BT 635 Chemo Informatics (3-0-0-6)

Prerequisites: Nil

Course Contents:

The Molecular Paradigm: Molecular objects and design objectives, Structure databases, Representation & manipulation of 2D and 3D molecular structures, Molecular descriptors. Similarity models, Virtual Screening.

Target identification & Protein optimization. Receptor-Ligand interaction, Molecular docking. Combinatorial chemistry and library design. Ligand based approaches to *insilico* pharmacology. Computational tools for drug discovery. Applications in Bio-molecular systems: Ligand based design of compound libraries on identified targets.

Texts:

1. A. R. Leach and V. Gillet, An Introduction to Chemo-informatics , st Edn., Springer, 2007
2. G. Schneider, and K. H. Baringhaus, Molecular Design: Concepts and Applications, 1st Edn., Wiley-VCH: Weinheim, New York, 2008.
3. J. L. Faulon and A. Bender, Handbook of Chemo-informatics Algorithms , 1st Edn., Chapman & Hall, 2010.
4. J. Bajorath, Chemoinformatics & Computational Chemical Biology , 1st Edn., Springer, 2011.
5. E. J. Corey, B. Czako and L. Kurti, Molecules & Medicine. 1 st Edn., Wiley 2007.