Molecular docking studies of extracts and essential oils isolated from a medicinal plant of Ammodaucus leucotrichus as potential inhibitors of Rheumatoid Arthritis disease.

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Subject description: Traditionally, it was thought that only human collagenases (matrix metalloproteinases-1, -8 and -13) were capable of initiating collagen degradation. Trypsin is also capable of cutting the triple helix of human collagens, and is at the root of rheumatoid arthritis.

Objectives: The trypsin inhibitor , is considered a valid target for the discovery of new active compounds for the treatment of rheumatoid arthritis.In this study, a series of 61 compounds from the methanolic extract of A.leuchotruchus identified by GC-MS were used for a molecular docking study to identify interactions between compounds and active site amino acids.

Methods: Network pharmacology was adopted to detect the active components of our medicinal plants obtained by PubChem in 3D form, and the main target in the treatment of RA was obtained from the PDB. Key components and the target were selected for molecular anchoring. .

Results and discussion: We studied methanol extracts of A. leuchotricus to identify significant functional groups and phytochemical constituents. With an IC50 of 966.48 ±9.95 µg/mll, GC-MS analysis of A. leuchotricus methanol extract revealed the presence of 61 phytochemical constituents and showed impressive anti-inflammatory activity.These 61 substances were then examined for bioactivity using in silico molecular docking techniques. The results showed that the majority of phytochemicals discovered could have an inhibitory action on trypsin.

Conclusion: In this study, we identified 61 active components of ALME, trypsin is an important therapeutic target for the treatment of rheumatoid arthritis, our AMLE has a significant effect for the inhibition of trypsin in vitro and in silico which confirms the importance of our plant with regard to rheumatoid arthritis.

Keywords: GC_MS,A. leuchotricus ,in silico ,molecular docking-, trypsin, rheumatoid arthritis.