Chapter-3

Plan of Work
The plan of work is divided into three steps:-

**STEP-1: 2D QSAR study of nitric oxide synthase inhibitors and interpretation of models to design potent new compounds.**

The development of 2D QSAR models towards the known lead structure in a rational way is done by calculating structural molecular descriptors and selection of important set of descriptors to develop higher levels of predictability. We will therefore apply it to the various series of reported compounds to predict the effective nitric oxide synthase inhibitors with high biological activity and low toxic effects. Various steps are involved in this process to get the new compounds as follows:

![Diagram](image)

**Fig. 3.1** Various steps involved in QSAR
STEP-2: Docking studies of the designed compounds obtained by using QSAR

In this step, we will perform the docking study on the predicted compounds obtained by Step-1. Docking is useful to check the binding affinity of the compound or drug with the receptor. Here, we will dock our predicted compounds with their respective NOS enzyme (iNOS or nNOS).

STEP-3: Synthesis and biological evaluation of the designed compound

In this step, we will synthesize the designed compound obtained by Step-1 and which shows the good drug-receptor interaction with the enzyme. Further, we will perform the biological evaluation of the synthesized compound.