20BT005 CHEMOINFORMATICS & PHARMACOGENOMICS

Hours Per Week :

L	T	P	C
3	-	3	5

Total Hours :

L	T	P
45	-	45

WA/RA	SSH/HSH	CS	SA	S	BS
-	-	-	-	-	-

Course Description and Objectives:

The objective of this course is to provide introduction to chemoinformatics and pharmacogenomics, an interdisciplinary area on the interface of chemistry, informatics, paharmacy and biology. The student will be provided with understanding of fundamentals of chemoinformatics and its applications.

Course Outcomes:

The student will be able to:

- Explain basic concepts of chemoinformatics.
- Explain and implement computation of molecular descriptors and chemical similarity.
- Classify small molecules and interpret results from chemoinformatics analysis.

SKILLS:

- ✓ *Acquire chemical data*
- ✓ *Analyze QSAR/QSPR models*
- ✓ *Analyze genomics datasets*

ACTIVITIES:

- Develop SMILES string for compounds.
- To construct QSAR models.
- To analyze genomic datasets.

UNIT - I

Introduction to the world of Chemical Informatics: Overview of the class; defining chemical informatics; chemical and bioinformatics; chemical informatics and the pharmaceutical industry; example applications

UNIT - II

Representing 2D Structures: Kinds of 2D structure representation; atom lookup and connection tables; graph theory; SMILES; SD files; Fragment codes & Fingerprints; descriptors

UNIT - III

2D Chemical Database Applications: Types of searching; substructure searching with SMARTS; similarity searching with fingerprints; demonstrations of searching systems

UNIT - IV

QSPR & QSAR: Feature selection, Model building, QSAR biological and physicochemical parameters, QSAR applications in drug design, QSAR model selection and validation, CoMFA

UNIT - V

Pharmacogenomics: introduction, variants and SNPs, personalized medicine, PK/PD in pharmacogenetics, clinical significance and practice, benefits and limitations

LABORATORY EXPERIMENTS

Laboratory Experiments Total hours: 30

1. To study & to analyze the information from the various chemical databases available on the World Wide Web
2. To obtain information about the given chemical compounds
3. To get the ways & results to perform the given queries
4. To calculate molecular properties using Osiris
5. To create a chemical database using UCSF Chimera
6. To create a chemical database using VEGAZZ
7. To convert, filter and manipulate chemical data using Open Babel
8. To explore bioinformatics tools for performing QSAR studies

TEXT BOOK:

1. Leach, Andrew R., and Valerie J. Gillet “An introduction to chemoinformatics”, 1st edition Springer, 2007".

REFERENCE BOOK:

1. Thomas Engel (2006). “Basic Overview of Chemoinformatics”, 1st edition J. Chem. Inf. Model. 46 (6): 2267–77.

2. Lee, Ming Ta Michael, and Teri E. Klein. “Pharmacogenetics of warfarin: challenges and opportunities.” Journal of human genetics 58, no. 6 (2013): 334-338.