

## **Chapter 17 - Modeling cannabis and Catha edulis bioactives and derivatives: insights from computational and theoretical predictions**

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### **Abstract**

In silico drug design studies have been conducted over the years particularly in most parts of the developed world. They have opened up a wider opportunity to study millions of potential drug leads over a short period of time without necessarily going onto the wet lab bench and without costs associated with them. Today, these have spread even wider in areas that are resource-strained. With the backbone of artificial intelligence and machine learning, in silico studies have helped mankind to find potential solutions to many ailments without risking humans and animals in early studies. They generally focus on physicochemical properties of the compounds being studied and produce outcomes that are reliable to inform next scientific, social, and economic decisions. Cannabis, Khat, and other plant secondary metabolites have been studied in silico leading to the establishment of several drug banks and compound management databanks for use in subsequent wet lab studies. In silico studies present an open source of information in the buildup of backup drug series as well as almost immediate responses to emerging diseases and pandemics. The future of in silico design studies remains an open array of opportunities in drug discovery. With more investments in the science and technology of cannabis and khat products among others in all parts of the world, concerted efforts will make do with a lot of benefits for mankind.