ORIGINAL RESEARCH ARTICLES

EXPLORATION OF CROSS-RECEPTOR MODULATION AND DRUG REPURPOSING FOR POLYCYSTIC OVARY SYNDROME (PCOS): A COMPREHENSIVE ANALYSIS OF NPACT DATABASE AND FDA-APPROVED COMPOUNDS

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ABSTRACT

Polycystic ovary syndrome (PCOS) is a multifactorial endocrine disorder involving hormonal imbalance, insulin resistance and metabolic and reproductive dysfunctions. Conventional treatments mainly offer symptomatic relief without addressing the complex hormonal crosstalk central to PCOS pathophysiology. This study employed molecular docking using Molecular Operating Environment (MOE) software to investigate interactions between selected phytochemicals from the NPACT database and FDA-approved drugs with key hormonal receptors: estrogen receptor (ER), androgen receptor (AR), gonadotropin-releasing hormone (GnRH) receptor, follicle-stimulating hormone (FSH) receptor, and insulin receptor. Several phytochemicals demonstrated strong binding affinities and favorable receptor-ligand interactions, surpassing some FDA-approved drugs. These candidates exhibited the potential to modulate androgen levels, regulate gonadotropins, and enhance insulin signaling. The results emphasize the potential of phytochemicals in targeting multiple hormonal pathways to develop effective, multi-targeted therapies for PCOS. Further experimental studies are warranted to validate their efficacy and establish their role as alternative or adjunct therapies in PCOS management.