M. Tech. Bioinformatics (Evening)
(with effect from July 2018)

2nd Year **4th Semester**

S.No.	Course Category	Subject Code	Subject	Periods and Credits				Evaluation Scheme				Subject Total
								Sessional (CA)			ESE	
				L	T	P	C	CT	TA	Total		
1	ESA	CS-513	Database Management System	3	1	0	4	25	15	40	60	100
2	DC	BEE-620	Computer Aided Drug Design	3	1	0	4	25	15	40	60	100
3	DC	BEE-625	Computer Aided Drug Design Lab	0	0	4	2	30	30	60	40	100
Total				**6**	**2**	**4**	**10**	**80**	**60**	**140**	**160**	**300**
* A zero-credit foundation course. Candidate has to pass this course by securing at least 50% marks.												

L: Lecture **T**: Tutorial **P**: Practical **C**: Credit **CA**: Continuous Assessment
CT: Class Test **TA**: Teacher's Assessment **ESE**: End Semester Examination
DC: Departmental Core **DE**: Departmental Elective

DATABASE MANAGEMENT SYSYTEM
CS-513

Pre-requisite	Co-requisite	L	T	P	C
None	None	3	1	0	4

Objective: The objective of the course is learning and understanding the concept of database and its management. The application of the course also focuses on database development technologies and data warehousing.

UNIT I	DBMS: Introduction - concepts and overview - Types DBMS- Relational and transactional Database, Database planning and Design concepts: General Database Planning and Design – Documentor forms - preparation and architecture. Entity-Relational ship Model- entities, Attributes, keys, tables design, relationships, roles and dependencies. Advanced E-R model. - concepts.	**8**
UNIT II	Relational DB: Introduction to relational DB and transactions. SQL-statements-Data Definition-Manipulation-control-Objects, - Views, sequences and Synonyms. Working with code and forms- Frontend development-query sublanguage-modifying relations in SQL.	**8**
UNIT III	Internals of RDBMS: Physical data structures, query optimization. Join algorithmstatisca andcost base optimization. Transaction processing. Concurrency control and recovery management. Transaction model properities, state serializability, lock base protocols, two phase locking.	**8**
UNIT IV	Database technologies: JDBC, ODBC standard and CORBA - extended entity relationshipmodel, object data model UML diagram. File organizations and data structures. Distributed databaseenvironment and its overview. Different databases and internet. Use of XML.	**8**
UNIT V	Datawarehouse: Descriptive Data Summarization, Data Cleaning, Data Integration and Transformation, Data Reduction, Data Discretization and Concept Hierarchy Generation, Data Warehouse and OLAP technology - A Multidimensional Data Model - From Data Warehousing to Data Mining - Efficient Methods for Data Cube Computation - Further Development of Data Cube and OLAP Technology.	**8**

References:

1. Abraham Silberschatz, Henry F. Korth and S. Sudhashan, Database system concepts. McGraw Hill Publications.
2. Elmasri Ramez and Novathe Shamkant, “Fundamentals of Database systems”, Benjamin cummings Publishing Company. ISBN-10: 0321369572.
3. P. Ramakrishnan Rao: Database Management system, McGraw Hill Publications. 9780071230575
4. Jim Gray and A. Reuter “Transaction processing : Concepts and Techniques” Morgan Kaufmann Press. ISBN-10: 1558601902.
5. V.K .Jain. Database Management system. Dreamtech Press ISBN 8177222279.
6. Date C.J. “Introduction to database management” Wesley.
7. Ullman, JD “Principles of Database systems” Galgottia publication.
8. James Martin Principles of Database Management systems” PHI.

COMPUTER AIDED DRUG DESIGN
BEE-620

Pre-requisite	Co-requisite	L	T	P	C
None	None	3	1	0	4

Objective: The objective of the course is learning and understanding the entire picture of the latest developments in the field of Drug Designing. The application of the course focuses on recent insilico structure and ligand based approaches to modern day drug design.

UNIT I	**Stages of Drug Designing**	**8**
	Drug Discovery Pipeline: Strategies to identify possible drug targets, Validation and Druggability of targets, Discovery of Lead compounds, Optimization of Lead compounds to Candidate drugs, Clinical Trials and its applications.	
UNIT II	**Drug Targets**	**8**
	Potential Drug Targets: Family of G-Protein Coupled receptors (GPCRs), Ion Channels: Molecular structure and significance; Aquaporins as Drug Targets, DNA as anti-cancer targets.	
UNIT III	**Direct Drug Design**	**8**
	Structure based Drug Design: Molecular Docking-principles and concepts, Representation of molecules, Searching and Scoring of potential solutions, Special aspects of docking: protein flexibility and water molecules. Common Docking programs: AUTODOCK, GOLD.	
UNIT IV	**Indirect Drug Design**	**8**
	Ligand based Drug Design: Quantitative Structure Activity Relationship (QSAR) – principles and concepts, Statistical Methods used in QSAR analyses, Pharmacophore Modeling: Criteria for satisfactory pharmacophore model, Basics of Hip Hop and Hypogen Model, Applications of pharamacophore model.	
UNIT V	**Drug Pharmacokinetics**	**8**
	Pharmacokinetic analyses of Drugs: Quantitative Structure Property Relationship (QSPR) studies –important parameters and significance, ADME- TOX studies, Concept of Drug-likeliness and its applicability.	

References Books:

1. Harren Jhoti, Andrew R. Leach; Structure- based Drug Discovery, Springer, 2007, ISBN 1402044070

2. Andrew Leach; Molecular Modelling: Principles and Applications (2nd Edition), Prentice Hall, 2001, ISBN 13: 9780582382107
3. R E Hubbard; Structure-based Drug Discovery: An Overview, Royal Society of Chemistry, 2006
4. Barry A. Bunin, Brian Siesel, Guillermo Morales, Jurgen Bajorath; Chemoinformatics: Theory, Practice, & Products, Springer Science & Business Media, 2006.

Research Publications:

1. Zhang W, Pei J, Lai L. Computational Multitarget Drug Design, J ChemInf Model, 2017. doi: 10.1021/acs.jcim.6b00491
2. Leelananda SP, Lindert S. Beilstein. Computational methods in drug discovery, J Org Chem,. 2016 Volume 12. Pg- 2694-2718.

Websites:

1. simulation software: www.schrodinger.com
   Online document/video/audio

2. Jenny Viklund & Fredrik Rahm (Sprint Bioscience): Marvin Live for structure-based drug design: Chem axon:
   https://www.youtube.com/watch?v=5gzxQC_mMX0
2. Webinar recording: a sequel for beginners: ligand-based drug design — the basics
   https://www.youtube.com/watch?v=ef5EaooBYUU

COMPUTER AIDED DRUG DESIGN LAB
BEE-625

Pre-requisite	Co-requisite	L	T	P	C
None	None	0	0	4	2

Objective: To obtain hands-on-training on the different tools for computer-aided drug design

List of Experiments	
	1. To retrieve the protein structures form PDB and perform its energy minimization studies by applying suitable force fields. 2. To visualize and comment on the active sites of the retrieved protein structures using Accelrys Discovery studio visualizer. 3. To identify the ligand binding sites in the protein molecules using Q-site Finder. 4. To retrieve the chemical compounds from the PubChem database in the sdf format and convert it into suitable pdb, asn and mol format using Open Babel. 5. To perform the protein-ligand docking experiments using AutoDock Tools and draw out important inferences. 6. To perform the protein-protein docking experiments using Z-DOCK server and draw out important inferences. 7. To check the Drug-Likeliness properties of the given chemical compound using Lipinski's Rule of Five. **8.** To carry out the *in silico* toxicity studies of the given chemical compound and draw out the important inferences.

References Books:

1. Andrew Leach; Molecular Modelling: Principles and Applications (2nd Edition), Prentice Hall, 2001, ISBN 13: 9780582382107.
2. Barry A Bunin, Brian Siesel, Guillermo Morales, Jurgen Bajorath; Chemoinformatics: Theory, Practice, & Products, Springer Science & Business Media, 2006.
3. Wolff, M E Ed.; Burger's Medicinal Chemistry and Drug Discovery, John Wiley and Sons, 2010, New York.
4. H. Fenniri; Combinatorial Chemistry–A practical Approach, Oxford University Press, 2000, UK.
   a. D. Frenkel, B. Smit; Understanding Molecular Simulation: From Algorithms to Applications, Elsevier 2012.
   b. Stephen Misener, Stephen A. Krawetz . Bioinformatics Methods and Protocols, Humana Press, 1999, ISBN 978-0-89603-732-8.4.

Online document/video/audio:

1. Computational chemistry in drug discovery. European Bioinformatics Institute - EMBL-EBIhttps://www.youtube.com/watch?v=9DESulCWbRQ
2. Andrew McCammon: Molecular Dynamics and Drug discovery, www.youtube.com/watch?v=ui1ZysMFcKk