Bridging Traditional Knowledge and Modern Network Pharmacology: Exploring the Role of Karunguruvai Rice in PCOS Management

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Abstract

Polycystic Ovary Syndrome (PCOS) is a multifactorial endocrine and metabolic disorder characterized by hormonal imbalance, insulin resistance, and ovarian dysfunction, affecting a large proportion of reproductive-aged women worldwide. Traditional grains such as Karunguruvai rice, indigenous to Tamil Nadu, have long been utilized in Siddha medicine for their detoxifying and therapeutic properties. The present study explored the molecular basis of Karunguruvai rice in managing PCOS using an integrative network pharmacology and molecular docking approach. Gas Chromatography–Mass Spectrometry (GC–MS) analysis identified thirteen major bioactive compounds, including lactose and linoelaidic acid. Target prediction via SwissTargetPrediction and PharmMapper, followed by disease gene collection from DisGeNET, OMIM, NCBI Gene, and GeneCards, revealed 32 overlapping targets associated with PCOS. Protein–Protein Interaction (PPI) network construction using STRING and Cytoscape identified key hub genes — EGFR, NOS3, ESR1, HMOX1, HSP90AA1, MAPK8, and PPARG. Gene Ontology (GO) and KEGG pathway enrichment analyses demonstrated that these targets were primarily involved in PI3K Akt, MAPK, Estrogen signaling, and Insulin resistance pathways. Molecular docking results confirmed strong binding affinities of lactose and linoelaidic acid with major targets such as HSP90AA1, PPARG, HMOX1, and NOS3, indicating potential regulatory effects on oxidative stress, metabolic balance, and hormonal function. Overall, this study provides molecular-level evidence supporting the traditional therapeutic potential of Karunguruvai rice as a functional dietary intervention for managing PCOS through multi-target modulation of key signaling pathways.

Keywords: Karunguruvai rice, Secondary metabolites, PCOS, Network pharmacology, Hub genes, Molecular docking, Bioactive compounds.