THE USAGE OF MOLECULAR DOCKING AS A PRE-LAB SCREENING TOOL FOR TESTING THE EFFECTIVENESS OF PHYTOCHEMICALS FROM PLANT EXTRACTS

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30 years
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1992-2022

Natural compounds especially phytochemicals and their potential medical benefits have intrigued scientists for a long time. However, the identification of beneficial plant extracts or single compounds is a complicated and time-consuming process as extensive studies are associated with it.

***An insilico* approach (Figure 1) is useful in shortening the screening time for appropriate plant extracts and their active compounds. By docking single compounds identified in the plant with target proteins of certain diseases, we can predict the action of these compounds on enzymes/receptors that are involved in inter- or intracellular pathways critical for the chosen disease. The docking approach can shorten the time and help to design specific studies.**

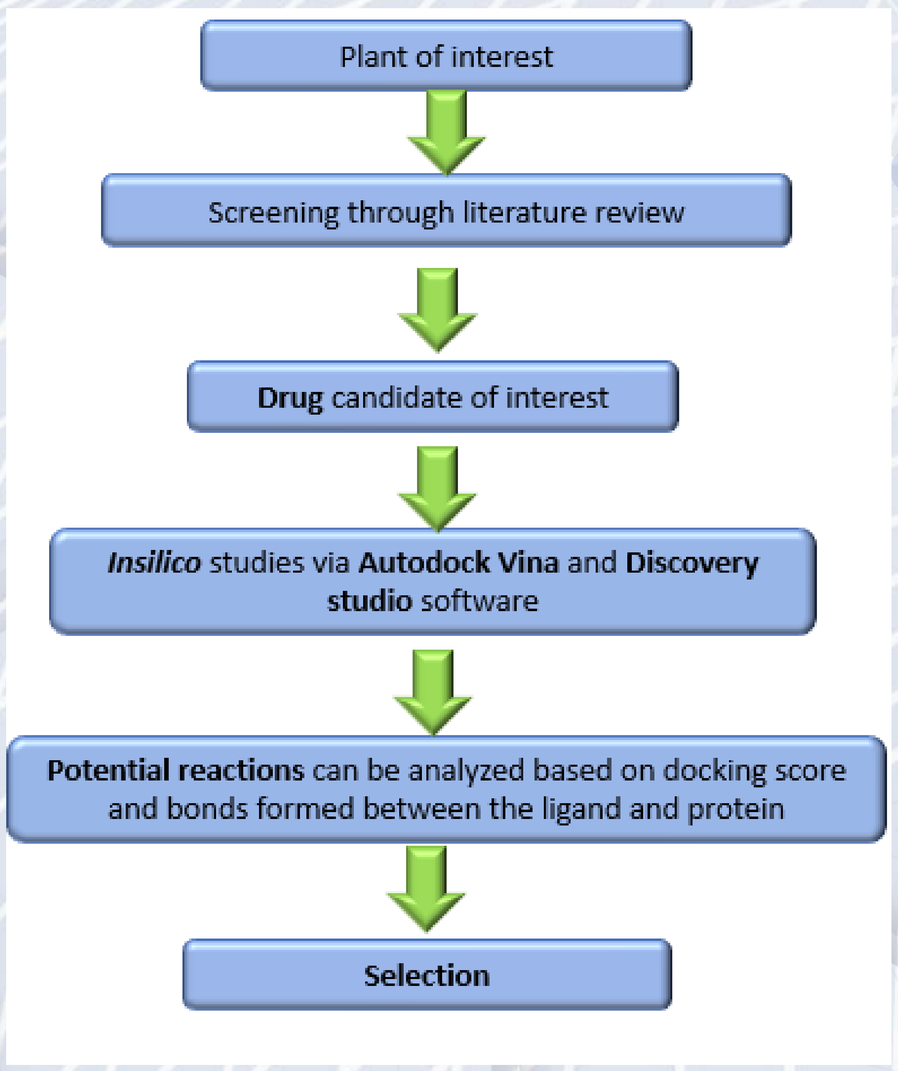

Figure 1 : Flowchart showing the *insilico* approach

Example: Through Autodock Vina and Discovery Studio as screening tools, phytochemicals identified in *Tinospora crispa* (*T.crispa*) and *T.cordifolia* were docked with advanced glycation end product receptor (RAGE) to observe their affinity towards the protein.

This project is funded by the TZC (FO5/TZC/1917/2019) and MOHE (FO5/FRGS/2033/2020)

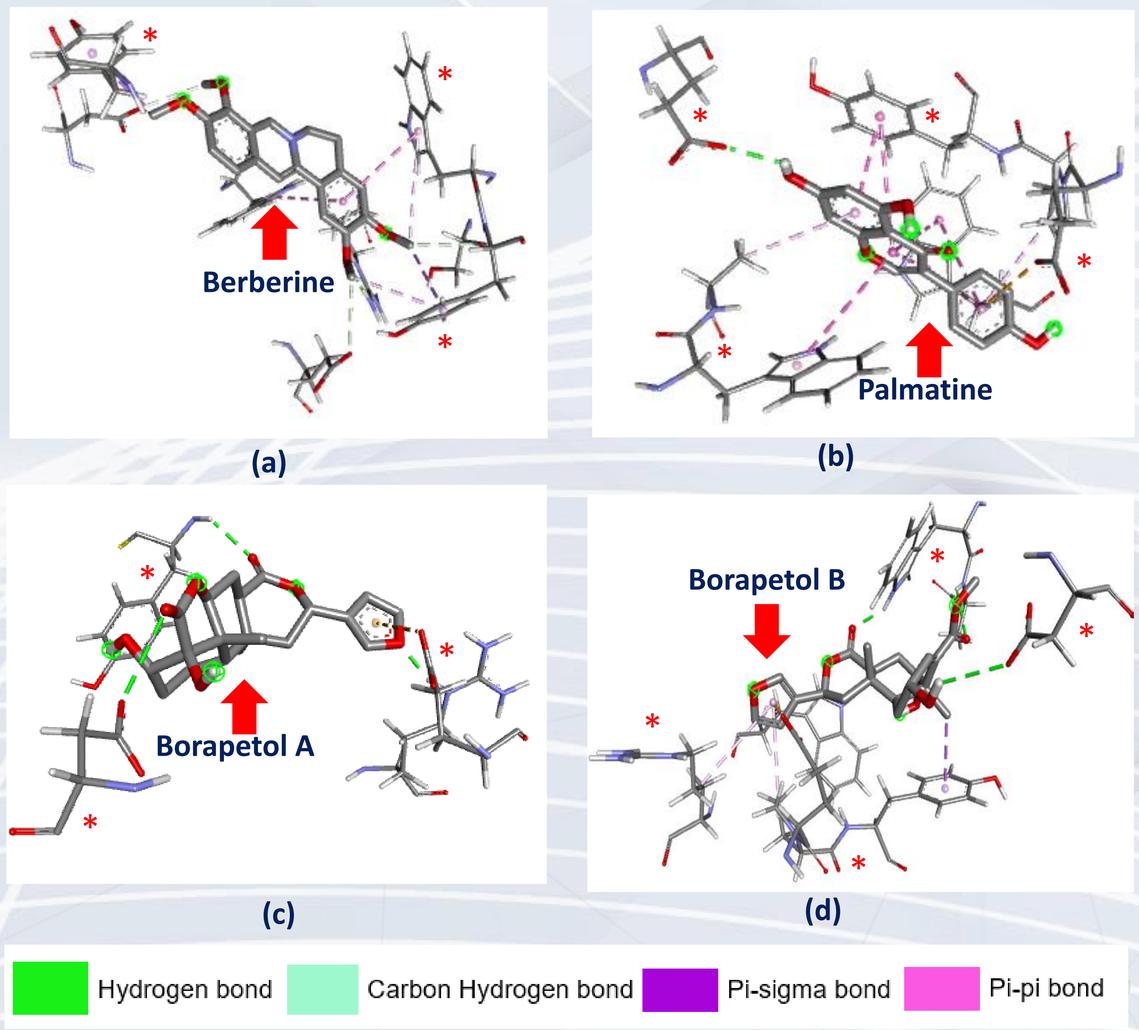

Figure 2: (a) Berberine docked with RAGE. (b) Palmatine docked with RAGE. (c) Borapetol A docked with RAGE. (d) Borapetol B docked with RAGE.
*** Amino acids of RAGE that bind to ligands.**

Table 1: Binding energy of ligands docked with RAGE

Ligands interacted with RAGE	Docking energy value (kcal/mol)	Binding energy*
Borapetol A	-10.7	Highest
Berberine	-8.6	High
Palmatine	-8.1	Average
Borapetol B	-8.0	Lowest

***When compared among the ligands**

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