

DRUG DISCOVERY, DESIGNING CHEMISTRY AND PHARMACEUTICAL ANALYSIS &

BIOBETTERS AND REGULATORY AFFAIRS

June 27-28, 2018 | Vancouver, Canada

Systems pharmacology and computer-aided analysis of chamomile for predicting potential advantages and adverse effects

Amir Zarrinhaghighi and Bahareh Moazen
Shiraz University of Medical Sciences, Iran

Chamomile is the common name of daisy-like plants of the family Asteraceae. *Matricaria chamomilla* L. is the most common type of this plant. Chamomile is used in traditional medicine in different countries such as Traditional Chinese Medicine (TCM) and Traditional Iranian Medicine (TIM). Chamomile has many benefits in different medical conditions such as: fever, inflammation, muscle spasm, menstrual disorders, insomnia, ulcer, wounds, gastrointestinal disorders, rheumatic pain, hemorrhoid and etc. But further researches is necessary for the confirmation of them and many researches are planned for this purpose. Chamomile contains a wide range of compounds, and to identify their advantages it's crucial to investigate more. Although multiplicity of this compounds makes the research difficult, Virtual screening and computational methods help us make it easier. Furthermore, network analysis and systems pharmacology are powerful tools for this reason. So the present study was undertaken to identify properties of chamomile and possible toxic features of this plant. In this research known compounds of chamomile were collected from Dr. Duke's Phytochemical and Ethnobotanical Databases (<https://phytochem.nal.usda.gov>). After that ADME/tox and QSAR properties of compounds were analyzed by Schrodinger (Maestro) package. Other possible pharmacologic properties were predicted by systems pharmacology approach by Cytoscape and available networks from Reactome database (<https://www.reactome.org>) based on QSAR data. Totally 152 compounds were collected from Dr. Duke database for Chamomile. Analysis of compounds show what potential usage and possible adverse effects chamomile could have by molecular and systems pharmacological approach. This study introduces a new method for having a better sight in experimental studies and helps us to walk on the right path for clinical trials on medicinal plants.

Biography

Amir Zarrinhaghighi received his PharmD in Pharmacy from Shiraz University of Medical Sciences (Shiraz, Iran) in 2016. He served as community pharmacist since 2014 in Shiraz. Also he is active in systems pharmacology and immunoinformatics. Amir was one of the co-founders of KAPA (student group for promoting creativity in high school students) and Pharmaceutical Strategic Studies Office. He was the scientific manager in 19th Iranian Pharmaceutical Students Seminar in Shiraz. He was chosen as the best poster presentation for 3 times in 17th, 18th, and 19th Iranian Pharmaceutical Students Seminar.

zarrinhaghighi.a@gmail.com

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