Molecular mechanism study of curcumin treatment for constipation based on network pharmacology and molecular dockings

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Purpose: To explore the mechanism of curcumin in treating constipation through network pharmacology combined with molecular docking technology.

Methods: The method is based on collecting curcumin and constipation targets from multiple databases, establishing a target prediction network for curcumin treatment of constipation, submitting common targets to the STRING database, analyzing connectivity using Cytoscape software, conducting gene ontology (GO) functional analysis and Kyoto Encyclopedia of Genes and Genomes (KEGG) pathway enrichment analysis on the top 20 ranked genes, and molecular docking of the obtained targets to study the mechanism of curcumin treatment of constipation.

Results: As a result, 232 targets related to curcumin, 563 targets related to constipation, and 54 common targets between curcumin and constipation were obtained from the database. GO functional analysis shows that these targets are associated with 635 pathways; KEGG pathway enrichment analysis showed 134 related pathways. The molecular docking results showed that curcumin has good binding ability to targets such as mitogen activated protein kinase 3 (MAPK3), interleukin (IL) 6, serine/threonine kinase 1 (AKT1), vascular endothelial growth factor A (VEGFA), signal transduction and transcription activator 3, albumin, Jun oncogene, tumor necrosis factor (TNF), IL1B, tumor protein p53, C-C motif chemokine ligand 2, and fibronectin 1.

Conclusion: The therapeutic effect of curcumin on constipation is achieved through multiple targets and pathways; Specifically, curcumin may regulate MAPK by binding to core targets MAPK3, IL6, AKT1, VEGFA, and TNF IL6、TNF、 Phosphatidylinositol 3-kinase/protein kinase B and VEGF signaling pathways play a role in treating constipation.