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Molecular Mechanism of Ferula Asafoetida for the Treatment of Asthma: Network Pharmacology and Molecular Docking Approach

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Abstract

Asthma is a significant health-care burden that has great impact on the quality of life of patients and their families. The limited amount of previously reported data and complicated pathophysiology of asthma make it a difficult to treat and significant economic burden on public healthcare systems. Ferula asafoetida is an herbaceous, monoecious, perennial plant of the Umbelliferae family. In Asia, F. asafoetida is used to treat a range of diseases and disorders, including asthma. Several in vitro studies demonstrated the therapeutic efficacy of F. asafoetida against asthma. Nevertheless, the precise molecular mechanism is yet to be discovered. In the framework of current study, network pharmacology approach was used to identify the bioactive compounds of F. asafoetida in order to better understand its molecular mechanism for the treatment of asthma. In present work, we explored a compound-target-pathway network and discovered that assafoetidin, cynaroside, farnesiferol-B, farnesiferol-C, galbanic-acid, and luteolin significantly influenced the development of asthma by targeting MAPK3, AKT1 and TNF genes. Later, docking analysis revealed that active constituents of F. asafoetida bind stably with three target proteins and function as asthma repressor by regulating the expression of MAPK3, AKT1 and TNF genes. Thus, integration of network pharmacology with molecular docking revealed that F. asafoetida prevent asthma by modulating asthma-related signaling pathways. This study lays the basis for establishing the efficacy of multi-component, multi-target compound formulae, as well as investigating new therapeutic targets for asthma.

Keywords: Ferula asafoetida; Asthma; Network pharmacology; Molecular docking

Introduction

Asthma refers to a common respiratory disease with high morbidity and mortality. Asthma has affected more than 300 million individuals around the globe which makes it the most common respiratory disease. Asthma is a chronic inflammatory disease of the airways that causes wheezing and other symptoms like coughing, dyspnea, and chest tightness, as well as fluctuating expiratory airway blockage [1]. Asthma has become a noteworthy health issue due to its increasing morbidity rate throughout the past few years globally due to environmental and lifestyle changes. Currently, inhaled corticosteroids (ICS) are the effective for the long-term asthma treatment and the addition of long-acting β2-agonists further help in controlling asthma. Long-term exposure of ICS may lead to adverse effects on the patient's health. In Pakistan respiratory diseases such as asthma is common because of severe environmental conditions and limited access of population to medical facilities. People usually rely on herbal medicine to cure respiratory diseases and it is also practiced around the globe. Pakistan produces a variety of medicinal plants with over 6000 species in account of its diverse climate conditions. Multiple studies demonstrated that few distinct natural components and herbs can express anti-inflammatory properties. Being an emerging area of pharmacology, "network pharmacology" is considered a new approach to drug designing [2]. To date, this technique has been successful in elucidating the multi-target effects of medicinal plants for curing enormous types of diseases and disorders. The traditional medicine is one of the safest medicines demonstrated by extensive studies [3]. Network pharmacology, a systematic biology approach has revolutionized the interaction studies between active herbal ingredients and potential targets of disease. It provides feasible and reliable ways to explore potential molecular mechanisms and key targets. The concept of network pharmacology relies on the concept of "network target, multicomponent therapeutics", which shifts the paradigm away from the concept of one gene, one target, and one disease [4].

The compounds of F. asafoetida and the putative mechanism behind its anti-asthmatic activity were investigated utilizing network pharmacology integrating with molecular docking in the current study. According our understanding this is the leading study to classify the underlying mechanism of F. asafoetida for asthma treatment using bioinformatics and network pharmacology [5].

Methodology

Active compounds in F. Asafoetida

Information related to active compound of F. asafoetida was retrieved from literature and publically available databases. F. asafoetida related compounds were collected from phytochemical based databases, including traditional Chinese medicines integrated database (TCMSP) KNApSAcK-3D, and Dr. Duke's Phytochemical and Ethnobotanical Database [6]. The keyword "F. asafoetida" was used in the databases, while literature mining was conducted on PubMed, and Google Scholar. All of the predicted F. asafoetida constituents were virtually screened based on oral bioavailability (OB) and drug likeness (DL). Only those compounds were preferred for subsequent analysis which met the precise standards of DL ≥ 0.18 and OB ≥ 30 %. Regarding this, Admet SAR2.0 and Molsoft were used to compute the OB and DL of all active constituents, respectively. Meanwhile, PubChem and ChemSpider were used to collect chemical information of predicted

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compounds such as CID number, structure, and molecular weight [7].

Target prediction

Prediction of target genes is an initial stage to reveal the molecular interaction of therapeutic plants for treatment of various types of diseases and disorders. Based on simplified molecular-input line-entry system (SMILES), targeted gene(s) of compounds were retrieved through Swiss Target Prediction and STITCH databases. In case of STITCH database, SMILES of each compound were inputted with the search restricted to "Homo sapiens". And accumulating the targets with a combined-score ≥ 0.7 On the other hand, the SMILES numbers of compounds were then uploaded into the Swiss Target Prediction online platform. As the predicted of target genes were performed on the basis of structural similarity using a reverse pharmacophore combination method consequently, targets with probability ≥ 0.7 was selected [8].

Prediction of target genes related to disease was performed using GeneCards and DisGeNET databases. Furthermore, these databases offer brief genomic data as well as functional annotations for well-studied human genes. All redundant genes were removed, and the common name of the target gene was obtained using UniProtKB function in UniProt with "Homo sapiens" as the organism. The final overlapping target genes between F. asafoetida and asthma-targeted genes were recognized and visualized by Venny [9].

Network construction

The protein–protein interactions (PPI) network of overlapped genes were obtained through STRING database, which offers experimental as well as predicted relationship information based on systematic co-expression approach, observation of shared selective signals across genomes, and automated scientific literature text mining[10]. In framework of current study, interactions having combined score ≥ 0.4 were selected for further analysis. Cytoscape 3.2.0 was then used to generate three types of networks to further analyze the multi-scale action mechanisms of F. asafoetida compound for treatment of asthma (1) network of compound-target, (2) Target-pathway network, and (3) compound-target-pathway network [11]. In network, nodes represented the compound, targets, and pathways while solid lines described the interaction between nodes. The degree that is a topological parameter reveals the significance of component/target/pathway in the network [12].

Discussion

Asthma is dreadful heterogeneous inflammatory disease of the human respiratory tract with increase morbidity rate throughout the world. The rate of asthmatic patient rise approximately 2.5 million each year. Asthma cannot be effectively treated in many cases, despite the enormous availability of drugs and therapeutic approaches. Moreover, 50 % of asthmatic patients have symptoms on regular basis; nearly all patients have difficulty in breathing and coughing. It is reported that, an oral anti-asthmatic medicine has a major side effect on a patient health. Moreover, the advancement of novel drug is often restricted due to the lack of absorption, distribution, metabolism, and excretion (ADME) properties, and these highly-priced natures imposes an additional trouble in the process of drug development. Therefore, ADME based screening has acquired more attention from scientists studying the drug discovery process. For this purpose, the use of network pharmacology can aid in the systematic and holistic evaluation by spotting key bioactive compounds and the potent targets from a large amount of data. Based on systems biology, high throughput screening and network pharmacology can help to discover promising candidate genes to control asthma. In order to analyze the interaction between body and drug based upon system biology, high throughput screening and network pharmacology to discover promising candidate genes to control asthma.

Conclusion

Network pharmacology was applied in the present study for identification of mechanism of the plant F. asafoetida for the treatment of asthma. Traditional herbal medicine aims to improve the patient whole-body balance by using herbal formula having suppressed side effects. Our findings suggested that these compounds (Cynaroside, Farnesiferol-B, Farnesiferol-C and Assafoetidin) can play a significant role to elucidate the mechanism of F. asafoetida for the treatment of asthma. Thus, network pharmacology has vast number of applications and serves as a promising approach for the future drug discovery process to diminish the incidence of asthma.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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