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A REVIEW ON ANALYSING AYURVEDIC MEDICINES THROUGH MOLECULAR DOCKING -THE NEED OF THE HOUR

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ABSTRACT

Ayurveda describes about numerous formulations with multidimensional therapeutic action across various systems of human body. There is a growing relevance of molecular docking when it comes to validating and analysing Ayurvedic drugs through modern scientific methods. Due to complexity of the drugs, mechanisms underlying the broad spectrum effects are difficult to be explored using conventional biomedical parameters. Currently, reverse pharmacology is commonly adopted to scientifically evaluate the action of Ayurvedic formulations. Molecular docking is one such in-silico drug discovery technique which helps in identifying and predicting therapeutic potential of the drug/ formulation. The present review analysed twelve recent scientific research conducted and published in indexed journals related to molecular docking in Ayurveda. An attempt is made to elaborate the application of molecular docking ranging from studies on hormonal modulation, diabetic retinopathy, COVID 19, Nipah Virus, Alzheimer's disease, atherosclerosis, metabolic disorders etc. The review indicates that molecular docking can aid

in identifying bioactive constituents, thus supporting innovations in formulation developments.

KEYWORDS: Ayurveda, Rasashastra, Molecular Docking.

INTRODUCTION

Ayurveda is the science of life which has gifted us with numerous formulations for countless disorders of human body. Most of the *Rasaushadi* and *Kashtaushadhi* mentioned under various contexts in *Rasashastra* and *Ayurvedic* classics have multidimensional action. It is observed that in many formulations, the list of indication mentioned in the classical reference covers multiple system disorders, the mode of action of which is difficult to explain using modern parameters.

The concept of drug discovery is concerned with development of medications which can be efficacious against a particular disease-causing factor. It includes various steps ranging from target discovery, Hit generation to Post approval surveillance. In case of *Ayurveda*, Reverse pharmacology approach is preferably adopted since we have classical references enumerating the list of indications of each formulation. Ayurvedic Drug Research has shifted towards validation of the actions mentioned and its application in current health scenario using various scientific tools available.

Molecular docking is an in-silico method useful in drug discovery which includes a recognition process for identifying potential target proteins using certain software. The result obtained can be further used to validate the in-vitro and in-vivo studies of the drug.

METHODOLOGY

A review was conducted based on scientific publications in Indexed journals of *Ayurveda* related to molecular docking in Ayurveda. 196 articles published in last five years were enlisted by Pubmed related to Molecular docking in *Ayurveda* out of which 12 scientific articles were considered for current review.

RESULT

The current analysis is based on 12 scientific articles published in pubmed during the last five years examining the therapeutic benefits of various herbs, active principles and compound formulations mentioned in classical references for a range of diseases mentioned:

1. Shatavari phytoconstituents: It was concluded that it has potential effects for hormone modulation through molecular interactions with female hormonal receptors.[1]
2. Diabetic Retinopathy: Molecular docking was used to find out whether active constituents from Solanum xanthocarpum and Plumbago zeylanica could modify pathways linked to diabetic retinopathy.[2]
3. Sesbania grandiflora for Liver Health: Hepatoprotective and cytoprotective activity was assessed using Flavonoid interactions with PPARα and using in- vitro, in-vivo models.[3]
4. AYUSH-64 against Omicron: Strong binding and therapeutic potential against primary SARS-CoV-2 protease and spike protein was exhibited by AYUSH-64 phytochemicals.[4]
5. Nipah Virus treatment: Based on molecular docking and dynamics simulations, the study proposed potential Ayurvedic alternatives with strong binding affinity to NiV proteins.[5]
6. MAPK1 in Alzheimer's: Study identified potential inhibitors of MAPK1 to develop new treatment for Alzheimer's disease.[6]
7. Atherosclerosis Treatment: A polyherbal formulation showing strong anti-oxidant activity and safety in cell-based assays was evaluated.[7]
8. Oroxylum indicum against Epstein-Barr Virus: Oroxylum indicum was evaluated for dual targeting potential for treating both Epstein-Barr virus and Naso-pharyngeal carcinoma.[8]
9. Clerodendrum glandulosum: Study evaluated antihyperglycemic and anti-oxidant properties of leaf extract of Clerodendrum glandulosum and its potential in managing diabetes.[9]
10. Cerebroside Sulfotransferase as a Drug Target: A 3D model of CST for substrate reduction therapy in metachromatic leukodystrophy.[10]
11. Pyrazole Derivatives for COVID-19: Antiviral candidates from pyrazole derivatives with strong binding affinity to SARS-CoV-2 main protease was identified.[11]
12. Herbal Phytoconstituents for Breast Cancer: New therapeutic approaches with herbal compounds to target breast cancer related genes was studied.[12]

DISCUSSION

Molecular docking can play a significant role in advancing Ayurvedic medicine by bridging traditional knowledge with modern scientific research. Most of the times, formulations explained in classical references indicates that one particular formulation can be used in various disorders affecting various system. The mechanism of this multidimensional action of herbs or compound formulations can be understood by using molecular docking.

Molecular docking aids in validating ayurvedic herbs and formulations thus playing a role in formulation development. It helps in identification of bioactive compounds which can help in drug discovery. The steps in molecular docking are briefed in Fig1. It can be used as a tool for developing personalized medicine based on the concept of Prakruti. Molecular docking can be a potential tool when it comes to combination therapies. Thus, it can be used to understand whether a particular active principle or a compound drug will possess key binding molecules with binding affinity for treating diseases.

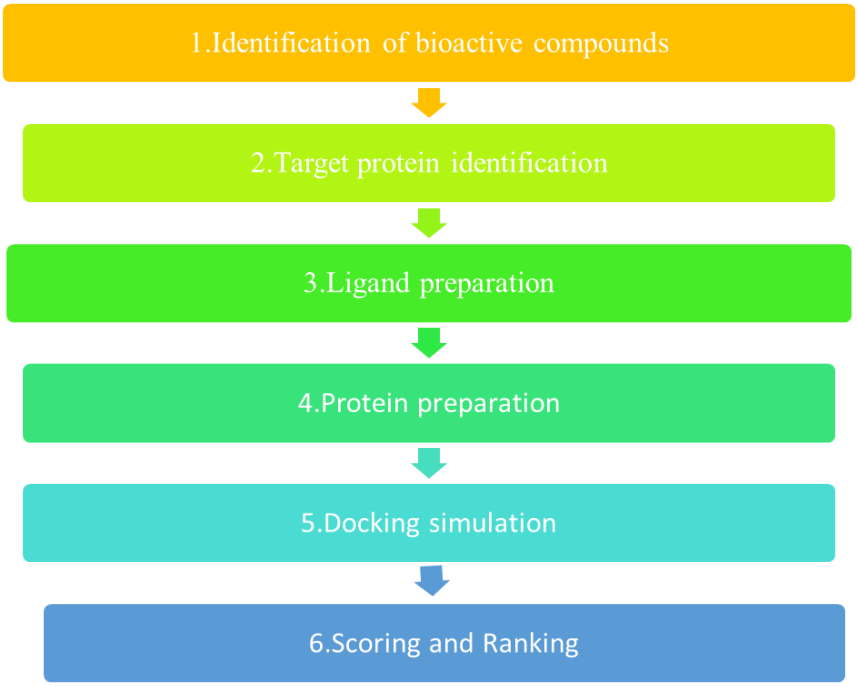

Fig 1: FLOW CHART DEPICTING STEPS IN MOLECULAR DOCKING.

CONCLUSION

The review implies that molecular docking can be useful for drug discovery in Ayurveda especially in evaluating the spectrum of indications mentioned in classical formulations.

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