

The use of herbal medicinal products and supplements has increased tremendously over the past three decades with not less than 80% of people worldwide relying on them for some part of primary health care. However, the pharmacological actions of most herbal medicines could not be understood, because they are extremely complex when compared to conventional drugs. One herb usually has several different activities, and many herbal medicines combine several herbs. Ten years ago the network pharmacology was proposed by updating the research paradigm from "one target, one drug" mode to a new "network target, multi-components" mode. Subsequently, a set of network pharmacology methods were created to prioritize disease-associated genes, to predict the target profiles and pharmacological actions of herbal compounds, to reveal drug-gene-disease co-module associations, to screen synergistic multi-compounds in a high-throughput manner, and to interpret the combinatorial rules and network regulation effects of herbal medicine. We have an in-house database that includes plants, chemicals information. We plan to compile these data using the above mentioned methods to get some results.

Additionally, In this project the students will employ various supervised machine learning methods such as Nearest Neighbor methods, Matrix factorization methods etc. to predict the drug target interaction. The students will develop a machine learning workflow in three stages.

(I) preprocessing input data of the drug and the target

(II) training the underlying model based on similarity methods

(III) using the predictive model to make predictions on the test dataset

In the end they can evaluate the machine learning models and learn which model performs better for a given dataset.