QSAR BASED DRUG DESIGN, DISCOVERY AND BASIC BIOINFORMATICS

COURSE OBJECTIVE (CO)

1. To understand the basic workflow of Quantitative Structure Activity Relationship (QSAR)

2. To understand the methodology of structure drawing, energy minimization, descriptor calculation

3. Know the hands on technology of docking, analysis of its results, interpretation of best docking conformer

4. Knowledge of 2D QSAR model equation, understand the relationship between biological activity and descriptors

5. Understand tools of basic bioinformatics

COURSE OUTCOME (CO)

At the end of the course, the student will be able to

1. Understand quantitative correlation between any set of medicinal compounds and their biological activities.

2. Construct chemical structures *in silico* and perform further processing on them

3. Perform, analyze and interpret manual docking working with protein and chemical structures of medicinal interest.

4. Create new QSAR model equations in the subset of medicinal compounds and biological activities

5. Utilize basic tools of bioinformatics to manipulate, engineer or design newer proteins; identify unknown receptors, delineate mutations and other parameters of active proteins of physiological systems.