Course Structure and Syllabi of PhD in Computational Sciences (2017 --)

Semester I						
S.No.	Subject Code	Subject Name	Credit Hours			Maximum Marks
			Theory	Practical	Total	
1	CCS.701	Research Methodology	2		2	50
2	CCS.702	Statistics	2		2	50
3	CCS.703	Review Writing and Presentation		8	4	100
Opt any two of the following courses:						
4	CCS.704	Computational Chemistry	4		4	100
5	CCS.705	Sequence and Structural Bioinformatics	4		4	100
6	CCS.706	Biomolecular Structure Modelling and Drug Design	4		4	100
7	CCS.707	Biomathematics	4		4	100
8	CCS.708	Computer applications	4		4	100
9	CCS.709	Introduction to Quantum Dynamics	4		4	100
Total					16	400

Semester I

Subject Code: CCS.701
Subject Name: Research Methodology

L	T	P	Credits	Marks
2	0	0	2	50

Course Objective: The objective of this subject is to ensure that a student learns basis of scientific research to arrive at and verify the conclusions drawn.

Unit 1 5 Lectures

General principles of research: Meaning and importance of research, critical thinking, formulating hypothesis and development of research plan, review of literature, interpretation of results and discussion.

Unit 2 10 Lectures

Technical writing: Scientific writing that includes the way of writing Synopsis, research paper, poster preparation and presentation, and dissertation.

Unit 3 5 Lectures

Library: Classification systems, e-Library, web-based literature search engines

Unit 4 16 Lectures

Entrepreneurship and business development: Importance of entrepreneurship and its relevance in career growth, characteristics of entrepreneurs, developing entrepreneurial competencies, types of enterprises and ownership (large, medium SSI, tiny and cottage industries, limited, public limited, private limited, partnership, sole proprietorship) employment, self-employment and entrepreneurship, financial management-importance and techniques, financial statements- importance and its interpretation, and Intellectual Property Rights (IPRs).

Recommended Readings

1. Kothari, C. R. (2014). Research methodology (s). New Age International (p) Limited. New Delhi. 2. Sahay, Vinaya and Pradumna Singh (2009). Encyclopedia of Research Methodology in life sciences. Anmol Publications. New delhi
3. Kauda J. (2012). Research Methodology: A Project Guide for University Students. Samfunds literature Publications.
4. Dharmapalan B. (2012). Scientific Research Methodology. Narosa Publishing House ISBN: 978-81-8487-180-7.

Subject Code: CCS.702
Subject Name: Statistics

L	T	P	Credits	Marks
2	0	0	2	50

PART-A

10 Hours

General Statistics: Difference between parametric and non-parametric statistics, Univariant and multivariant analysis, Confidence interval, Errors, Levels of significance, Hypothesis testing. Measures of central tendency and dispersal,

PART-B 5 Hours

Histograms, Probability distributions (Binomial, Poisson and Normal), Sampling distribution, Kurtosis and skewness; Comparative Statistics: Comparing means of two or more groups: Student's t-test, Paired t-test, Mann-Whitney U-test, Wilcoxon signed-rank.

PART-C 16 Hours

One-way and two-way analysis of variance (ANOVA), Critical difference (CD), Fisher's LSD (Least significant difference), Kruskal–Wallis one-way ANOVA by ranks, Friedman two-way ANOVA by ranks, Chi-square test

PART-D 15 Hours

Regression and correlation: Standard errors of regression coefficients, Comparing two regression lines, Pearson Product - Moment Correlation Coefficient, Spearman Rank correlation coefficient, Power and sampling size in correlation and regression.

Suggested Reading

1. Gupta, S. (2008). Research methodology and statistical techniques. Deep & Deep Publications (P) Limited, New Delhi.
2. 6. Norman, G. and Streiner, D. (2008). Biostatistics: The Bare Essentials.3/e (with SPSS). Decker Inc. USA.
3. Rao, P. P., S. Sundar and Richard, J. (2009). Introduction to Biostatistics and Research
4. Methods. PHI learning. 11. Christensen, L. (2007). Experimental Methodology. Boston: Allyn & Bacon.

Subject Code: CCS.703
Subject Name: Review Writing and Presentation

L	T	P	Credits	Marks
0	0	8	4	100

Course Objectives and Learning Outcomes: The objective of this course would be to ensure that the student learns the aspects of the Review writing and seminar presentation. Herein the student shall have to write a 5000 words review of existing scientific literature with simultaneous identification of knowledge gaps that can be addressed through future work.

The evaluation criteria for "Review Writing and Presentaion" shall be as follows:

Maximum Marks: 100

S.No.	Criteria	Marks
1.	Review of literature	25
2.	Identification of gaps in knowledge	15
3.	References	10
4.	Content of presentation	15
5.	Presentation Skills	20
6.	Handling of queries	15
Total		100

Subject Code: CCS. 704
Subject Name: Computational Chemistry

L	T	P	Credits	Marks
4	0	0	4	100

Course Objectives and Learning Outcomes: The objective of this subject is to ensure that a student learns basis of computational chemistry to ensure that they understand the intricacies of applying computational chemistry methods in their research work.

Part-A 10 Hours

Fundamental Background: Postulates of quantum mechanics, Eigen values and Eigen functions, operators, hermitian and unitary operators, some important theorems. Schrodinger equation-particle in a box (1D, 3D) and its application, potential energy barrier and tunneling effect, one-dimensional harmonic oscillator and rigid rotor.

Part-B 15 Hours

Many Electron atoms: Angular momentum, eigenvalues of angular momentum operator, Particle in a Ring, Hydrogen Atom. Electron correlation, addition of angular momentum, Clebesch-Gordan series, total angular momentum and spin-orbit interaction.

Part-C 16 Hours

Ab Initio Methods: Review of molecular structure calculations, Hartree-Fock SCF method for molecules, Roothaan-Hartree-Fock method, selection of basis sets.
Electron Correlation and Basis Sets: Configuration Interaction, Multi-Configuration Self-Consistent Field, Multi-Reference Configuration Interaction, Many-Body Perturbation Theory, Coupled Cluster, Basis sets.

Part-D 15 Hours

DFT and Force Field methods: Energy as a functional of charge density, Kohn-Sham equations. Molecular mechanics methods, minimization methods, QSAR.

ESSENTIAL BOOKS:

1. Introduction to Computational Chemistry, F. Jensen, 2nd edition, Wiley-Blackwell (2006).
2. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedman, 3rd edition, Oxford University Press, Oxford (1997).
3. Quantum Chemistry, H. Eyring, J. Walter and G.E. Kimball, (1944) John Wiley, New York.
4. Quantum Chemistry, I.N. Levine, 5th edition (2000), Pearson Educ., Inc., New Delhi.
5. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure, A. Szabo and N. S. Ostlund, (1982), Dover, New York.

Subject Code: CCS. 705
Subject Name: Sequence and Structural Bioinformatics

L	T	P	Credits	Marks
4	0	0	4	100

Course Objectives and Learning Outcomes: The objective of this subject is to ensure that a student learns advanced concepts in Bioinformatics.

Unit-1 14 Hours

Biological data Types of biological data (various omics)

Biological Databases Nucleic acid and protein sequence and protein structure databases Overview of available Bioinformatics resources on the web

Unit-2 14 Hours

DNA sequence analysis

Sequence annotation and sequence analysis - Phylogeny of gene (blast, fasta, HMMer) and residue conservation. Primer design and Tm Calculation, DNA Restriction pattern analysis.Condon bias and its effect on the protein expression with reference to various expression system.

Unit-3 14 Hours

Bioinfo tools

Protein sequence and structure insights (PSSI) X-ray, NMR, Comparative modeling, ab initio, threading methods. Structure refining techniques Energy minimization approaches (Steepest descent, Conjugate gradient etc), Basis of Molecular dynamics simulations and its application.

Unit-4 14 Hours

Simulation methods : algorithm for time dependence; leapfrog algorithm, Verlet algorithm, Boltzmann velocity, time steps, duration of the MD run, Starting structure, analysis of MD job, uses in drug designing, ligand protein interactions. Various methods of MD, Monte Carlo, systematic and random search methods. Differences between MD and MC, Energy, Pressure, Temperature, Temperature dynamics, simulation softwares. Various methods of MD, Monte Carlo, systematic and random search methods.

Suggested Readings

1. Andrew R.Leach Molecular Modelling Principles and applications . (2001) II ed . Prentice Hall.
2. A.D. Baxevanis *et. al.*, Current Protocols in Bioinformatics, (2005) Wiley Publishers
3. David W.Mount Bioinformatics (2001) Cold Spring Harbor Laboratory Press, ISBN 0-87969-608-7
4. Computational Molecular Biology by P. A. Pevzner, Prentice Hall of India Ltd, (2004) ISBN81-203-2550-8
5. D.E.Krane and M.L.Raymer Fundamental concepts of Bioinformatics (2003) Pearson Education ISBN 81-297-0044-1
6. N.Gautham Bioinformatics Narosa publications. (2006) ISBN-13: 9781842653005
7. Fenniri, H. “Combinatorial Chemistry – A practical approach”,(2000) Oxford University Press, UK.
8. Lednicer, D. “Strategies for Organic Drug Discovery Synthesis and Design”; (1998) Wiley International Publishers.
9. Gordon, E.M. and Kerwin, J.F “Combinatorial chemistry and molecular diversity in drug discovery” (1998) Wiley-Liss Publishers.

Subject Code: CCS.706
Subject Name: Biomolecular Structure Modelling and Drug Design

L	T	P	Credits	Marks
4	0	0	4	100

Course Objective and Learning Outcomes: The objective of this subject is to ensure that a student learns modelling of biomolecular structures.

Unit 1 14 Hours

Introduction to Molecular Geometry, Coordinate Space for Optimization of Algorithm of Molecular Geometry, Z-Matrix, Molecular Vibrations, Electrostatic Charges, Electrostatic Charges, Multipole Moments,

Unit 2 14 Hours

Modelling and structure: From protein sequence to structure, theoretical and practical aspects of protein sequence alignments, secondary, tertiary structure prediction, comparative modeling, Docking, protein-protein and protein-ligand docking.

Unit 3 14 Hours

Computational drug designing: Structure-based drug design, virtual screening, quantitative structure activity relations, Cheminformatics, Historical Perspective and Viewpoint of Pharmacophore, Functional Groups Considered as Pharmacophores, Ehrlich’s “Magic Bullet”, Fischer’s “Lock and Key”, Two-dimensional Pharmacophores, Three-dimensional Approach of Pharmacophores, Criteria for Pharmacophore Model,

Unit-4 14 Hours

Pharmacophore Model Generation Software Tools, Molecular Alignments, Handling Flexibility, Alignment Techniques, Scoring and Optimization, Pharmacophores, Validation and Usage, Automated Pharmacophore Generation Methods, GRID-based Pharmacophore Models, Pharmacophores for Hit Identification, Pharmacophores for Human ADME/Tox-related Proteins.

Suggested Readings:

1. Molecular and Structural Database, Protein Data Bank, Bioactivity Databases, Gene and Protein Sequence Databases,Cambridge Crystallographic Database, Compound Storage and Management.
3. Lednicer, D. “Strategies for Organic Drug Discovery Synthesis and Design”; (1998) Wiley International Publishers.
7. Gordon, E.M. and Kerwin, J.F “Combinatorial chemistry and molecular diversity in drug discovery” (1998) Wiley-Liss Publishers.

L	T	P	Credits	Marks
4	0	0	4	100

Subject Code: CCS.707
Subject Name: Biomathematics

Course Objectives and Learning Outcomes:The course aims at enabling learners to:
• become precise, exact and logical.
• acquire knowledge of mathematical terms, symbols, facts and formulae.
• develop an understanding of mathematical concepts.
• develop problem solving ability.
• acquire skills in applying the learning to situation including reading charts, tables, graphs etc

Unit 1 14 Hours
Vectors Scalars and vectors Vectors as directed line segments Magnitude and direction of a vector; Null vector and Unit vector Equality of vectors Position vector of a point Algebra of vectors
Addition and subtraction of vectors and their properties Multiplication of a vector by a scalar and their properties, Resolution of a vector Resolution of a vector in two dimensions; Resolution of a vector in three dimensions; Section formula

Unit 2 14 Hours
Discrete and Continuous Distributions Binomial, Gaussian, Chi-Square test, Student's t-Test, F-test, Z-test

Unit 3 14 Hours
2D Coordinate geometry: line, circle, ellipse, parabola, hyperbola, 3D Geometry: equations of Sphere and cone

Unit 4 14 Hours
Probability Theory Sample Space and Events, Axioms of Probability, Conditional Probability, Independent Events, Baye's Formula.

Unit 5 14 Hours
Matrix algebra, addition, subtraction, multiplication, inverse and transpose and determinants

Suggested readings
1. Wayne W. Daniel, Biostatistics, 9e Wiley (2004) ISBN: 978-0-471-45654-4
2. Bernard Rosner, Fundamentals of Biostatistics 6e (2006) Thomson Brooks/Cole ISBN: 0-534-41820-1

L	T	P	Credits	Marks
4	0	0	4	100

Subject Code: CCS.708
Subject Name: Computer Applications
Course Objectives and Learning Outcomes: The objective of this subject is to ensure that a student learns application of computer for research data management.

Unit 1 14 Hours
Fundamentals of Computers: Block Diagram of Computer, Hardware Components, Introduction to computer network and World Wide Web, Sharing Data over Network, Internet Terminology, Searching over Internet, Google: advance Search Operations, Email, Checking Plagiarism using Internet
Unit 2 14 Hours
Introduction to Word Processing and Microsoft Office, Creating and Saving Documents, Text Formatting, Tables, Document Review Option, Mail Merge, Inserting Table of Contents, Reference Management.
Introduction to Spreadsheet and Microsoft Excel, Text Formatting, Formulas, Charts, Table formatting, Sorting Records, Filtering the content.

Unit 3 14 Hours
Computer Configuration, Memory Hierarchy, Software Structure, Introduction to Operating System, Operating System types and functions. Introduction to Disk Operating System, DOS Internal and External Commands, Introduction to Windows operating System, Windows Task Manger.

Unit 4 14 Hours
Introduction to MS Paint, Figure Designing components in MS Paint
Introduction to Microsoft PowerPoint, Layout Selection, Designing and Formatting Slides, Slide Design and background formatting, Bullets and Numbering, Transition Style, Custom Animations, Hyperlink to Local files and Web Pages, Movies and Sound, Slide Timings.

Suggested Reading
1. Gookin, D. (2007). MS Word for Dummies. Wiley.
2. Harvey, G. (2007). MS Excel for Dummies. Wiley
3. Sinha, P.K., Computer Fundamentals, BPB Publications.

Course Title: Introduction to Quantum Dynamics

Paper Code: CCS.709
Total Lecture: 72

L	T	P	Credits	Marks
4	0	0	4	100

Course Objective and Learning Outcomes: This course will introduce the basic aspects of time dependent quantum wavepacket dynamics to Ph.D. students.

Unit I 18 Hours

Separation of electronic and nuclear motions: adiabatic representation, Born-Oppenheimer approximation, Hellmann-Feynman theory, diabatic representation, transformation between two representations, crossing of adiabatic potentials. TDSE: separation of variables and reconstitution of the wavepacket, expectation values, free-particle wavepacket: centre and dispersion of the wavepacket.

Unit II 18 Hours

Gaussian wavepacket: Gaussian free particle, general properties of Gaussian wavepackets, Gaussian in a quadratic potential. Correspondence between Classical and Quantum Dynamics: Ehrenfest's Theorem, Bohmian Mechanics and the Classical limit.

Unit III 18 Hours

Spectra as Fourier transforms of wavepacket correlation functions. 1D barrier scattering: wavepacket formulation of reflection and transmission coefficients, cross-correlation function and S-matrix.

Unit IV 18 Hours

Numerical methods for solving the TDSE: spectral projection and collocation, pseudospectral basis, gaussian quadrature, represntation of the hamiltonian in the reduced space, discrete variable representation, Fourier method, time propagation.

Books

1. D. J. Tannor, *Introduction to Quantum Mechanics: A Time-dependent Perspective*, University Science Books, 2006.
2. Edited by R E Wyatt and J Z H Zhang, *Dynamics of Molecules and Chemical Reactions*, CRC Press, 1996.
3. K. C. Kulander, *Time-dependent Methods for Quantum Dynamics*, Elsevier Science, 1991.
4. J. Z. H. Zhang, *Theory and application of Quantum Molecualr Dynamics*, World Scientific Publishing Company, 1998.
5. Edited by M Brouard and C Vallance, *Tutorials in Molecular Reaction Dynamics,* Royal Society of Chemistry, 2010.
6. Edited by D. A. Micha, I. Burghardt, *Quantum Dynamics of Complex Molecular Systems*, Springer-Verlag, 2006.