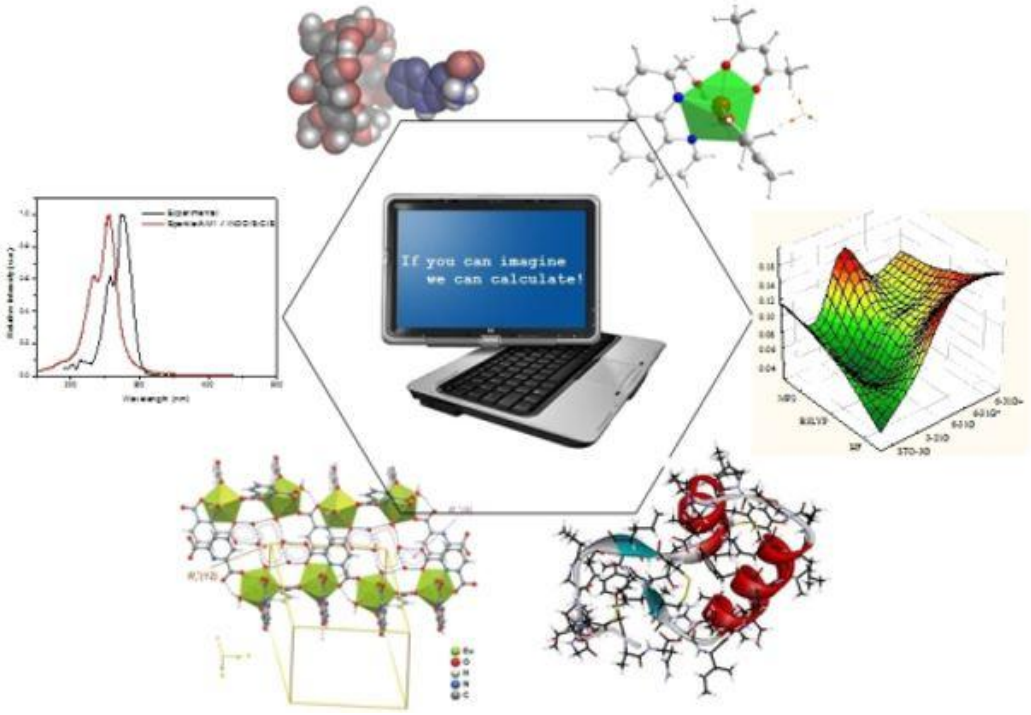
Computer-Aided Drug Discovery

Introduction

Computer-aided drug design (CADD) is a widely used technology using computational tools and resources for the storage, management, analysis and modeling of compounds. It relies on digital repositories for the study of designing compounds with physicochemical characteristics, predicting whether a given molecule will be combined with the target, and if so how strongly. Computer-based methods can help us to search new hits in drug discovery, screening many irrelevant compounds at the same time and study the structure-activity relationship of drug molecules.



The advantages of CADD

The traditional strategies for discovering new drug usually begin with taking a lead structure, and then develop a chemical program to find an analog molecule which can exhibit the desired biological properties. The process often involved a long cycle and a large number of experiments, in which medical chemist utilizing their experience and intuition to ultimately select a candidate for further development. The whole process is laborious, expensive and inelegant. Contrary to traditional drug design methods, CADD has been applied as a highly effective tool for systematic assessment of potential lead candidates before they are synthesized and tested. In this way, it saves time as well as cost in drug discovery.

BOC Sciences's Computer-Aided Drug Discovery (CADD) team can help you accelerate drug development and clinical development by designing novel compounds to provide research projects and develop advanced solutions for researchers around the world. Our team has a wealth of experience in informatics, virtual screening and molecular modeling to provide customers with a full range of computer-aided drug design support and services.