Review Article

EXPLORING PHYTOESTROGENS AND AI-ASSISTED DOCKING IN FEMALE NEUROPROTECTION AND COGNITIVE AGING

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Cognitive aging and the heightened prevalence of Alzheimer's disease in post-menopausal women highlight the pivotal neuroprotective role of estrogens in maintaining neuronal integrity. Declining estrogen levels after menopause accelerate oxidative stress, mitochondrial dysfunction, and synaptic loss, thereby predisposing women to neurodegenerative disorders. Phytoestrogens—plant-derived polyphenolic compounds with structural similarity to 17β-estradiol—have emerged as promising alternatives to hormone replacement therapy owing to their selective estrogen receptor modulation and antioxidant capacity. However, variable receptor affinity, bioavailability limitations, and incomplete mechanistic understanding constrain their translational use.

Recent advances in artificial intelligence (AI) and molecular docking now enable the rapid prediction of receptor–ligand interactions, pharmacokinetic behavior, and toxicity of phytoestrogen analogues. AI-assisted structure–activity relationship (SAR) modeling and virtual screening can identify novel derivatives with improved selectivity toward estrogen receptor-β and enhanced blood–brain barrier permeability. Integrating computational intelligence with sustainable drug discovery not only accelerates neurotherapeutic design but also aligns with eco-friendly and precision-medicine goals.

This review provides a comprehensive synthesis of current evidence on phytoestrogens in female neuroprotection, elucidates molecular and cellular mechanisms, and examines how AI-driven modeling, docking, and ADMET prediction contribute to rational, sustainable drug discovery for cognitive aging.

Keywords : Phytoestrogens; Cognitive aging; Neuroprotection; Estrogen receptor-β; Artificial intelligence; Molecular docking; Structure–activity relationship (SAR); Alzheimer's disease; Sustainable drug discovery; Machine learning.