In Silico Drug Discovery using Natural Products

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ABSTRACT

During the past fifty years in the life sciences two revolutions, Natural Product Chemistry and Computational Chemistry, have enhanced the knowledge on which modern medical science and pharmaceutical discovery are based. One of the most important challenges in the research will be the development of new drug compounds. Mainly due to the lack of proper understanding of biological systems, several problems concerning many existing drugs are still present including side effects. The ability to predict the structures with better understanding is thus expected to lead to advances in modern drug discovery.

In this presentation, we intend to integrate advance computational techniques, named structure and ligand-based drug discovery, to accomplish the task of lead selection and optimization. The main objective is to create comprehensive and reliable in silico systems that will improve the process of drug discovery using natural product.

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