STRUCTURE AND SYLLABUS OF PhD COURSEWORK

TO BE DISSCUSSED IN THE

BOARD OF STUDIES (CENTRE FOR COMPUTATIONAL SCIENCES)

FOR

PhD Computational Sciences

2015-16

Central University of Punjab
Bathinda-151001

Programme Objective:

The objective of coursework for PhD Computational Sciences (Computational Chemistry) Programme is that the student gains solid understanding of the research methodology. In addition, the courses are designed to help the student to study the relevant literature in his area of interest and narrow down to a problem of interest that he is going to pursue for his PhD research. Summarily, based on the research training provided in this course, the students should be enabled to understand concurrent scientific literature, identify the knowledge lacunae, shortlist attainable objectives, design comprehensive methodology and carry out further research leading to his PhD degree. In addition, extensive stress on logic based discipline would ensure development of scientific temperament among the students. Therefore graduated students of MSc Chemistry (Computational Chemistry) would be valuable asset for the nation by virtue of their scientific abilities. The student can expect successful career/employment in academic / research / industry by undertaking this course. A special effort has been made to enable the student clear national level tests for teaching ability and research fellowships especially, CSIR-NET.

Eligibility Criteria for PhD Computational Sciences

Master's degree in any branch of Life Sciences / Chemical Sciences / Pharmaceutical Sciences / Bioinformatics / Computational Sciences (or Applications) / or M. Tech. in CSE / IT / BioTechnology with at least 55% marks from a UGC recognised Indian or a foreign University (as considered equivalent by UGC).

Course structure for Ph.D. in Computational Sciences

Students will move into working towards their Ph.D thesis after successful completion of one semester course work.

Semester I						
S.No.	Subject Code	Subject Name	Credit Hours			Maximum Marks
			Theory	Practical	Total	
1	CCS.701	Computer applications	4		4	100
2	CCS.702	Review Writing and Presentation		16	8	200
Opt any one of the following courses:						
3	CCS.703	Research Methodology and Statistics-I	4		4	100
4	CCS.704	Research Methodology and Statistics-II	4		4	100
Opt any one of the following courses:						
4	CCS.705	Computational Quantum Chemistry	4		4	100
5	CCS.706	Sequence and Structural Bioinformatics	4		4	100
6	CCS.707	Biomathematics	4		4	100
7	CCS.708	Quantum Wave packet Dynamics	4		4	100

Syllabi for PhD Course work
Central University of Punjab

Semester I

Subject Code: CCS.701
Subject Name: Computer Applications

L	T	P	Credits	Marks
4	0	0	4	100

Objectives

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. Sinha, P.K., Computer Fundamentals, BPB Publications**.**

Subject Code: CCS.702
Subject Name: Review Writing and Presentation

L	T	P	Credits	Marks
0	0	16	8	200

Objective: 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: 200

S.No.	Criteria	Marks
1.	Review of literature	50
2.	Identification of gaps in knowledge	30
3.	References	20
4.	Content of presentation	30
5.	Presentation Skills	40
6.	Handling of queries	30
Total		200

Subject Code: CCS.703
Subject Name: Research Methodology and Biostatistics-I

L	T	P	Credits	Marks
4	0	0	4	100

Course Objective: The objective of this subject is to ensure that a student learns basis of scientific research and statistical methods to arrive at and verify the conclusions drawn. This course is intended for those students who have already done a course in Research Methodology at the Master's level. This would be more of an applied course with extensive problem solving and actual application of theoretical concepts (which students may have learnt at Masters' program).

PART-A **10 Hours**

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. Technical writing: Scientific writing, Writing synopsis, Research paper, Poster preparation and Presentations and Dissertation.

PART-B **15 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, Histograms, Probability distributions (Binomial, Poisson and Normal), Sampling distribution, Kurtosis and skewness

PART-C **16 Hours**

Comparative Statistics: Comparing means of two or more groups: Student's t-test, Paired t-test, Mann-Whitney U-test, Wilcoxon signed-rank, 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. Kothari, C. R. (2014). Research methodology (s). New Age International (p) Limited. New Delhi.
3. Sahay, Vinaya and Pradumna Singh (2009). Encyclopedia of Research Methodology in life

sciences. Anmol Publications. New delhi
4. Kauda J. (2012). Research Methodology: A Project Guide for University Students. Samfunds Literature Publications.
5. Dharmapalan B. (2012). Scientific Research Methodology. Narosa Publishing House ISBN: 978-81-8487-180-7.
6. Norman, G. and Streiner, D. (2008). Biostatistics: The Bare Essentials.3/e (with SPSS). Decker Inc. USA.
7. Rao, P. P., S. Sundar and Richard, J. (2009). Introduction to Biostatistics and Research
8. Methods. PHI learning. 11. Christensen, L. (2007). Experimental Methodology. Boston: Allyn & Bacon.

Subject Code: CCS.704
Subject Name: Research Methodology and Biostatistics-II

L	T	P	Credits	Marks
4	0	0	4	100

Course Objective: The objective of this subject is to ensure that a student learns basis of scientific research and statistical methods to arrive at and verify the conclusions drawn. This course is intended for those students who have not done a course in Research Methodology at the Master's level. This course would be a mix of basic content which is taught at the Master's level and applied content with extensive problem solving and actual application of theoretical concepts. Thus, although the course content of Part A and Part B of this course is similar to that of the course CCS-703, the level of depth will be different in both courses. However, Part C and D will be at the same level for both CCS.703 nad CCS.704 courses.

PART-A **10 Hours**

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. Technical writing: Scientific writing, Writing synopsis, Research paper, Poster preparation and Presentations and Dissertation.

PART-B **15 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, Histograms, Probability distributions (Binomial, Poisson and Normal), Sampling distribution, Kurtosis and skewness

PART-C **16 Hours**

Comparative Statistics: Comparing means of two or more groups: Student's t-test, Paired t-test, Mann-Whitney U-test, Wilcoxon signed-rank, 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. Kothari, C. R. (2014). Research methodology (s). New Age International (p) Limited. New Delhi.
3. Sahay, Vinaya and Pradumna Singh (2009). Encyclopedia of Research Methodology in life sciences. Anmol Publications. New delhi
4. Kauda J. (2012). Research Methodology: A Project Guide for University Students. Samfunds Literature Publications.

5. Dharmapalan B. (2012). Scientific Research Methodology. Narosa Publishing House ISBN: 978-81-8487-180-7.
6. Norman, G. and Streiner, D. (2008). Biostatistics: The Bare Essentials.3/e (with SPSS). Decker Inc. USA.
7. Rao, P. P., S. Sundar and Richard, J. (2009). Introduction to Biostatistics and Research
8. Methods. PHI learning. 11. Christensen, L. (2007). Experimental Methodology. Boston: Allyn & Bacon.

Subject Code: CCS. 705

Subject Name: Computational Quantum Chemistry

L	T	P	Credits	Marks
4	0	0	4	100

Course Objective: 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.

L	T	P	Credits	Marks
4	0	0	4	100

Subject Code: CCS. 706
Subject Name: Sequence and Structural 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.

L	T	P	Credits	Marks
4	0	0	4	100

Subject Code: CCS.707
Subject Name: Biomathematics

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

Subject Code: CCS.708
Subject Name: Quantum Wave Packet Dynamics

L	T	P	Credits	Marks
4	0	0	4	100

Unit I[1-6] **14 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[1-6] **14 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[1-4] **14 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.

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.

Unit IV[1-2] **14 Hours**

Statistical versus non-statistical reaction, beyond Transition State Theory: rigorous Quantum approaches for determining chemical reaction rates: Classical Rate theory, Transition State Theory, Quantum Transition State Theory, Semiclassical Transition State Theory, Rigorous Quantum Rate Theory.

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.