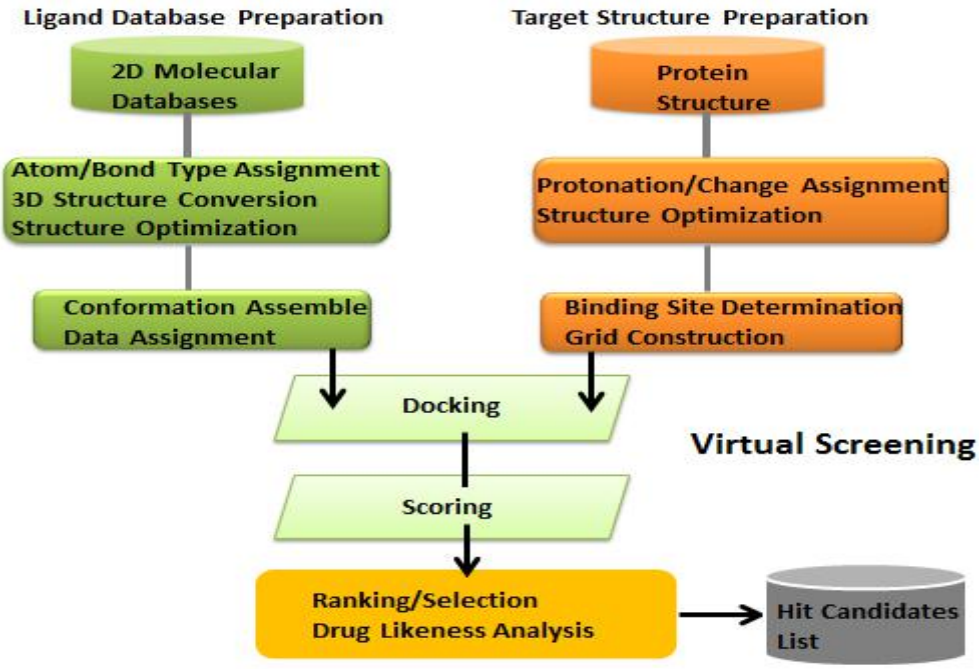
Virtual Screening

Research on the development of new drugs generally starts with target selection followed by hit identification, hit-to-lead confirmation, lead optimization and clinical candidate selection. Virtual screening has been widely applied in early-stage drug discovery. As an alternative or complementary approach to high-throughput screening (HTS) assays with high cost and low hit rate, virtual screening is an efficient computational method to identify drug candidates *in silico* from large chemical compound databases. Its usefulness has been verified by current applications that successfully retrieved hit and lead identifications against various disease targets.



Types of Virtual Screening in BOC Sciences

Virtual screening can be divided into two broad categories, namely structure-based virtual screening (SBVS) and ligand-based virtual screening (LBVS).

- SBVS utilizes the three-dimensional (3D) structure of the biological target (determined either experimentally through X-ray crystallography or NMR or computationally through homology modeling) to dock the candidate molecules and rank them based on their predicted binding affinity or complementarity to the binding site.

- LBVS on the other hand, strategies utilize structure-activity data from a set of known actives in order to identify candidate compounds for experimental evaluation. LBVS methods include approaches such as similarity and substructure searching, quantitative structure-activity relationships (QSAR), and pharmacophore- and three-dimensional shape matching.