Pharmacoinformatics-based investigation of bioactive compounds of Rasam (South Indian recipe) against human cancer

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ABSTRACT:

Background and Objectives: Spice-rich recipes are referred to as “functional foods" because they include a variety of bioactive chemicals that have health-promoting properties, in addition to their nutritional value. Using pharmacoinformatic-based analysis, we explored the relevance of bioactive chemicals found in *Rasam* (a South Indian cuisine) against oxidative stress-induced human malignancies.

Methods: The *Rasam* is composed of twelve main ingredients, each of which contains a variety of bioactive chemicals. Sixty-six bioactive compounds were found from these ingredients, and their structures were downloaded from Pubchem. To find the right target via graph theoretical analysis (mitogen-activated protein kinase 6 (MAPK6)) and decipher their signaling route, a network was built. Sixty-six bioactive compounds were used in the silico molecular docking study against MAPK6 and compared with the known MAPK6 inhibitor drug (PD-173955).

Results: The top four compounds were chosen for further study based on their docking scores and binding energies. In silico analysis predicted ADMET and physicochemical properties of the selected compounds and were used to assess their drug-likeness. Molecular dynamics (MD) simulation modelling methodology was also used to analyze the effectiveness and safety profile of selected bioactive chemicals based on the docking score, as well as to assess the stability of the MAPK6-ligand complex. Surprisingly, the discovered docking scores against MAPK6 revealed that the selected bioactive chemicals exhibit varying binding ability ranges between −3.5 and −10.6 kcal mol^{-1}. MD simulation validated the stability of four chemicals at the MAPK6 binding pockets, including Assafoetidinol A (ASA), Naringin (NAR), Rutin (RUT), and Tomatine (TOM).

Conclusion: According to the results obtained, fifty of the sixty-six compounds showed higher binding energy (−6.1 to −10.6 kcal mol^{-1}), and four of these compounds may be used as lead compounds to protect cells against oxidative stress induced human malignancies.