STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600 086
M.Sc. DEGREE: BIOINFORMATICS

SYLLABUS
(Effective from the academic year 2019 -2020)

INTRODUCTION TO BIOINFORMATICS

CODE: 19BI/PE/IB23   **CREDITS : 3**
                                                            L T P : 3 0 0
                                          TOTAL TEACHING HOURS : 39

OBJECTIVES OF THE COURSE
- To become familiar with bioinformatics and how it's changing complex biological research
- To enable textual mining of biological literature and bioinformatics tools that are required to query biological data
- To understand the application of information technology in biological research

COURSE LEARNING OUTCOMES
On Successful completion of the course, the student will be able to

- Better understanding of the bioinformatics concepts
- Emphasis the application of bioinformatics and biological databases to problem solving in real research problems
- Perform a complete analysis of the genes and protein
- Understand the evolutionary concepts related to biological query

Unit   1   **(8 Hours)**
Introduction to Bioinformatics
1.1 Introduction to Bioinformatics, Classification of biological databases, Biological data formats, Application of bioinformatics in various fields
1.2 Introduction to single letter code of amino acids, symbols used in nucleotides
1.3 Data retrieval systems- Entrez and SRS

Unit   2   **(8 Hours)**
Sequence and Structure analysis
2.1 Introduction to Sequence alignment. BLAST, Multiple sequence alignment
2.2 Structural Databases – PDB and other online tools
2.3 Visualizing tools – Rasmol, Pymol

Unit   3   **(7 Hours)**
Phylogenetic analysis
3.1 Evolutionary analysis: distances, Cladistic and Phenetic methods
3.2 Clustering Methods. Rooted and unrooted tree representation
3.3 Bootstrapping strategies, Tools for Phylogenetic tree construction

Unit 4   **(8 Hours)**

Genomics

4.1 Genome - Gene finding methods,

4.2 Gene prediction tools

4.3 Repeat Sequence finder

Unit 5   **(8 Hours)**

Proteomics

5.1 Proteomics - Protein structure – levels of organisation

5.2 Protein separation techniques – SDS-PAGE

5.3 Restriction Enzymes and Mapping

BOOKS FOR STUDY

Pevsner and Jonathan.*Bioinformatics and Genomics Functional.* USA: John Wiley,2003.

Baxevanis, Andreas D. and Francis B.F. Ouellette. *Bioinformatics- A Practical Guide to the Analysis of Genes and Proteins*. USA: John Wiley, 2001.

David W. Mount. *Bioinformatics Sequence and Genome Analysis*. INDIA: CBS Publishers, 2003.

BOOKS FOR REFERENCE

Baldi P. and Brunak S. *Bioinformatics: Machine Learning Approach*. USA: MIT Press, 2003.

Chen, Yi-Ping Phoebe. *Bioinformatics Technologies*. Germany: Springer, 2005.

Durbin R, S. Eddy, A. Krogh and G. Mitchison.*Biological Sequence Analysis: Probabilistic Models of Proteins and Nucleic Acids.* USA: Cambridge University Press, 2005.

Higgins, Des and Willie Taylor. *Bioinformatics – Sequence, Structure and Databanks – Practical Approach***.** UK: Oxford University Press, 2001.

Lesk, Arthur M. *Introduction to Bioinformatics.* UK: Oxford University Press, 2014.

JOURNALS

BMC Bioinformatics

Bioinformatics

Journal of Bioinformatics and Computational Biology

Journal of Biomedical Informatics

Journal of Integrative Bioinformatics

PLoS Computational Biology

WEB RESOURCES

http://bioinformaticsweb.net/tools.html

https://www.bits.vib.be/index.php/training/122-basic-bioinformatics

http://bioinformaticssoftwareandtools.co.in/

http://www.genscript.com/tools.html

PATTERN OF ASSESSMENT

Continuous Assessment Test: **Total Marks: 50**   **Duration: 90 minutes**
Section A – 10 x 1 = 10 Marks (All questions to be answered)
Section B – 2 x 10 = 20 Marks (2 out of 4 to be answered)
Section C – 1x 20 = 20 Marks (1 out of 2 to be answered)

Other Components: **Total Marks:50**
Assignment/Test/Seminars

End Semester Examination: **Total Marks: 100**   **Duration: 3 Hours**
Section A – 20 x 1 = 20 Marks (All questions to be answered)
Section B – 4 x 10 = 40 Marks (4 out of 7 to be answered)
Section C – 2 x 20 = 40 Marks (2 out of 4 to be answered)

STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600 086
M.Sc. DEGREE: BIOINFORMATICS

SYLLABUS
(Effective from the academic year 2019 -2020)

COMPUTER AIDED DRUG DESIGN

CODE: 19BI/PE/CD23   **CREDITS : 3**
L T P : 3 0 0
TOTAL TEACHING HOURS : 39

OBJECTIVES OF THE COURSE
- To understand the general pathway for drug discovery and development
- To define new methodologies for analysis of ligands with their bound protein target
- To gain an in-depth overview of methods and techniques applied in computer assisted drug design (CADD)
- To learn about computer-aided drug design, safety evaluation, bioavailability and clinical trials

COURSE LEARNING OUTCOMES
On Successful completion of the course, the student will be able to

- Identify the key elements in drug and explain new methodologies for drug design
- Describe the role and importance of the various disciplines involved in the different phases of drug discovery and development
- Review and evaluate preclinical and clinical pharmaceutical studies
- Follow new ideas in utilizing main approaches of ligand screening methods

Unit 1   **(7 Hours)**
     Drug Discovery and Development

1.4 Drug Development Process Overview - The Changing Landscape of drugs development

1.5 Drug Discovery Phases

1.6 Preclinical Phase studies

Unit 2 (8 Hours)

Regulations in Drug Discovery

2.1 FDA regulations on Drug Development

2.2 Indian Regulatory Systems

2.3 Ethical Considerations and Special Populations

Unit 3 (8 Hours)

Drug Target Identification

3.1 Computational inferences used to identify and validate small molecule drug targets

3.2 Databases for Drug targets, Retrieving protein structure and visualisation

3.3 Target Discovery and Validation, Active Site Prediction

Unit 4 (8 Hours)

Ligand Based Drug Design

4.1 Screening of lead molecules - Natural products and their analogues

4.2 Chemical Databases – PubChem, Drug Bank

4.3 Chemical file formats, Retrieving drug molecules

Unit 5 (8 Hours)

Pharmacokinetics and Molecular Docking

5.1 Pharmacokinetics - ADME Prediction

5.2 Pharmacodynamics

5.3 Molecular Docking - Scoring and evaluation

BOOKS FOR STUDY

Claudio N. Cavasotto. *In Silico Drug Discovery and Design: Theory, Methods, Challenges, and Applications*. USA: Taylor & Francis Group, 2017

Charifson P S. *Practical Application of Computer Aided Drug Design*. New York: Dekker, 1997

BOOKS FOR REFERENCE

Andrew R. Leach. *Molecular Modeling: Principles and Applications*. USA: Prentice Hall, 2007.

Daan Frenkel and Berend Smit. *Understanding Molecular Simulation: From Algorithms to applications*. USA: Academic Press, 2002.

Alan Hinchliffe. *Molecular Modelling for Beginners*. USA: John Wiley & Sons, 2008

Luca Monticelli, Emppu Salonen. *Biomolecular Simulations: Methods and Protocols.* USA: Humana Press, 2016**.**

JOURNALS
Journal of Molecular Graphics and Modelling
Journal of Computer-Aided Molecular Design
Current Computer Aided-Drug Design

WEB SOURCES

http://accessengineeringlibrary.com/browse/computer-aided-drug-design-and-delivery
systems
http://www.southernresearch.org/life-sciences/lead-discovery-and-optimization/medicinal-chemistry/computational-chemistry
http://www.ch.ic.ac.uk/local/organic/mod/

STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600 086
M.Sc. DEGREE: BIOINFORMATICS

SYLLABUS
(Effective from the academic year 2019 -2020)

COMPUTER AIDED DRUG DESIGN

CODE: 19BI/PE/CD23   **CREDITS : 3**
                                                         L T P : 3 0 0
                                    TOTAL TEACHING HOURS : 39

OBJECTIVES OF THE COURSE
- To understand the general pathway for drug discovery and development
- To define new methodologies for analysis of ligands with their bound protein target
- To gain an in-depth overview of methods and techniques applied in computer assisted drug design (CADD)
- To learn about computer-aided drug design, safety evaluation, bioavailability and clinical trials

COURSE LEARNING OUTCOMES
On Successful completion of the course, the student will be able to

- Identify the key elements in drug and explain new methodologies for drug design
- Describe the role and importance of the various disciplines involved in the different phases of drug discovery and development
- Review and evaluate preclinical and clinical pharmaceutical studies
- Follow new ideas in utilizing main approaches of ligand screening methods

Unit   1   **(7 Hours)**
        Drug Discovery and Development
   1.7   Drug Development Process Overview - The Changing Landscape of drugs development
   1.8   Drug Discovery Phases
   1.9   Preclinical Phase studies

Unit   2   **(8 Hours)**
       Regulations in Drug Discovery
       2.4 FDA regulations on Drug Development
       2.5 Indian Regulatory Systems
       2.6 Ethical Considerations and Special Populations

Unit   3   **(8 Hours)**
       Drug Target Identification
       3.4 Computational inferences used to identify and validate small molecule drug
          targets
       3.5 Databases for Drug targets, Retrieving protein structure and visualisation
       3.6 Target Discovery and Validation, Active Site Prediction

Unit   4   **(8 Hours)**
       Ligand Based Drug Design
4.4 Screening of lead molecules - Natural products and their analogues
4.5 Chemical Databases – PubChem, Drug Bank
4.6 Chemical file formats, Retrieving drug molecules

Unit   5   **(8 Hours)**
       Pharmacokinetics and Molecular Docking
       5.4 Pharmacokinetics - ADME Prediction
       5.5 Pharmacodynamics
       5.6 Molecular Docking - Scoring and evaluation

BOOKS FOR STUDY

Claudio N. Cavasotto. *In Silico Drug Discovery and Design: Theory, Methods, Challenges, and Applications*. USA: Taylor & Francis Group, 2017

Charifson P S. *Practical Application of Computer Aided Drug Design*. New York: Dekker, 1997

BOOKS FOR REFERENCE

Andrew R. Leach. *Molecular Modeling: Principles and Applications*. USA: Prentice Hall, 2007.

Daan Frenkel and Berend Smit. *Understanding Molecular Simulation: From Algorithms to applications*. USA: Academic Press, 2002.

Alan Hinchliffe. *Molecular Modelling for Beginners*. USA: John Wiley & Sons, 2008

Luca Monticelli, Emppu Salonen. *Biomolecular Simulations: Methods and Protocols*. USA: Humana Press, 2016**.**

JOURNALS
Journal of Molecular Graphics and Modelling
Journal of Computer-Aided Molecular Design
Current Computer Aided-Drug Design

WEB SOURCES

http://accessengineeringlibrary.com/browse/computer-aided-drug-design-and-delivery systems

http://www.southernresearch.org/life-sciences/lead-discovery-and-optimization/medicinal-chemistry/computational-chemistry

http://www.ch.ic.ac.uk/local/organic/mod/

PATTERN OF ASSESSMENT

Continuous Assessment Test: **Total Marks: 50**   **Duration: 90 minutes**
Section A – 10 x 1 = 10 Marks (All questions to be answered)
Section B – 2 x 10 = 20 Marks (2 out of 4 to be answered)
Section C – 1x 20 = 20 Marks (1 out of 2 to be answered)

Other Components: **Total Marks: 50**
Assignment/Test/Seminars

End Semester Examination: **Total Marks: 100**   **Duration: 3 Hours**
Section A – 20 x   1 = 20 Marks (All questions to be answered)
Section B –   4 x 10 = 40 Marks (4 out of 7 to be answered)
Section C –   2 x 20 = 40 Marks (2 out of 4 to be answered)