthine oxidase - zinc enzymes – carbonic anhydrase, carboxy peptidase and vitamin B12 coenzymes.

REFERENCES

1. Biochemistry, Lehinger J, **1993**, John Wiley and Sons
2. Biochemistry, D.Voet and J.G.Voet. 2 Ed, **1995**, John Wiley & Sons. Inc.
3. Fundamentals of Biochemistry, Jain J.L, **2000**, Chand & Co. New Delhi.
4. Biochemistry, Davison, V.L. & Sitlmon, D.L., 4thed, **1999**, Lippinocoth, William & Willeing.
5. Biochemistry, U.Satyanarayana & U.Chakrapani, **1999**, Books & Allied Pvt. Ltd
6. BioChemistry, Lubert Stryer, Fifth Edition, **2005**, W. H. Freeman and company, New York.
7. Concepts of Biochemistry by A.C. Deb, **1990**, New Central Book Agency, Kolkata
8. Biotechnology by U. Satyanarayana, **2008**, Books and Allied Pvt Ltd.

I Semester / Elective Paper 2			
E 1 B	**Metabolic Concepts of Bioenergetics**		**11PEMD1B**
Hrs / Week : 5	**Hrs / Sem : 75**	**Hrs / Unit : 15**	**Credit : 4**

UNIT – I Bioinformatics introduction
Objective : *An Introductory study about Bioinformatics*

Bioinformatics overview, definition and History, Information Networks – Internet in Bioinformatics – Bioinformatics and tools on the Internet. Genome database – Annotation of Genome – Structure Annotation- Gene Medication approaches – Open reading frame prediction – Hideen Markov model, prediction of promoter sequences – functional annotation prediction of gene function, sequence similarity – gene family and metabolic pathway.

UNIT – II Protein Structure and Function
Objective : *To study about the Protein, its structure and functions*

Relationship between protein structure and function: Prions, structure prediction and human proteomics. Use of Computer simulation and knowledge based methods in the design process. Denovo design making use of databases of sequences and structure.

UNIT –III Genomes
Objective : *A basic study about human genome*

Human genome and genomic analysis – Sequences repeats, transposatle elements, gene structure, pseudogens – gene analysis – gene order – chromesome rearrangement – compositional analysis – Clustering of genes and composite genes.

UNIT –IV Proteomics
Objective : *To study about the proteome*

Introduction to proteome – proteome and technology –Information and the proteome – primary attributes for protein identification, protein species of origin protein N and C-terminal sequences tags – cross species protein identification.

UNIT –V Database for proteins

Objective : *A detailed study about database related to proteins and genomes*

Proteome databases – Protein sequences databases, SWISS-PROT, Tr EMBL specialized protein sequence databases PROSITE, BLOCKS, 2-D PAGE databases PDB, genomic databases, OMIM Metabolic databases, some specific metabolic databases – Application of proteomics to medicine proteomics, toxicology and pharmaceuticals.

REFERENCES

1. Genomes, T. A Brown, **2002**, BIOS Scientific Publishers, Ltd., Oxford, U.K.
2. Bioinformatics, Sequences and Genome analysis, David W. Mount, Cold Spring, **2001**, Harbour Laboratory Press, New York.
3. Discovering Genomics, Proteomics and Bioinformatics, Campbell, A. Molcolm and Heyer, Laurie J. Benjamin Cummings, **2008**, Pearson
4. Proteomics, S.R. Pennington and M.J. Dunn, **2002**, Viva Books Pvt. Ltd., New Delhi.
5. Structure and Mechanism in Protein Science, **1999**, Fersht, A.W.H. Freeman.
6. Website – www. Amazon.com

Core Practical paper -1		
CP1	**Drug synthesis, Natural product extraction and evaluation of activities of drugs**	**11PCMDP1**
Hrs / Week : 5	**Hrs / Sem : 75**	**Credit : 4**

I. Drug Synthesis

1. Asprin
2. Phenacetin
3. Acetylcysteine
4. Paracetamol
5. Benzoyl Glycine
6. Flavone
7. Benzyl Benzoate
8. Dichloramine-T
9. Salicyladehyde
10. Coumarin -3-carboxylic acid
11. *para*-Bromoacetanilide
12. Fluorescein.
13. Anthrone
14. *p*-Hydroxypropiophenone
15. Flopropione
16. Resacetophenone
17. Coumarin
18. Metamfepramone
19. Gramine
20. Acetaminophen

II. Synthesis of the following heterocyclic compounds

a) Benzimidazole.
b) Benzotriazole.
c) 2,3-diphenylquinoxaline.
d) Oxadiazole.
e) Thiadiazole.

III. Extraction of natural products

a). Eugenol from cinnamon leaf oil or cloves.

b). Piperine from black pepper.

c). Curcumin from turmeric.

d). Pectins from orange peels.

e). Carotene from carrots.

IV. Screening for following activities

1. Anti-inflammatory
2. Anti-bacterial

REFERENCES:

1. Lab Experiments in Organic Chemistry by Arun Sethi, **2003**, New Age international publishers
2. Systematic identification of organic compounds by R.L. Shriner R C Fuson D Y Curtin
3. Identification of organic compound by N D Cheronis and J B Entrikin
4. Organicum – Practicul handbook of Organic chemistry by B J Hassard
5. Organic Experiments by Fisser Williamson
6. A handbook of organic analysis by H T Clarke
7. Introduction to organic chemistry by S Heathcock
8. Experimental organic chemistry by H Dupont Durst and George W Gokal
9. Operational organic chemistry by John W Lehman
10. Natural Product Chemistry by Raphael Ikan
11. Natural product Chemistry Edited by Atta Ur Rahman
12. Phytochemistry Vol I – The process and product of photosynthesis edited by Lawrence P Miller
13. Organic Synthesis Collective volume I, II, III, IV, V and VI
14. Organic Chemistry by L G Wade
15. Practical heterocyclic chemistry by A O Fitton, and R K Smalley
16. Reactions of organic chemistry by Hickinbotton
17. Practical organic chemistry by F G Mann and B.C Saunders
18. Textbook of Practical Organic Chemistry by A I Vogel
19. Unitized experiment in organic chemistry by R Q Brewster, C A Vanderef and W E Mcewen
20. Systematic Organic Chemistry by W M Cumming, I U Hopper and T S Wheeler
21. Practical chemistry an integrated course by J W Buttle and D J Daniels

Elective Practical Paper - 1		
EP1	**Linux, Bio-Java, Perl Program, and Quantum mechanical calculations**	**11PEMDP1**
Hrs / Week : 5	**Hrs / Sem : 75**	**Credit : 3**

I.PROGRAMMING USING LINUX

1. Simple Linux Commands:

alias, at, banner, cat, cd, chmod, chown, chroot, cp, dd, grep, gzip, gunzip, kill, ln, ls, mail, man, mcopy, mdel, mdir, more, ps, pwd, rm, rmdir, shutdown, sort, su, tar, unzip, vi, wc, who, whoami, zip.

2. Communication Commands:

write, wall, talk, mesg, motd.

3. Administration Commands:

adduser, cpio, fdformat, halt, hostname, ifconfig, login, logout, lpc, lpd, lprm, mount, mv, passwd, ping, quota, route, umount.

II. Programming using Perl

1. Translating DNA in to proteins.
2. Read a FASTA file and extract the sequence data.
3. Read a DNA FASTA file and translate to protein and format the output.
4. Translate DNA sequence in all six reading frames.
5. Subroutine to parse a REBASE data file.
6. Make restriction for user queries.
7. Extract Annotation and sequence from GenBank record.
8. Parsing GenBank annotations using arrays.
9. Parsing GenBank annotations using arrays, take 2.
10. GenBank library Subroutine.
11. List contents of a folder and its sub folder.
12. Extract sequence chains from PDB file.
13. Extract atomic coordinate from PDB file.
14. Parse Alignments from BLAST output file
15. Write a format that creates a FASTA style output

III. Quantum Mechanical Calculation

1. Draw the structure of simple molecules (CH_4 / Ethane / Water/ toluene/ benzene/ HCHO) in:

- GaussView Chem3D

Observe the amount of effort required in each case.

2. Use GaussView version of the above molecules as .mol file and read it with Gaussian. Run geometry optimizations using

(a) Hartree-Fock (HF / STO-3G)

(b) HF / 3-21G

(c) HF / 6-31G*

Observe the time taken for running each molecule. Save the output file.

3. Read the .mol file with GaussView and set up a Gaussian job for the above molecules and run geometry optimization using DFT with B3LYP / 6-31G* and cc-pVDZ (reasonable accuracy) basis set. Save the output file.

4. Draw ethylbenzene molecule in GaussView and optimize the geometry using semi empirical method (PM3, AM1).

5. Load the result back into GaussView and set up three Gaussian job for geometry optimization:

- using HF/STO-3G method (minimal accuracy)
- using HF/cc-pVDZ method (reasonable accuracy)
- using HF/cc-pVQZ method (high accuracy)

Compare the time taken and analyze the results [bond length, bond angle and dihedral angle].

6 Optimize the geometry of methane at MP2/cc-pVDZ level and compute the energy at the minimum using MP2, MP4, CISD(T), CCSD and CCSD(T) methods. Use scf=dsymm to enforce the use of tetrahedral symmetry, otherwise the calculation may take a long time.

7. Optimize the geometry of cyclobutaneusingB3LYP / 6-31G* or HF / 6-31G* and run a vibrational analysis job (use freq keyword). Visualize the resulting normal mode vibrations in GaussView.

8. Run the geometry optimization for benzene cation radical with an option to keep the checkpoint file (%Chk=filename.chk). Transform the checkpoint file into platform-independent ASCII (fchk filename.chk), and open the resulting .fchk file in GaussView. Generate the total electron density and spin density plots.

9. Set up a potential energy scan with respect to the C=C bond stretch in ethylene using MP2/cc-pVDZ method with and without counterpoise BSSE correction. Observe the difference in the bond breaking profile.

10. Use optimized methane geometry to perform a thermodynamic analysis (see the FREQ keyword documentation on Gaussian website).

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1. http://www.Indiana.edu/-cheminfo/ca_mvts.html
2. http://www.umass.edu/microbio/rasmol/history.htm
3. http://www.openrasmol.org/
4. http://www.mc.manchester.ac.uk./about/events/molecularvisualizationday
5. http://www.cscs.ch/~mvalle/teaching/manchester.html
6. www.gaussian.com

II Semester / Paper 4			
C 4	Drug Synthesis		11PCMD21
Hrs / Week : 5	Hrs / Sem : 75	Hrs / Unit : 15	Credit : 5

UNIT – I: CLASSIFICATION, NOMENCLATURE AND SYNTHESIS OF DRUGS

Objective: *To get an introductory idea about pharmacology and drugs*

Drugs -definition, Requirements of an ideal drug -Sources – Historical evolution of drugs – Nomenclature of drugs – Chemical (IUPAC) – Heterocyclic – Non-stereo chemical – Chirality of drugs - Terminology & description of the terms –Pharmacology – Pharmacy – Molecular pharmacology – Medicinal chemistry – Pharmacokinetics – Pharmacodynamics – Metabolites & antimetabolites – Pharmacophore - Bacteria – Bacterial cell – Gram stain – Importance – Fungi – Viruses – Classification – Chemical structure –therapeutic actions -– Generic and trade name of drugs.

Unit – II: Antibiotics

Objective: *To study about different antibiotics and their activity*

Definition and Classification - Chemical reaction of penciline – pencilinetypes – structure and mode of action of penciline – V, methillium sodium, ampicillin, piperacillin sodium, cephalexin, ceptralerin, ceptradine, cefoxitin and cefixime – amino glycoside and antibiotics – streptomycin – neomycin - kanamycin – structure, mechanism, of action and structure activity relationship. – chloramphenil and tetrayclic structure, synthesis, mechanism of action – SAR.

Unit –III: Cardiovascular drugs & antimycobacterial drugs

Objective: *To know about the cardiovascular and antimycobacterial drugs and its structure*

Cardiovascular drugs – classification – cardiac glycosides – structure and mechanism of action of digitoxin and digoxin - Antihypertensive & Hypotensive drugs – Structure & mechanism of cloridine, hydralazine, Mrthyldopa, diazoxide – Salient features of antiarrhythmic agents - Structure & mechanism of quinidine, disopyranide, lorcainide and amiodarone – Vasopressor drugs – structure, synthesis and mode of action of prenylamine – Antimycobacterial drugs – Classification – First line drugs- pyrazinamide – Second line drugs – Synthesis and mechanism of action of oflaxacin, ciprofloxacin.

UNIT – IV STEROIDS

Objective: *To have an idea about the various steroids and their action*

Steroids – nomenclature – classification – steroids – sex hormones – synthesis and mechanism of action:androsterone, testosterone, oxandroloneestrone, estriol, estradiol, diethylstilbesterol, hexesterol, dienesterol, progesterone – adrenocortical steroids –

classification – biological activity of profiles – structure and uses of hydrocortisone, cortisone, methylprednisolone, prednisoloneand betamethasone.

Unit -V: Synthon approach and Combinatorial Synthesis

Objective: *To study about the synthesis, by a disconnection approach using retero analysis and to have a basic idea about combinational synthesis*

Synthon approach:

Definition of terms - disconnection, synthon, functional group Inter-conversion (FGI), Basic rules in Disconnection. Use of synthon approach in synthesis of the following compounds: Trimethoprim, Terfenadine, Ibuprofen, Propanolol, Fentanyl, Ciprofloxacin, Cimetidine, Piroxicam, Rosiglitazone, Diclofenac, Captopryl, Nifedipine, Losartan potassium.

Combinatorial Organic synthesis

Methods and Techniques of Combinatorial Synthesis - chemical Peptide and small molecule libraries, applications, methodology, assays and screening of combinatorial libraries. High Throughputs Screening (HTS) - Introduction

REFERENCES:

1. Organic Chemistry, I.L. Finar, Vol II, **1975**, ELBS.
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II Semester / Paper 5			
C 5	Computational Chemistry		11PCMD22
Hrs / Week : 5	Hrs / Sem : 75	Hrs / Unit : 15	Credit : 5

Unit – I: Quantum Chemistry –II

Objective: *To know the concept of wave function of many electron system and approximate methods.*

Wave function of many electron systems – Helium atom - Pauli's exclusion principle – Slater determinants – Angular Momentum - Commutators relations – step-up and step-down operators - angular momentum in many electron atom – Spin – orbit interaction – vector model of the atom – LS and JJ coupling - Term symbols – General time –independent perturbation theory – Applications to hydrogen and Helium atoms - Variation theorem – Application to hydrogen and helium atoms – Time dependent perturbation theory

Unit - II: Quantum Chemistry - III:

Objective: *To know the concept of Molecular orbital (MO), Valence bond (VB) and Huckel Molecular Orbital (HMO) theories.*

Born-Oppenheimer approximation –MO theory - LCAO approximation – MO method for H_2^+ and H_2 – VB treatment of H_2 molecule – Excited state of Hydrogen molecule – Comparison of MO and VB theories - Hybridization – solving wave functions for sp, sp^2, sp^3 hybrid orbitals,- Huckel molecular Orbital theory for the linear conjugated system - HMO theory of ethylene, butadiene and benzene –Calculation of bond order and charge density calculation.

Unit - III: Quantum Chemistry - IV:

Objective: *To know the concept of Hartree-Fock, Parsier-Parr-Pople, Semi-empirical and abinitio methods.*

Self-consistent- field approximation – Hartree's theory - Hartree-Fock SCF theory –Virial theorem –Koopmann theorem- Parsier-Par-Pople (PPP) approximation -Extended Huckel theory. Semi-empirical SCF theory – NDO – INDO - CNDO - MINDO - AM1 - PM3 methods – Basis sets – Slater type orbitals and Gaussian type orbitals – Classification of basis sets –STO-3G, 3- 21G, 3-21+G and 6-31G* - *ab initio* methods (preliminary ideas).

Unit - IV: Numerical methods - II

Objective: To know the concept of potential energy surface and various optimization techniques.

Potential energy surface – Global energy minimum – transition state – saddle point - Energy Minimization – Non- derivative minimization methods – simplex methods and sequential univariate method – Derivative minimization methods – First order minimization method – Steepest descent method, Conjugate gradient methods - Second derivative methods – Newton

– Raphson method – Quasi Newton method - Applications of energy Minimization – Normal mode of analysis – Study of intermolecular process.

Unit - V - Numerical differentiation and integration:

Objective: *To know the concept of various methods of numerical differentiation and integration.*

Numerical differentiation: Newton's forward difference formula- Newton's backward difference formulae-Stirlings method.

Numerical integration: Newton's Cotes quadrature formulae- Trapezoidal rule – Simpson's one-third rule – Simpson's three eight rule – Weddle's rule – Romberg's method - Numerical solutions of ordinary differential equations: Taylor's series method –Runge Kutta method.

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II Semester / Paper 6			
C 6	**Bioinformatics and Cheminformatics**		**11PCMD23**
Hrs / Week : 5	**Hrs / Sem : 75**	**Hrs / Unit : 15**	**Credit : 5**

UNIT –I: Introduction to bioinformatics and databases

Objective: *To know the basic idea about bioinformatics and databases*

Bioinformatics- applications- Databases- Characteristics and categories of databases – Navigating databases – Sequence databases – Nucleotide sequence databases- EMBL, DDBJ, GenBank- Secondary nucleotide sequence databases – UniGene, STACK, Ribosomal databases, HIV sequence database, REBASE- Protein sequence databases- UniProtKB, SWISSPROT, TremBL, PDB-

UNIT II– Structure databases and tools

Objective: *To have an idea about structure databases and data submission and analysis tools*

Structure database – PDB, MMDB, CATH, FSSB, DALI, SCOP- Enzyme Databases- MEROPS, BRENDA –Disease database- OMIM, Genecards- Literature databases- Pubmed.

Tools- Need- Data submission tools – Nucleotide sequence submission tools, BankIt for GenBank, Sequin for GenBank, webin for EMBL,Sakura for DDBJ, Protein submission tools- Spin for Swissprot, AutoDep and tbl2asn – Data analysis tools- Nucleotide sequence submission tools- Transeq, CpGreport, GCUA, BLAST- Blastn, BLASTx, ORF Finder, Vecscreen, Protein sequence tools- BLASTp, PSI-BLAST, tBLASTx, CDART.

Unit –III: Representation and manipulation of 3d molecular structures

Objective**:** *To understand the various representations of 3D Molecular structures in cheminformatics.*

Introduction - Experimental 3D Databases- 3D Pharmacophores - Implementation of 3D Database Searching-Theoretical 3D Databases - Structure-Generation Programs - Conformational Search and Analysis - Systematic Conformational Search - Random Conformational Search - Other Approaches to Conformational Search - Comparison and Evaluation of Conformational - Search Methods - The Generation of Distance Keys for Flexible Molecules - Methods to Derive 3D pharmacophores-Pharmacophore Mapping Using Constrained - Systematic Search –Pharmacophore mapping Using Clique Detection - The maximum likelihood method for pharmacophore mapping – Pharmacophore mapping using a Genetic Algorithm - Other approaches to pharmacophore mapping - Practical Aspects of Pharmacophore Mapping - Applications of 3D pharmacophore mapping - 3D Database Searching

Unit –IV: VIRTUAL SCREENING

Objective*: To know about virtual screening of molecules for drug molecules*

Introduction-"Drug-Likeness" and Compound Filters - Structure-Based Virtual Screening - Protein–Ligand Docking - Scoring Functions for Protein–Ligand Docking - Practical Aspects of Structure-Based Virtual Screening - The Prediction of ADMET Properties - Hydrogen Bonding Descriptors - Polar Surface Area - Descriptors Based on 3D Fields - Toxicity Prediction.

UNIT – V: Applications of Bioinformatics and Cheminformatics

Objective*: To have an idea about the applications of bio informatics and cheminformatics.*

Transcriptomics – probes – Northern hybridization – differential display – microarrays – types of microarray – designing a micro array – cDNA microarray experimental – micro array data variability – Normalization – image analysis

Metabolomics – reconstruction of metabolic pathway from complete geneome sequence – metabolic pathway databases.

Pharmacogenomics – Drugs – agonist – antagonist – inhibitor – drug receptor – types – Drug designing – structure based drug design – drug discovery and development process – pharmacokinetics – simple nucleotide polymorphism – benefits and limitations

Cheminformatics: Prediction of properties – Estimation of log $P_{o/w}$, log S & toxicity – Prediction of spectral properties – chemical shift and mass spectra - Prediction of chemical reactions

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II Semester / Elective Paper - 1			
E2 A	**Molecular Biology**		**11PEMD2A**
Hrs / Week : 5	**Hrs / Sem : 75**	**Hrs / Unit : 15**	**Credit : 4**

UNIT– I: Cell structure and transport

Objective: *To understand the structure of cell and the transport of ions within the cell*

General structure of prokaryotes and Eukaryotes – models for structure of plasma membrane – bilayer model – Micellar model – transport through the plasma membrane – passive and active transport – ion selective channels – structure and functions of nucleus, nucleolus, mitochondria, endoplasmic reticulum – golgi apparatus – lysosomes.

UNIT – II: **Ribosomes and Cell – Cell signaling**

Objective: *To know about the ribosomes and cell – cell signaling process*

Ribosomes – Eukaryotic, prokaryotic, mitochondrial and chloroplast – structure – quasi symmetrical model and lakes asymmetrical model – function of rRNA in the ribosomes.

Cell – Cell signaling: signal receptors – cell surface receptor types – structure and mechanism of action of G-protein couple receptor – intra cellular receptor – signal transduction pathways.

UNIT– III: **DNA**

Objective: *To know about DNA and enzymes*

DNA as the genetic material – direct and indirect evidence – one gene one enzyme concept – biochemical mutation in man – multiple allele – cistron concept – denaturation of DNA and melting curve – C value paradox – satellite DNA – origin and evolution of pseudo genes – overlapping genes – split genes – exon theory - topoisomerase – Type I and Type II – super coiling of DNA

UNIT – IV: Replication and transcription

Objective: *To have an idea about replication and transcription*

Replication – External proof – Enzymes in DNA replication – prokaryotic DNA polymerase – Eukaryotic DNA polymerase – unidirectional and bidirectional replication – models of replication

Transcription – RNA polymerase – Prokaryotic and Eukaryotic – transcription in prokaryotes and eukaryotes - post transcriptional modification in mRNA – mechanism – transplicing of mRNA

UNIT – V: Reverse transcription and translation

Objective: *To know about the reverse transcription and translation process*

ReverseTranscription – Structure and function of reverse transcriptionase

Translation – Translation – genetic code – wobble hypothesis – mechanism – protein biosynthesis – chaperones – protein targeting to mitochondria and nucleus.

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1. Molecular Cell Biology of the cell, Albert's, B., Johnson, A., Lewis, J., Raff, M., K and Walter, P. Fourth Edition, **2002**, Garland Science, Taylor and Francis Group, USA.
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II Semester / Elective Paper – 2			
E 2 B	**Enzyme Technology**		**11PEMD2B**
Hrs / Week : 5	**Hrs / Sem : 75**	**Hrs / Unit : 15**	**Credit : 4**

UNIT-1 : Enzyme

Objective : To understand classification, nomenclature and purification of enzyme

Enzyme Classification and nomenclature – isolation and purification properties of enzymes – enzyme specificity effect of pH, temperature, concentration of enzyme, concentration of substrate on enzyme activity and stability – units of enzyme activity and stability – co-enzymes and co-factors.

UNIT-2 : Kinetics and mechanism of enzyme catalyzed reaction

Objective : To understand the kinetics and mechanism of enzyme catalyzed reaction

Kinetics and mechanism of enzyme catalysed reaction – Steady state kinetics – Derivation of Michealis-Menton equation – significance of V_{max} and k_m–L–plot – Multistage enzyme kinetics – pre-steady state relaxation kinetics – King and Allman procedure – Negative and positive cooperativity (feed back inhibition) – enzyme inhibition – enzyme immobilization and its application.

UNIT-3 : Mechanism of enzymes and types

Objective : To understand the mechanism of enzyme reaction and other types of enzymes

Active sites – Mechanism of enzyme action – lysoyme, chymotrypsin, DNA polymerase RNAse, isoenzymes (lDH), alloteric enzyme, ribozyme & abzyme.

UNIT-4 : Multi Enzyme Complex

Objective : To have an idea about the multi enzyme complex advantage and biosensors

Multienzyme complexes – structure and function of pyruvate dehydrogenase and fatty acid synthase complex – Advantages of multienzyme complex – Commercial application of enzymes in food pharmaceutical and other industries – enzymes for diagnostic applications – Biosenors

UNIT-5 : Extremozymes

Objective : To have an idea about Extremozymes and industrial applications

Extremozymes – Extremophiles – Thermophiles – Halophiles – Psychrophiles – Industrial application – protein engineering (site – directed mutagenesis).

References

1. Biochemistry, Lehinger, J., **1993**, CBS. Publishers.
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III Semester - Core Paper – 7			
C7	**Drug Design and Development**		**11PCMD31**
Hrs / Week : 5	**Hrs / Sem : 75**	**Hrs / Unit : 15**	**Credit : 5**

Unit-I: Introduction and Objective of Drug Designing

Objective: To have a basic idea about Drug Designing and SAR

Economic aspects of drug designing – Procedures followed in drug designing – Lead based methods – Approaches to lead discovery – Drug discovery without a lead-*de novo* drug designing – Structure Activity Relationships: Quantitative analysis of structure activity relationships – Hansch Paradigm for pharmaceuticals – Apparent lack of structure activity relationships – True structure activity relationships.

Unit-II: Thermodynamic calculations of molecular descriptors

Objective: To study about the thermodynamic calculations of molecular descriptors

Electronic, Steric and Hydrophobic substituents constant – Structural and theoretical parameters – Bioisostreism – Wilson method and its significance – Acid base properties, ionization – partition coefficients (hydrophobicity) – Hammett constants – Taft's steric factor – resonance effect – inductive effect – Masca Model of pharmacochemistry - Multivariate Statistics – Probability of Type I and Type II Error, Multivariate test criteria – Multivariate bioassay –Experimental design, Multivariate variance analysis (MANOVA), Discriminant Analysis (Discra) and Classification (Clasca) - Multivariate Sp test – Profile analysis - Multivariate covariance analysis (MACOVA)

Unit-III: Electronic aspects of Drug Action

Objective: To understand the drug design on the basis of molecular orbital method

Molecular Orbital (MO) Calculations-HMO theory of phenyl acetate-Chemical reactivity-dynamic and static methods – Perturbation theories for drug action – Inouye's two-point receptor and Klopman and Hudson's Poyelectronic theory–Pullman's di-positive bond theory – Role of charge transfer processes in drug action – Conformational aspects of Drug-Receptor Interactions – Acetylcholine Receptor- Serotonin receptor – Adregenicreceptor- Cortisol receptor- Specific Applications to drug systems – Acetylcholinesterase inhibitors – Sulfonamides.

Unit-IV: **Drug-Receptor Interaction**

Objective: To have an understanding about Drug-Receptor interaction and peptidomimetics

Theories and forces involved in drug-receptor interaction – Stereo-chemical and conformational aspects of drug receptor interaction – Agonists and Antagonists – Designing of receptor antagonists – Receptor binding as a tool in designing biologically active steroids.

Peptidomimetics**:** Peptidomimetics – Rational design of Peptidomimetics, nonpeptide, ligands for peptide receptors – Applications of oligonucleotides in anti-viral and anti-tumoral chemotherapy – Antisense nucleotides designing.

Unit-V: **Prodrugs and Soft drugs**

Objective: To study about the drug action

Basic concepts – Mechanism of drug action – Common promoities – Reversal of prodrugs-chemical and enzymatic – Application of prodrug approach to alter taste and odour reduction of pain at injection site – reduction of gastrointestinal irritability – Alteration of drug solubility – increasing chemical stability – Prevention of presystematic metabolism – Prolongation of drug action – site specific drug delivery – Reduction in drug toxicity – Alteration of drug metabolism – soft drugs – design of soft drugs.

References

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III Semester- Core Paper–8			
C8	**Molecular Modeling**		**11PCMD32**
Hrs / Week : 5	**Hrs / Sem : 75**	**Hrs / Unit : 15**	**Credit : 5**

Unit I: Ensembles

Objective: To understand the concept of thermodynamics, partition function, virial theorem of various ensembles.

Micro canonical ensemble: Thermodynamics, Boltzmann's relation and the partition function, Classical virial theorem Conditions for thermal equilibrium, Free particle and ideal gas, Gibbs paradox, Harmonic oscillator and harmonic baths. Canonical ensemble: Thermodynamics, Phase distribution and partition function, Energy fluctuation, Examples - Free particle and the ideal gas, Harmonic oscillator and harmonic bath, Harmonic bend spring model. Isobaric ensemble: Thermodynamics, Phase space distribution and partition function, Pressure and work, virial theorem, Ideal gas in the isothermal-isobaric ensemble, Anisotropic cell fluctuations. Grand canonical ensemble: Thermodynamics, Phase space and the partition function, Ideal gas, Particle number fluctuation.

Unit – II: Molecular Dynamics – I

Objective: To understand the fundamental concept of molecular dynamics.

Basics of Laplace vision - Various types of potential – Lennard Jones type Potential, Truncated Lennard-Jones Potential, Kihara Potential , Exponential-6 potential, BFW Two body potential , *abintio* Potential, Ionic and polar potential- Periodic boundary conditions- minimum image convention – Energy conservation- Integrators: Verlet, Velocity-Verlet, Leap frog and Beeman's algorithms –Analysis of integrators- Lypunov instability- Time reversible and area- preserving integrators- Discontinuos potentials- Simple estimators- energies, temperature, velocity rescaling, pressure and heat capacity- Statistics of averages- Structured based averages- Methodology of Molecular dynamics – Initialization, equlibaration and production — Constrained dynamics - Shake and Rattle Algorithm.

Unit - III: Molecular dynamics- II

Objective: To understand the concept of molecular dynamics in the ensemble, thermostats and barostats.

Molecular dynamics in the Micro-canonical ensemble – Extended Hamiltonian- Canonical ensemble – Nose Hamiltonian, Nose-Hoover equations, Nose-Hover chains, Isoenthalpic – isobaric ensemble, Isothermal - isobaric ensemble- isotropic volume fluctuation, Anisotropic cell fluctuation, Roll algorithm.– Thermostats –Berendsen thermostat, Andersen thermostat, Nose thermostat, Nose-Hoover thermostat- Barostats – Symplectic Integrators – Multiple

Time step methods. Multi-canonical method - Wang Landu sampling – Transition martin estimators - Thermodynamic integration – Gibbs Duhem integration.

Unit- IV: Free – Energy calculations:

Objective: To understand the concept of the methods of determining free energy calculations.

Free energy -Basic approaches to free energy calculations, Free energy perturbation (FEP) theory – Pictorial representations – Simple applications-Charging a spherical particle dipolar states at an aqueous interface- Improving efficiency of FEP- Histogram reweighing- Free energies from Histograms, Ferrenberg-Swendsen reweighing method - Weighted histogram analysis method (WHAM) – Stratification- Importance sampling and stratification with WHAM - Flat histogram methods.

Unit – V: Computer Simulation methods:

Objective: To understand the basic concept of computer simulation and Monte-Carlo simulation methods.

Monte Carlo methods – Differences between Molecular Dynamics and Monte Carlo method – Practical aspects of Computer Simulations - Boundaries – Periodic and Non-Periodic Boundary Methods - Monitoring the equilibration – Truncating the potential and the minimum energy convention - Long range forces – Ewalds Summation Method - Reaction Field method – Cell multipole method for non-bonded interactions – Analysis of simulation – error estimation

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3. Computational Medicinal Chemistry in Drug Discovery, PatricBultinct, Hans De Winter, Wilfried Langenaeker, Jan P Tollenaere (Ed), CRC Press, **2009**, First Indian Edition
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III Semester- Core paper 9			
C9	Genomics and Proteomics		11PCMD33
Hrs / Week : 5	Hrs / Sem : 75	Hrs / Unit : 15	Credit : 5

UNIT-1: Data Analysis Algorithms

Objective: To know the basic idea about data analysis algorithm

Basic terminology used in sequence similarity, identity and homology, Definitions of homologues, orthologues, paralogues and xenologues. Sequence Comparison algorithms – Dot plots, Substitution matrices Algorithms, PAM matrix construction algorithm, BLOSUM Matrix Construction Algorithm-Sequence Alignment Algorithm-Penalties for insertions and deletions-Pair wise sequence alignment: Basic concepts of global sequence alignment-Needleman and Wunsch algorithm-Local sequence alignment- Smith and Waterman algorithms- Multiple alignment-FASTA-BLAST

UNIT-II: Multiple alignment and Phylogenetic analysis

Objective: To have an idea about multiple alignment and phylogenetic analysis

Multiple sequence alignments (MSA): The need for MSA, basic concepts of various approaches for MSA (e.g. progressive, hierarchical etc.). Algorithm of CLUSTALW and PileUp and their application for sequence analysis (including interpretation of results), concept of dendrogram and its interpretation, Use of HMM-based Algorithm for MSA (e.g. SAM method)

Phylogenetic trees and Phylogenetic Analysis-Phylip-Phyml-Gene prediction-Genscan-GrailEXP-Protein Structure and Prediction-Prosite, 3DPSSM.Modeling tools- Rasmol 2.6-Tools for 3D protein modeling- Deep View 3.7.

Unit – III: Gene, Genome Expression and Array Databases

Objective: To have a basic idea about prokaryotic and eukaryotic genome

Organization of the prokaryotic and eukaryotic genomes – Genome maps and types – Genome sequencing – Finding the genes – Statistical methods: site-specific scoring matrices, artificial neural networks, Marker models and Hidden Markov models, levels of reliability - Gene identification – gene prediction rules-Annotation of genome – Genome diversity – Taxonomy and significance of genomes – Bacteria, Yeast, Caenorhabditis – Homosapiens and Arabidopsis

Microarray – Gene expression, methods for gene expression analysis – DNA array for global expression profile– Array databases – Applications of DNA microarray – Analysis of gene expression – Bifferential gene expression under different conditions and during development of organisms.

UNIT-IV: Human Genome

Objective: To study about the human genome

Human Genome – Mapping of Human Genome – Construction of physical maps – Basics of radiation hybrid maps – Sequencing of the entire human genome – Annotation and analysis of genome sequences – Sequence repeats – transposable elements – Gene structure – Pseudogenes – Gene analysis – Gene order – Chromosome rearrangement – Compositional analysis – Clustering of genes – Composite genes – Basics of Single Nucleotide Polymorphisms – Detection and its implications.

UNIT-V: Proteomics, Protein Interactions and Homology modeling

Objective*: To understand the proteome and proteome technology using various techniques and the interaction of protein*

Proteome technology – Introduction – Expression proteomics – express profile – Cell map proteomics – Protein separation technology-2D – Gel Electrophoresis - Affinity chromatography for cell map proteomics – Forward and Reverse Proteomics, Protein–Protein Interactions – Yeast two hybrid – Co-Precipitation – Phage Display –Domain fusion – Gene Neighborhood –Gene Cluster – Mirror Tree – Analysis of genome wide Protein–Protein interactions in yeast – Genome wide yeast to hybrid analysis of other organisms – Protein fragment complementation assays – Homology Modeling – Principles , Steps of Comparative modeling – Accuracy of Homology models.

REFERENCE

1. Principles of Genome Analysis and Genomics, S.B. Primrose, R.M. Twyman, Third Edition, **2003**, Blackwell Publishing Company, Oxford, UK.
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3. Bioinformatics and Functional Genomics, J. Pevsner, **2003**, John Wiley and Sons, New Jersey, USA,
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7. An Introduction to Genetic Analysis, 7th edition, Anthony JF Griffiths, Jeffrey H Miller, David T Suzuki, Richard C Lewontin, and William M Gelbart. **2000**, W. H Freeman, New York.
8. Advanced genetic analysis: finding meaning in a genome, R. Scott Hawley, Scott W Hawley, Michelle Y Walker, **2003**, Wiley-Blackwell.
9. Principles of genome analysis and genomics, Sandy B Primrose, Richard Twyman, **2002**, Wiley-Blackwell.
10. Genomics: The Science and Technology behind the Human Genome Project, Charles R. Cantor, Cassandra L. Smith, **1999**, Wiley-Interscience.

III Semester- Elective Paper 3			
E3A	**Chromatography and Spectroscopy**		**11PEMD3A**
Hrs / Week : 5	**Hrs / Sem : 75**	**Hrs / Unit : 15**	**Credit : 4**

UNIT – I: Separation techniques

*Objective**:** To study about the various purification methods*

Chromatographic techniques: Principles of separation and application of Column, Paper, Thin layer, Gas chromatography, HPLC, HPTLC, Size exclusion chromatography, Affinity chromatography, Instrumentation of HPLC, Preparative and micropore columns, Reverse phase columns, Mobile phase selection and detectors in HPLC.

UNIT-II: **NMR Spectroscopy**

Objective: To study about the use of NMR in the protein structure determinations

Spectroscopy – Basic principles of NMR: Chemical shift, *J-J* couplings, Dipolar coupling, Nuclear Overhausser effect – Multidimensional NMR Spectroscopy: From 1-D to 2-D to n-D – homonuclear coherence transfer and mixing: COSY, DEPT, NOESY, TOCSY – NMR for biomolecular structure determination – NMR data collection and analysis of protocol for HTP protein structure determination.

UNIT- III: Spectroscopy methods for Protein Structure Determination

Objective: To study about various spectroscopic techniques for the structural determination of protein

Circular Dichroism (CD) – Principles and determination of protein structure - CD Spectra and Secondary Structure – Analysis of protein folding, non- folding and misfolding – Fluorescnce Spectroscopy – Principles of FRET –investigation of protein folding by FRET – RAMAN – IR spectroscopy.

Unit – IV: Mass spectrometry

*Objective**:** To understand the principles and applications of mass spectrometry*

Mass spectrometry – Principle – Instrumentation – m/e, m/z, fragmentation pettern – Mclafferty rearrangement - Relative abundance of isotopes, chemical ionization, FABMS, EIMS, MALDI ICPMS – Interface types – GC-MS and LC-MS.

Unit - V: **Advanced Optical Spectroscopy**

*Objective***:** *To have an idea about the various optical spectroscopic techniques.*

Optical spectroscopy – Light-matter interaction, Einstein coefficients, Selection rules for electronic transitions – Jablonskii diagram – fluorescence and phosphorescence, LASERS

Principles, Instrumentation (block diagram) and its significance - UV-Vis spectrophotometry, Steady-state fluorimetry, Time-resolved fluorimetry, Transient absorption spectroscopy, Surface Plasmon spectroscopy, Evanescent wave spectroscopy, Multiphoton spectroscopy, Single-molecule spectroscopy, Fluorescence correlation spectroscopy.

REFRENCES:

1. Instrumental Methods of Analysis, Willard, H.H., Merrit, L.L., Dean, J.A., Settle P.A., **1974**, Van Nostrand.
2. Principles of Instrumental Analysis, Skoog, D.A., Heller, F.J., Nieman, T.A., **2006**, WB Saunders.
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III Semester / Elective paper 3			
E3B	**Structural Genomics**		**11PEMD3B**
Hrs / Week : 5	**Hrs / Sem : 75**	**Hrs / Unit : 15**	**Credit : 4**

UNIT-I: Basic Concept of Structural Genomics

Objective: To know the basic concepts of Structural Genomics

Structural basis of biological phenomena – Challenges in computing with structural data – Fundamental principles of protein / DNA / RNA structure –Vibrational, rotational and torsion angles – protein secondary and tertiary structure – protein domains and folds – Protein Function and Folding – Folding Process– Folding Pathways – Forming Disulphide Bridges – Molecular Chaperones – Sequence-Structure-Function Paradigm – Automated search of natively folded protein fragments for high-throughput structure determination in structural genomics – Sequence-to-Structure-to-function paradigm, Molecular visualization, visualization styles and software.

UNIT-II: X-ray Crystallography in Protein Structure Determination

Objective: To understand the X-ray crystallography for protein structure determination

Crystal systems – Bravias lattices – Description of a Crystal – Symmetries and space groups – Miller indices – Wiess Indices – Brags indices – Diffraction from Crystals – X ray diffraction – single crystal and powder –Protein Structure Determination by X-ray Crystallography – Overview of Crystallography – Sample Preparation and Crystallization – The Phase Problem – molecular replacement method and direct method – Fourier Analysis – structure factor equation and solving the structure.

UNIT-III: **Basic Techniques in Bioinformatics**

Objective: To study about the basic techniques in bioinformatics

Electrophoresis – Agarose Gel Electrophoresis – polyacrylamide gel electrophoresis – sodium dodecylsulphate (SDS) PAGE – isoelectric focusing – Two dimensional (2D) Gel electrophoresis – Blotting technique – Southern Blotting, Northern Blotting, Western Blotting, Dot Blot – DNA Microarrays – Gene Sequencing technique – *ab initio* approaches – Web based promoter prediction programs for prokaryotes and eukaryotes – Glimmer3 – Important Features of GENSCAN – TwinScan – Gene Prediction using neural network – Gene discovery using EST and cDNA - web based programs for searching homology in EST or cDNA.

UNIT-IV: Genomics

Objective: To study about gene and genomics

Kyoto Encyclopedia of Genes and genomes – KEGG Databases, pathway – New KEGG pathway – Maps Developed upto August 2008 – New BRITE Hierarchies Added up to August

2008 – New KEGG Drug Structure Maps Developed During Year 2007–2008 – New KEGG Organisms – National Institute of Agrobiological Science (Japan) DNA Bank – Major Activities of NIAS DNA Bank – Significance of genome sequencing – Complex organism have more DNA than do simpler ones – Gene Duplication can increase genome size and complexity – genomics of prokaryotes and eukaryotes – genome of bacteriopage – Genomes of Cyanobacteria, *Escherichia coli, saccharomyces cerevisae caenorhabditis elegans, drosophilia melanogaster* – Genome of Mosquito – *Arabidopsis thaliana* – Genome of mouse (*Mus musculus*).

UNIT-V: Prediction of Structure in proteomics

Objective: To understand the concepts of structural prediction for proteins

Methods for Prediction of Secondary and Tertiary Structures of Proteins: –Homology Modeling – Threading – *ab initio* Methods for Protein Structure – Prediction – Methods for comparison of 3D structures of proteins – RNA structure prediction – protein-small molecule interactions – macromolecular docking and protein-protein interactions – Structural genomics in drug discovery.

REFERENCES:

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2. Introduction to Protein Structure, Carl Branden and John Tooze, **1999**, Garland Science.
3. Protein Structure New approaches to disease and therapy, Max Perutz, **1992**, New York: W.H. Freeman and Co.,
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13. Bioinformatics, Prakash S Lohar, **2009**, MJP Publisher, Chennai.

III / IV Semester - Core Practical Paper – 2		
CP2	**Rational, Pharmacophore and Ligand Based Drug Design**	**11PCMDP2**
Hrs / Week : 5	**Hrs / Sem : 75**	**Credit : 4**

1. Analyze a PDB file using DS.
2. Build Protein, Nucleic acids, Small molecules and ligands in DS.
3. Sequence Analysis.
4. Homology Modeling.
5. Validation of Modeled Structure using profile 3D, Protein Report.
6. Minimization, Loop and Side chain Refinement.
7. Docking using ligand site
8. Docking using CDOCKBR
9. Docking using LIBDOCK
10. Binding site prediction.
11. Flexible Docking.
12. Create QSAR models using MLR, PLS, GRA.
13. Toxicity Prediction using TOPKAT.
14. Binding site prediction
15. ADMET property calculation
16. 3DQSAR P44 Genearation

REFERENCES

1. www.ncbi.in
2. www.accelyrs.us

III / IV Semester - Elective Practical Paper – 2		
EP2	**Chromatography and Bioinformatics**	**11PEMDP2**
Hrs / Week : 5	**Hrs / Sem : 75**	**Credit : 3**

1. Separation of mixtures using separating funnel

(i) Aniline and *m*-nitro toluene

(ii) Benzophenone and Benzoic acid

And checking their R_f values by TLC after separation.

Thin Layer Chromatography/ Paper Chromatography

2. Calculation of R_f value of individual amino acid

3. Identification and Calculation of R_f value for the following compounds

a. drugs: aspirin, acetaminophen, ibuprofen and caffeine

b. sulpha drugs: sulphadiazine, sulphacetamide, sulphathiazole

c. sugar: glucose, fructose, sucrose

Column Chromatograpgy

4. Separation of mixture of compounds

a. aminoacid

b. drugs : aspirin, acetaminophen, ibuprofen

c. sulpha drugs : sulphadiazine, sulphacetamide, sulphathiazole

d. sugar mixture : glucose, fructose, sucrose

5. Preparation of isopentyl acetate (micro scale procedure) and semimicroscale procedure and conformation by co-TLC method

6. Gel electrophoresis

i. AGE- DNA Separation

ii. PAGE- Protein Separation

7. Spectra UV/VIS

i. Estimation of DNA

ii. Estimation of Total count of Bacteria

BIOINFORMATICS

1. Bioinformatics Resources: NCBI, EBI, DDBJ, RCSB, ExPASy, Swissprot, Uniprot, NAD

2. Bioinformatics Resources at the species level

a. ICTV Database b. AVIS

c. VirGen d. Viral genomes at NCBI, VBRC, VBCA, PBRC and Subviral RNA database,

Species 2000, TreeBASEetc

3. Biological Databases

a. Nucleotide/ Genome Databases. b. Protein Sequence Database.

c. Structure databases. d. Protein Pattern Databases

4. File format conversion

a. FmtSeq b. ReadSeq c. Sequence manipulation Suite

5. Sequence Analysis

a. Dot Plot b. Pairwise alignment

c. Multiple Sequence Alignment

6. Search tools against Databases – BLAST and FASTA

7. Sequence patterns and profiles:

a. generation of sequence profiles- PSI-BLAST

b. derivation of and searching sequence patterns- PHI-BLAST

8. Software

a. BioEdit. b. GeneDoc c. ClustalW / X, MEGA, MEME

9. Visualization Tool

a. RasMol b. DS c. Swiss PDB viewer

REFERENCES:

1. Experimental pharmaceutical chemistry by Anees A Siddiqui and SeemiSiddiqui
2. www.ncbi.in
3. www.accelyrs.us

IV Semester / Paper – 10			
C10	**Advanced Topics in Drug Design**		**11PCMD41**
Hrs / Week : 5	**Hrs / Sem : 75**	**Hrs / Unit : 15**	**Credit : 5**

Unit–I: QSAR

Objective: To have an idea about QSAR and Its applications

QSAR – Hansch& Free – Wilson Analysis – Validation and selection of QSAR models – Nonlinear QSAR models – Dissociation and ionization –application of QSAR analysis – Scope & limitation – Similarity of QSAR, HQSAR, Binary QSAR & other approaches.

3D – QSAR – Model evaluation– QSAR and Medicinal Chemistry – Distribution of activities in Physicochemical property space – Assumption in 3D – QSAR – Bioactive conformation and biological activity – COMFA –the alignment problem – ALMOND – alignment – Independence

Unit–II: Molecular descriptors, Docking and Scoring

Objective: *To know about molecular descriptors, docking and scoring*

Molecular descriptors – types –2D and 3D fragments – topological indices – field based descriptors

Docking techniques – protein structure – rigid docking – docking with flexible ligands – flexible protein docking – scoring techniques – force field scoring – regression based scoring – knowledge base scoring – complementary score – comparison of scoring function – consensus scoring – applications – docking as a modeling tool : understanding the selectivity of thrombin/matriptase inhibitors – docking as an *insilico* screening tool – discovery of Bcl-2 inhibitors

Unit–III: Pharmacokinetics and Drug metabolism

Objective: To understand the basic concepts of pharmacokinetics and transport of drug across biological membrane

Pharmacokinetics and its role in drug discovery – drug absorption Distribution – Metabolism – Excretion ADME – Routes of drug administration - External (Oral, Sublingual) – Parenteral - Intravenous and Intraarterial, Intramuscular, Subcutaneous, Intraperitoneal, Nasal, Tropical, Inhalation, Intrathecal, Ophthalmic.

Drug metabolism- Oxidation (saturated carbon atoms, olefinic bonds, aromatic rings, carbon-nitrogen centres, carbon oxygen and carbon-sulphurcentres) – Reduction (Carbonyl, Nitro, Azo groups, N-oxides, Disulfides and sulfoxides) – hydrolysis- Conjugation (Glucuronide, sulfate, Glycine, Glutamine, Methylation, acetylation and Glutathione conjugation).

Unit–IV: Drug Modeling

Objective: To understand the potency, efficacy of drug

Potency – Efficacy – Therapeutic Index – Margin of safety – Dose optimization – Source of curability: Metabolism, Genetics, Environmental, drug-drug interaction – Mathematical approach to pharmacokinetics modeling – Pharmacokinetic – Pharmacodynamic modeling – ADME tool development.

Unit–V: Data mining in drug discovery

Objective:To understand the concepts of data mining

Principles – Model and pattern – process – Improving the link between analysis and data-data warehouse – Representation and descriptors – Tasks – Predictive – Components of data mining methods – Tools and methods – Cluster analysis – Self organizing maps – Decision trees – Multilayer perceptions – On-line analytical processing (OLAP) – OLTP data warehousing – Characteristics – Processes – Tools – Criteria – Application of data mining – Visualization of data mining models.

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2. Pharmacokinetic Optimization in Drug Research, B. Testa, H. van de Waterbeemd, G. Folkers, R Guy (Eds) **2002**, VCH Verlag.
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5. Drug Bioavailability : Estimation of Solubility, Permeability, Absorption, and Bioavailability, H van de Waterbeemd, H. Lennernäs, P. Artursson, P. Manhold, H. Kubinyi, G. Folkers, **2003**, VCH Verlag.
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IV Semester- Core paper 11			
C11	**Advanced Topic in Molecular Modeling**		**11PCMD42**
Hrs / Week : 5	**Hrs / Sem : 75**	**Hrs / Unit : 15**	**Credit : 5**

Unit I: Molecular dynamics- III

Objective: To understand the concept of various dynamics

Phase equilbria - chemical potential – Widom particle insertion method, NPT + Test particle method-Overlapping distribution method. Ensemble-based Free energies and equilibria – Gibbs ensemble, Gibbs-Duhem integration and Phase equilibria in the Grand canonical ensemble – Applications of Flat Histogram methods- Liquid-vapour equilbria using the Wang Landu sampling – Prewetting transition in confined fluidsusing transition matrix methods.

Unit – II Molecular Dynamics - IV

Objective: To understand the concept of thermodynamics integration

Symplectic algorithm – Liouville formalism – Discretization - Hard sphere model – Langerin dynamics – Brownian dynamics – Smoluchoriski equation – Discretization – Enhanced sampling methods – Methods for constrained and unconstrained simulations – Lagrangian formulation – Potential of Mean constrained force – Adaptive biasing force (ABF) field-Applications-Two simple systems and deca-L-alanine – Non-equilibrium methods – Jarzynski's identity – derivation – Hamiltonain dynamics – Moving harmonic Oscillator – Crooks relation.

Unit - III: Applications of Free energy Calculation - I

Objective: To understand the concept of applications of free energy, thermodynamics perturbation and linear response theories.

Application of free energy calculation to Chemistry and biology - Protein ligand association, recognition and association, free energies and transport phenomena, protein folding and stability, redox and acid based titration and High performance computing. Applications of thermodynamic perturbation formula – ligand folding, systematic sensitivity analysis, λ-dynamics, electrostatic perturbation. Applications of linear response theory - proton binding and pK_a shifts - Application and potential of mean force and Poison Boltzmann free energy approach (PBFA).

Unit IV: Monte Carlo Simulation Methods

Objective: To understand the theory and models of Monte Carlo Simulation methods

Monte Carlo Simulation - Simple Monte Carlo integration - Metropolis Method – Theory – Implementation – Random Number generators - Monte Carlo Simulation of Molecules –

Models used in Monte Carlo Simulations of polymers – 'Biased' Monte Carlo Methods – Tackling the problem of Quasi-ergodicity: J-walking and Multicanoncial Monte Carlo method – Monte Carlo Methods: Ising model - q-state model – Baxter and Baxter – Wu models - Clock models – Ising spin glass models - complex fluid models in exchange sampling :Long Range – Fast multiple method , Particle mesh method – Accelerating Monte Carlo sampling - parallel tempering - Hybrid Monte Carlo.

Unit-V: Conformational Analysis

Objective: To have an idea about conformational analysis

Conformational analysis – Symplematic methods for exploring conformational space – Model building approaches – Random search method – Distance geometry - Exploring Conformational Space – A Comparison of Different Approaches – Variations on the Standard Method – Systematic unbounded multiple minimum method – Low mode search - Finding the Global Energy Minimum: Evolutionary Algorithms and Simulated Annealing - Solving protein structures using restrained MD and simulated annealing.

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1. Molecular Modeling – Principles and Applications, Andrew R Leach, Second Edition, **2010**, Pearson.
2. Understanding Molecular Simulation from Algorithm to Application, DoenFrenkel, Bernd Smith, **1996**, Academic Press.
3. Computational Medicinal Chemistry in Drug Discovery, PatricBultinct, Hans De Winter, Wilfried Langenaeker, Jan P Tollenaere (Ed), First Indian Edition, **2009**, CRC Press.
4. Molecular Modeling and Drug Design, N. Claude Cohen, **1996**, Academic Press.
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IV Semester / Core Paper – 12			
C12	**Project Work**		**11PCMD43**
Hrs / Week : 5	**Hrs / Sem : 75**	**Hrs / Unit : 15**	**Credit : 5**

Project work

IV Semester- Elective Paper			
E4A	**Advanced Computational Chemistry and Clinical Study**		**11PEMD4A**
Hrs / Week : 5	**Hrs / Sem : 75**	**Hrs / Unit : 15**	**Credit : 4**

Unit – I: Electron Correlation Methods:

Objective: To understand the concept of electron correlation methods.

Configuration Interaction (CI) – CI matrix element – Size of the CI matrix – Truncated CI – Direct CI methods – RHF, OHF dissociation, the spin coordination – size consistency and size extensivity – Multiconfigurational SCF – Multi – reference CI – Many body Petrubation theory – Moller – Plesset Petrubation theory – Coupled Cluster (CC) methods – comparison between CC, CI and Petrubation theory.

Unit- II: Density Functional Theory

Objective: To know about the DF theories

Density Functional Theory: Kohegen – Khon existence theorem, Kohegen – Khon variational theorem, Kohn Sam SCF methodology, Exchange correlation function- Local Density approximation - Density Gradient Correction - adiabatic method- Advantages and Disadvantage of Density Functional Theory.

Unit – III: Transition Structure Optimization:

Objective: To have some idea about transition structure optimization

Transition structure optimization – Methods to locate saddle points – Linear and quadratic synchronous transit, Saddle optimization method, Chain method, penalty walk method, Sphere optimization technique, Gradient norm minimization, Gradient external methods, Locating the global minimum and conformational sampling - Genetic algorithm, Diffusion method, Distance geometry method - Intrinsic reaction coordinate methods, Continuum Solvation method.

Unit–IV: Bioavailability and Clinical Studies

Objective: To have an idea about bioavailability and clinical studies

In vitro disintegration – *in vitro* dissolution – Noyes Whitney equation – Methods of dissolution **– i***n vivo* and i*n vitro* correlations. Bioavailability: absolute and relative – Area

Under Curve (AUC) – Assessment of Bioavailability: from plasma levels, from urine level – from pharmacological response – Bioequivalence – Therapeutic equivalence – New drug development process: Preclinical trials – Phase I and Phase II clinical trials.

Unit-V: Drug delivery systems

Objective: To have an idea about Delayed and Sustained release delivery systems in GI Tract

Small intestine specific delivery – mechanism of enteric coatings – colon specific drug delivery – pH controlled release – time controlled release –suitable drug candidates for sustained release dosage forms – stability in GI tract – absorption – presystemic metabolism – Half-life of the drug after absorption – dissolution based sustained release dosage forms – repeat action drug delivery system – gastroretentive drug delivery system - density differences to gastric fluid – swelling and expandable gastroretentive drug delivery system – diffusion based sustained release dosage forms –reservoir systems – polymer used in development of reservoir systems –matrix systems – bioerodible sustain release dosage forms.

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IV Semester – Elective Paper			
E4B	**Medical Instrumentation and Clinical Chemistry**		**11PEMD4B**
Hrs / Week : 5	**Hrs / Sem. : 75**	**Hrs / Unit : 15**	**Credits : 4**

UNIT - I: Drug Concepts

Objective: To understand the concepts of drugs and their action.

Concepts – Classifications of drugs – Biological and Chemical classification nomenclature of drugs – International Non-proprietary Names (INNs). Metabolism of drugs – Factors affecting metabolism - chemical pathway of drug metabolism – Bio transformation - Oxidative, reductive and hydrolytic bio transformations – Conjugate reactions – Glucouranides, amino acids, ethereal sulphate, methylated, acetylated and glucothione conjugations. Absorption of drugs – Routes of administration – Factors affecting absorption. Assay of drugs – Chemical, Biological and immunological assay.

UNIT – II: Diagnostic Medical Instruments

Objective: To study the different techniques used for diagnosis.

Design of medical instruments – General components – Transducers – Types – Biopotential recorders – Electrocardiograph (ECG) – Principles, block diagram, measurement and analysis of the ECG.X-rays - principles, block diagram, measurement and analysis of the X-ray. Ultrasonic Scanning - principles, block diagram, measurement and analysis of the scans. C.T-Scan - principles, block diagram, measurement and analysis of the scan

UNIT – III: Clinical Chemistry.

Objective: To know the various clinical analyses.

Clinical chemistry – Composition of blood – Blood grouping - Determination of blood groups and matching – Blood pressure – Hyper tension. Determination of glucose in serum – Folin's method, Wu's method - determination of serum cholesterol – Sackett's method – Tests for cholesterol. Estimation of glucose in urine – Benedict's test – Tests for salts in serum – Tests for chlorides in serum – Tests for salts in urine – Tests for cholesterol in urine. Detection of diabetes and anemia. Estimation of hemoglobin (Hb concentration) – Estimation of red blood cells(count).Analysis of blood – determination of blood urea – urease method. Estimation of bile pigment in serum – estimation of total protein in serum – estimation of total proteins and albumin based on Biuret and BCG methods.

UNIT – IV: Diseases and treatment I

Objective: To study the important disorders of human body and the drugs for them.

Causes and treatment of some common diseases: Insect borne diseases – malaria and filariasis.Air borne diseases – diphtheria, woophing cough, influenza, cold, fever and tuberculosis. Water borne – cholera, typhoid and dysentery. Digestive disorders – jaundice – respiratory disorder – asthma – nervous disorder – epilepsy - other diseases – piles and leprosy. Important Indian medicinal plants and their uses. Functions, uses and effects of the following drugs. Cardiovascular drugs – antiarrythmic drugs - quinidine. Anti hypertensive drugs - clondine and reserpine. Anti anginal drugs - glyceryltrinitrate and isosorbidedinitrate. Sulpha drugs – sulphanilide and sulphadiazine.

UNIT - V - Diseases and treatment II.

*Objective**:** To understand the important diseases and their treatment.*

Cancer – causes, spread and treatment – structure and effects of chloramBusil, methotreate, plant products and hormones. Diabetes – control – structure and uses of insulin - Oral hypoglycemic drugs – tolbutamide and chloropropanamide. Anti-convulsant agents – structure and uses of barbiturates and sucinimides. Uses and effects of the following drugs:Analgesics – narcotic analgesics – action, uses and structural activity of morphine. Non narcotic analgesics – asprin and paracetamol. Anesthetic - general anesthetic – uses and disadvantages of vinlyl ether and halothane. Intravenous anesthetics – tripental sodium – local anesthetics – cocaine and chincocaine. Anti psychotic drugs – piperazine and bezamides. Anti anxiety drugs – benzodiazepine.

REFERENCE BOOKS :

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2. Text Book of Pharmaceutical Chemistry, Jeyashree Gosh, **2003**, S.Chand andCompany, New Delhi.
3. Medicinal Chemistry, G.R.Chatwal, **2002**, Himalaya Publishing House, New Delhi.
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