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Yun-Fei Chang, Yue Huang, Yi-Hua Ni, Cheng-Min-shui Department of Otolaryngology-Head and Neck Surgery, Children's Hospital of Fudan University, Shanghai, People's Republic of China These authors have made an equal contribution to this work Von: Geraniol is a cyclical monoterpene alcohol that is extracted from essential oils. A systematic analysis of its mechanism of action has not yet been carried out. Methods: In this study, geraniol drugs were evaluated using the Traditional Chinese Medicine Systems Pharmacology Database (TCMSP), and potential geranium targets were identified using the Comparative Toxicogenomics Database (CTD). In addition, the genetic ontology pathways (GO) and the Kyoto Encyclopedia of Genes and Genomes (KEGG) were analyzed using WebGestalt. Network drug-targeted pathways have been built using Cytoscape to give a visual representation. Results: Our findings showed that geranium has an excellent with 38 oasily identified target genes. GO, KEGG and network analysis showed that these targets were associated with cancer, inflammatory immunoreaction and other physiological processes. Conclusion: Geraniol is projected to target several proteins and pathways that form a network that can have a systematic pharmacological effect. Keywords: geranium, addiction, target prognosis, enrichment analysis, online pharmacology Introduction of natural products and traditional Chinese medicine (TCM) are the most common resources of active compounds for drug detection. Monoterpenes, for example, are food compounds extracted from the essential oils of many vegetables, fruits and especially TCM. Geraniol (Figure 1A) is an acyclic monoterpene alcohol that is found in the essential oils of aromatic plants.1 Geraniol, as has been shown to provide a wide range of pharmacological interventions such as anti-inflammatory, antimicrobial, antitumor, and so on.2-5 Close attention has been paid to geranium due to its potential role in the treatment of various diseases such as chronic or allergic, lung cancer, etc.6-8 These results suggest that geranium can be used as a valuable chemical probe or chemical promatology. , the discovery of hidden molecular relationships, as well as the identification of therapeutic molecules of purpose and pathways. Accordingly, the molecular mechanisms that geranium induces and the associated changes in cellular phenotypes are rarely studied. At the same time, the employment of computational methodologies to identify drug targets and core mechanisms is becoming mainstream in order to save money, time and effort.9.9.10 In particular, computational target identification and the following molecular mechanisms can speed up drug detection and drug development processes. Figure 1 (A) Chemical geraniol uploaded PubChem database (CID: 637566); (B) Working process to identify potential geraniol target genes that integrates ADME assessment, chemical gene interaction, GO and KEGG pathway analysis, and network building. Reductions: ADME, absorption, distribution, metabolism and allotment; GO, gene ontology; KEGG, Kyoto Encyclopedia of Genes and Genomes; CTD, Comparative Toxicomics Database. Therefore, we explained the pharmacological actions of geranium systematically using computational methodologies. First, the narcotic use of geranium was evaluated using the database server of the traditional Chinese medical systems (TCMSP) pharmacology database.11 Further in history, the target genes of a potential candidate were investigated by analyzing the interaction of chemical genes.12 In addition, gene ontology and pathway analysis were investigated using identified target genes. Finally, a drug-focused network has been established to ensure a systematic review of potential target genes and geranium mechanisms. The schematic diagram of analysis procedures for predicting the geraniol gene is shown in Figure 1B. Materials and methods assessing the properties of pharmacokinetics using the TCMSP database (is a resource of systemic pharmacology for TMC or related compounds.11 It can provide information on the properties of absorption, distribution, metabolism and secretion (ADME) of the drug with potential biological effects at a systematic level. for example, total bioavailability (OB), medicinal similarity (DL), permeability of Caco-2 (Caco-2), hemous heme barrier (BBB) and so on.13.14 Of all properties of pharmacokinetics, OB is the main feature of oral-managed drugs, as it acts as a vital role in assessing the effectiveness of the drug's distribution in system circulation. In the TCMSP database, OB was designed to OBioavail1.1 based on an internal model.11.13 For orally managed drugs, movement through the intestinal epithelial barrier is one of the biggest obstacles to human absorption and bioavailability.11.13 In this current study, the chemical name geranium was introduced into the field of search and its pharmacokinetic properties were investigated at the molecular level. Targeted identification by the Comparative Toxicomics Comparative Toxicogenomics (CTD, database is a reliable, publicly available database for toxicogenic information. It contains curated curated key information on the interactions of chemical genes/proteins, chemical diseases and gene diseases, from peer-reviewed scientific literature. CTD currently includes more than 30.5 million toxicogenic relationships related to chemicals, proteins and so on.12 Given the compound, CTD provide appropriate target genes sorted by interaction between them in descending order. Candidate goals of geraniol were predicted by the help of with default settings. GeneMANIA GeneMANIA analysis () is a convenient and flexible web server for generating hypotheses regarding gene function, analyzing gene lists, and prioritizing genes for functional analyses.15 Given the list of queries, GeneMANIA can list genes that have common properties, or function similarly to the original request. It also shows a functional network of relationships, outlining the link among the list, as well as curating genomics and data proteomics. Potential candidate genes were put into the search bar after selecting Homo sapiens from the body variant, and the results were additionally collected. Gene function and analysis of the enrichment pathways of web analysis of gene set tools (WebGestalt, can be used to thoroughly understand functional and ways of enriching information about the gene of interest.16 Potential targets of the candidate were to enter into the WebGestalt server using the method of excessive representation of the enrichment analysis with gene ontology (GO) and Kyoto Encyclopedia of Genes and Genomes (KEGG) databases. Go analysis is a widely used approach for annotating genes and gene products with features including molecular function, biological pathways and cellular components.17 KEGG is a useful resource for systematic analysis of gene functions and related high-level genomic functional information.18.19 Building a network In order to understand the complex relationships between compounds, goals and diseases, we used Cytoscape (v 3.6.1; to build and analyze tri-layer networks. The results of the Pharmacokinetics properties of geranium ADME describes the location of the pharmaceutical compound and TCMCP provides information on 12 very important characteristics on ADME related properties like Caco-2, Human OB, BBB, and Lipinski Rule of Five for drug screening and evaluation.11 AMDE-related geraniol properties have been thoroughly researched using TCMSP. It is noteworthy that OB geraniol was designed for 23.93%. The targets of geranium identification Potential geranium targets were predicted using CTD, as described in the Materials and Methods section.12 In total, 41 candidate targeted genes were identified by CTD. We then filtered out these genes using the threshold interaction of chemical genes ≥ 1 and removed non-human genes. Finally, there are 38 unique target genes for geranium (table 1). These 38 identified interacting genes were used for further research. Table 1 Targets analysis of geraniol GeneMANIA Among 38 targets and their interacting proteins, it was found that 37.05% had physical interactions, 20.16% had joint localization, and 19.43% displayed similar characteristics of co-expression. Other results, including pathways, common protein and genetic interactions, interactions, Shown in Figure 2. Figure 2 Protein network of geranium. Black nodes are target proteins, and connecting colors indicate different correlations. Functional links between targets have been explored using GeneMANIA. Genes in black circles were query terms, while the gray circle indicated genes associated with query genes. GO and path analysis For further study of the 38 identified target genes, GO and KEGG enrichment analyses were conducted using WebGestalt. As shown in Figure 3, seven upper functions were used as a response to stimulus (35/38), biological regulation (33/38), metabolic process (31/38), membrane (30/38), protein binding (30/38), multicellular body process (29/38), and cellular communication (28/38). These functional terms are important for anti-inflammatory interventions, especially for chronic or allergic rhinitis. Figure 3 GO map targets. (A) Biological Process Categories. (B) Cellular Component Categories. (C) Molecular function categories. As for path analysis, 38 targets are involved in 10 KEGG pathways with significant false detection rate (FDR)-adjusted P-cost, including apoptosis, cancer pathways, and so on, which were shown in Figure 4. Figure 4 KEGG is a way to analyze target-targeting genes. Network analysis, based on an analysis of targets and pathways, has built a whole set, targets and disease networks using Cytoscape (v 3.6.1). As shown in Figure 5, this compound, purpose and disease interaction network has 80 nodes and 129 edges. Red oblong, green inverted triangles and blue circles correspond to geraniol, target genes and paths, respectively. Figure 5 Geraniol-target the network path. Discussion of poor pharmacokinetics and toxicity are the most important reasons for costly delays in the discovery and development of drugs. There is, therefore, a growing belief that certain features in the drug discovery process should be prioritized.20 In silico analysis can improve prognosis and pharmacokinetic modeling, as well as metabolic and toxic endpoints; all of which speed up and simplify the drug detection process.9.10 Lipinski's Five Rule can identify some very important drug properties that should be taken into account by compounds developed for oral delivery.21 Rule of Five takes into account molecular weights (MWs) of 500 Da, LogP and 5, as well as the number of donors of hydrogen bonds and accepts less than 5 and 10, respectively. Today, Rule Five is generally referred to as the guiding principle for drug optimization.22 As shown in Table 2, the pharmacokinetic properties of geranium meet these requirements, meaning geranium is an excellent candidate for drug development. Table 2 Pharmacological and Molecular Properties of Geraniol(Abbreviation: Kako-2, Kako-2 Permeability; OB, oral bioavailability; DL, medicinal likeness; BBB, blood-brain-brain-brain When drugs are detected, identifying target genes is the first step. More and more active compounds or drugs are shown to interact with multiple genes or proteins.23-26 Different approaches for identifying the silico target have been developed and are widely applied to this goal. As calculated in Table 1, 38 potential geranium targets were identified using computational methods. GeneMANIA's results provided information on physical interactions, shared localization, joint expression, and common protein regions, implying that targets and their interacting proteins may have identical or similar functions. We have identified the inflammatory role of geranium in allergic rhinitis. Similarly, Madankumar et al. reported geranium renders antimicrobial, antioxidant, antitumor and anti-inflammatory effects through activation of apoptotic pathways.6.27 These results closely coincide with our findings from GO and KEGG analyses. The drug network shown in Figure 5 also showed that geranium had several purposes and further indicated that it had several pharmacological activities. Cho et al have also shown that geranium has a systematic pharmacological effect, focusing on multiple proteins and pathways.29 Multiple targeted therapeutic medications are more effective for treating complex diseases such as allergic rhinitis, cancer, and less vulnerable to adaptive resistance. Thus, geranium can be a promising resource that can be used as a chemical moiety, lead compound, or active ingredient for future drug discovery. To sum up, we would like to emphasize that geranium is an active ingredient or promising compound for the development of a safe and effective multi-purpose anti-cancer drug treatment. This study provides new insight into the perspectives and challenges for geranium research and its application in future clinical trials. Disclosure Authors do not report a conflict of interest in this work. Links 1.Lapczynski A, Bhatia SP, Foxenberg RJ, Letizia CS, Api AM. The aroma of the material is reviewed by geranium. Food chemistry toxics. 2008;46 (Suppl 11):S160-S170. doi:10.1016/j.fct.2008.06.048 2.Solerzano-Santos F, Miranda-Novales MG. Essential oils from aromatic herbs as antimicrobials. Kurr Opin Biotechnol. 2012;23(2):136-141. doi:10.1016/j.copbio.2011.08.005 3.Tiwari M, Kakkar. Plant-derived antioxidants-geraniol and camphen protect rats of alveolar macrophages against t-BHP-induced oxidative stress. 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