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Supplement



Fig. S1 The targets of *M. oleifera* were imported into the STRING database, multiple proteins were selected, and the species was restricted to Homo sapiens to obtain the protein-protein interaction relationship. The protein-protein interaction relationship was imported into Cytoscape 3.7.1 to construct the PPI network. Through the analysis of the topology structure of the network, the protein nodes with degree value greater than the median 30 were extracted, and the core target PPI network was reconstituted to further analyse the interaction between core proteins. The target pathway/functional network was constructed by Cytoscape 3.7.1. In the network, potential targets of for *M. oleifera* treating arthritis, hypertension, diabetes, and tumour, biological processes, and signaling pathways obtained through enrichment analysis were represented by nodes, and the interactions between them were represented by edges.

Network pharmacology analysis of MOL in the treatment of arthritis

A: MOL - Arthritis target PPI network B: GO enrichment analysis of potential targets of MOL in treating Arthritis C: MOL - Arthritis target-pathway network. Result was sorted by -logP value, select the top 10 items to plot (P<0.05).



Fig. S2 Network pharmacology analysis of MOL in the treatment of hypertension

A: MOL - Hypertension target PPI network B: GO enrichment analysis of potential targets of MOL in treating Hypertension C: MOL -Hypertension target-pathway network. Result was sorted by -logP value, select the top 10 items to plot (P<0.05).



Fig. S3 Network pharmacology analysis of MOL in the treatment of diabetes

A: MOL - Diabetes target PPI network B: GO enrichment analysis of potential targets of MOL in treating Diabetes C: MOL - Diabetes target-pathway network. Result was sorted by -logP value, select the top 10 items to plot (P<0.05).



Fig. S4 Network pharmacology analysis of MOL in the treatment of tumour

A: MOL - Tumour target PPI network B: GO enrichment analysis of potential targets of MOL in treating Tumour C: MOL - Tumour target-pathway network. Result was sorted by -logP value, select the top 10 items to plot (P<0.05).



Fig. S5 Docking fraction of active component-core target According to the drug-disease-pathway target map, the correlation degree values of disease-corresponding active components were obtained. The first 8 components were screened for molecular docking verification with the core targets. The results showed that the common core active components of MOL in the treatment of arthritis, diabetes, hypertension and tumor were as follows: Rutin, Cirsiliol, Caffeic acid, Quercetin-3-O -(6-malondiyl)-β -D-glucopyranoside, Astragalin





Arthritis-CYP2C9 (4jnm)-Rutin Score:-9.8 kcal/mol

Hypertension-CYP3A4 (5vcg)-(+)-pi-noresinol-4-O-β-D-glucopyranoside Score:-9.6 kcal/mol



Diabetes-CYP3A4 (5vcg)-Rutin Score:-10.1 kcal/mol

Tumour-EGFR(5x2c)-Rutin Score:-10.5 kcal/mol

Fig. S6 From the PubChem database (<u>https://pubchem.ncbi.nlm.nih.gov/</u>) in the main active ingredient of 2D structural (sdf.formula) of active ingredient in ChemDraw 3D 19.0 was converted to mol2. Format. PDB can be downloaded from RCSB Protein Database (<u>www.wwpdb.org</u>). Format the core target protein structure file. Autodocktools-1.5.6 and Auto Dock Vina was used to dock the core target with the main active ingredient. According to Docking Score evaluation, pymol 2.2.0 was used to conduct visual analysis of the screening result. Docking results of the core targets and the corresponding effective compounds of MOL.in diabetes, hypertension, arthritis and tumour.