NLP-Driven screening and Computational Identification of Bioactive Peptides from Fermented Foods for Therapeutic Intervention in PCOS Management

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Abstract

Polycystic Ovary Syndrome (PCOS) is one of the most common endocrine-metabolic disorders affecting women of reproductive age and is closely associated linked to inflammation, insulin resistance, and hormonal imbalance. While various therapeutic options are available, most treatments remain symptomatic and often exhibit limited long-term efficacy alongside notable side effects. Increasing evidence suggests that the gut microbiota plays a vital role in regulating metabolic and reproductive health. In this context, bacteriocins—bioactive peptides produced by microbes in fermented foods—have gained attention for their antimicrobial, anti-inflammatory, and immunomodulatory properties. This study developed an AI-assisted bioinformatics framework integrating Natural Language Processing (NLP), peptide database mining, structural modelling, and protein–peptide docking to identify potential antimicrobial peptides (AMPs) from fermented foods for PCOS management. NLP-based literature mining identified fermented foods and associated AMPs linked to PCOS pathophysiology. Cross-referencing UniProt, CAMP, and DRAMP databases yielded 102 AMPs, of which 50 were structurally modelled using AlphaFold and validated via PROCHECK-based Ramachandran analysis and key PCOS targets—EGFR and TLR2—were identified through protein–protein interaction analysis using STRING and Cytoscape (v3.9.1). Protein–peptide docking using ClusPro revealed Pediocin PA-1 immunity protein, Enteriocin P, and Plantaricin S beta as top candidates showing strong binding affinity and structural stability with PCOS-associated receptors. Molecular dynamics simulations further confirmed the stability of these peptide–protein complexes. These peptides, predominantly derived from *Pediococcus acidilactici* and *Enterococcus faecium* P13, are proposed to modulate inflammatory and metabolic pathways central to PCOS. The findings suggest that fermented-food-derived AMPs P13 may modulate key metabolic and inflammatory pathways in PCOS. This computational framework provides a foundation for developing natural peptide-based therapeutics and supports future experimental validation.

Keywords: Polycystic Ovary Syndrome (PCOS), Antimicrobial Peptides (AMPs), AI-assisted Bioinformatics, Protein–Peptide Docking, Gut Microbiota Modulation