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Anti-obesity Mechanisms of Artemisiae Argyi Folium (Aiye) by the Integration of GC-MS, LC-MS, Network Pharmacology, and Molecular Docking

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ABSTRACT

Obesity has become a global epidemic with a significant influence on the health and well-being of humans. The side effects of anti-obesity medication and complications of surgery become a concern. Therefore, searching for natural anti-obesity compounds with fewer side effects from traditional medicinal plants has become an urge. *Artemisiae argyi* Folium (Aiye) is a widely used medicinal material in traditional Chinese medicine for treating different diseases. Some studies revealed the effects of Aiye on lipase activity inhibition, intestinal barrier protection, body weight control, and blood lipid regulation. However, little research is exploring its anti-obesity compounds and their molecular mechanisms. Therefore, the current study aims to identify Aiye's chemical profile and predict its anti-obesity mechanisms.

The GC-MS and LC-MS analysis, network pharmacology, and molecular docking were integrated to identify the anti-obesity mechanisms of volatile and non-volatile compounds extracted from Aiye. The targets of the identified compounds were collected from SwissTargetPrediction and the SEA database. The DisGeNET, DrugBank, GeneCards, and OMIM databases were used to collect obesity targets. The network analysis was conducted by STRING and Cytoscape. The Gene Ontology (GO) and Kyoto Encyclopedia of Genes and Genomes (KEGG) enrichment analyses of core targets were performed on Metascape. The molecular docking was conducted by Autodock Tools.

A total of 49 essential oils and 30 phenolics in Aiye were identified by GC-MS and LC-MS, respectively. The essential oils owned 308 anti-obesity targets, while the phenolics possessed 486 anti-obesity targets. Enrichment analysis revealed that the essential oils and phenolics may combat obesity through the Wnt signaling pathway, PI3K-Akt signaling pathway, MAPK signaling pathway, prolactin signaling pathway, cAMP signaling pathway, etc. Twenty essential oils and eight phenolics whose target numbers exceeded the mean value were selected for molecular docking. HIF1A, NFKB1, JUN, SRC, EGFR, PPARG, and ESR1 were the seven central targets of essential oils. HIF1A, AKT1, TNF, IL6, ESR1, STAT3, and BCL2 were the seven central targets of phenolics. For the 140 docking results between essential oils and central targets, the binding affinity of 99 results was below -5 kcal/mol, and 17 of them were further below -7 kcal/mol. Moreover, of the 56 phenolics-target docking results, 45 had a binding affinity lower than -5 kcal/mol, and 13 were less than -7 kcal/mol. Overall, essential oils and phenolics showed moderate or strong binding affinity with their central targets.

The current research revealed the bioactive components, potential therapy targets, and signaling pathways of Aiye in combating obesity. Further in vitro and in vivo experiments were necessary to verify the anti-obesity targets and signaling pathways of the identified components of Aiye.

Keywords: *Artemisiae argyi* Folium; essential oils; phenolics; obesity; GC-MS; LC-MS; network pharmacology; molecular docking