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Network pharmacology and molecular docking techniques to elucidate the mechanisms of *Ocimum sanctum* against tuberculosis

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Aim of Study: Mycobacterium tuberculosis (TB) is a notable health care load that imposes a serious impacton the quality of life of patients. The least reported data and multiple spectra of pathophysiological mechanisms of TB make it a challenging task and a serious economic burden in health care management. The presented study aims to discover the potential phenomenon of *Ocimum sanctum* in themedicament of tuberculosis. This study uncovers the active ingredients [1], their potential targets, and signaling pathways in O. *sanctum* for the treatment of TB.

Methodology: In the framework of this study, we used network pharmacology approach to explore the "compound-target-pathway" network [2]. The targets of the active ingredients of *Ocimum sanctum* and tuberculosis were collected by SwissTargetPrediction, DisGeNet and GeneCard. After the screening of mutual targets of TB and active ingredients, enrichment analysis through DAVID was performed. Then the compound-target-pathway network was constructed with Cytoscape. Later, molecular docking was employed to validate the successful activity of the active compounds against potential targets of TB. *Results:* we get 8 active ingredients out of 48 available compounds of *O. sanctum*, after that we get 72 functionally enriched potential target of tuberculosis found in active ingredients. By network analysis fivehub genes (AKT1, MAPK14, TNF, CASP3 and MAPK1) were screened to check the interaction between active compounds and potential targets. The docked complexes reveal that compounds of *O. sanctum* like flavones, terpenoids and sterol play a crucial role in the medication of tuberculosis.

Conclusion: Lastly, we conclude that eight highly active constituents help in the medication of disease byregulating the expression of AKT1, MAPK14, TNF, CASP3, and MAPK1, which may act as potential therapeutic targets for TB. These results revealed that bioactive compounds of *O. sanctum* act on proteins along with their pathways to frame a network analysis in systems pharmacology, having great worth in

drug development and utilization. These findings serve as a starting point for further research to explore the potential mechanism of *O. sanctum* for TB treatment.

References

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