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Natural Inhibitors of β2-Adrenergic Receptor: A Computational Study for Targeting GPCR-Mediated Diseases

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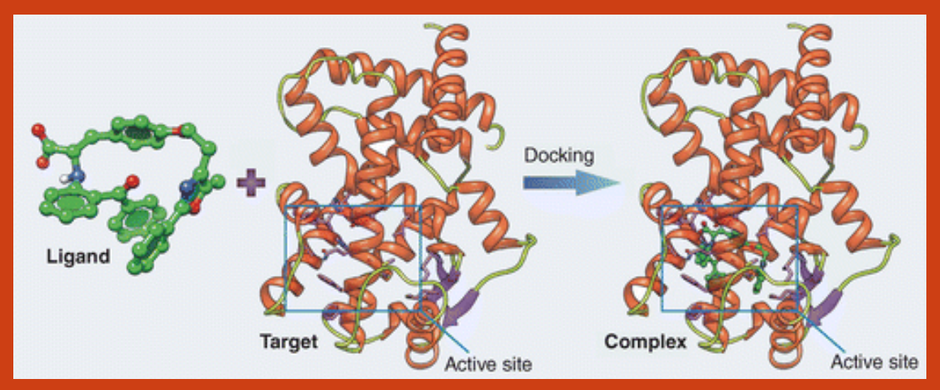
BACKGROUND

G-protein-coupled receptors (GPCRs) regulate essential physiological processes by converting extracellular signals into intracellular responses. Among them, the β2-Adrenergic Receptor (β2-AR) is crucial for smooth muscle relaxation, bronchodilation, and cardiovascular regulation, making it a key target for conditions such as asthma, hypertension, and chronic obstructive pulmonary disease. While synthetic drugs effectively target β2-AR, they often lead to adverse effects and drug resistance, highlighting the need for alternative therapeutic approaches.

METHODS

This study employed molecular docking using AutoDock 4.6 to investigate the interactions of natural compounds like; ephedrine, quercetin, catechin, and resveratrol with β2-AR. The receptor's 3D structure (PDB ID: 2RH1) was obtained, and docking simulations assessed binding energy, hydrogen bonding, and stabilizing interactions between each ligand and the receptor's active site



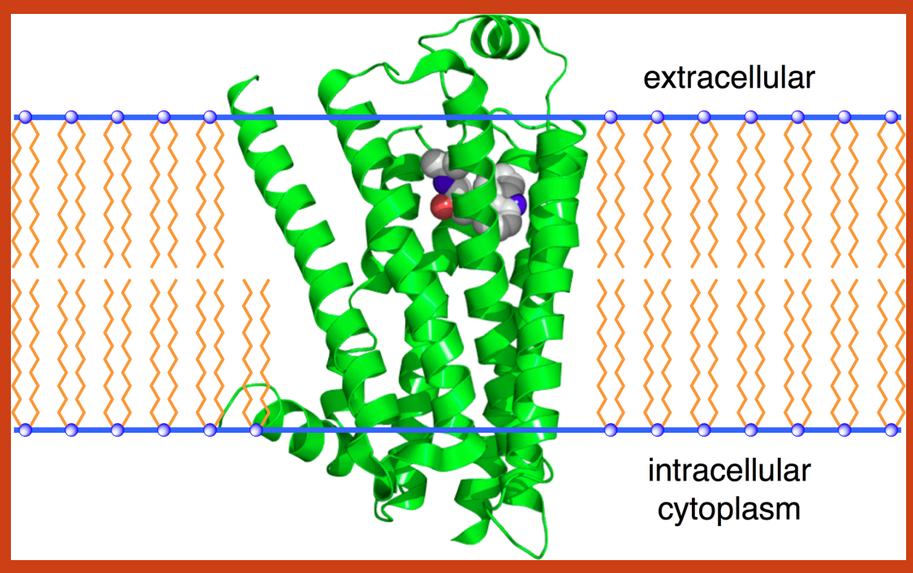
RESULTS

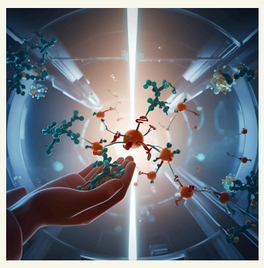
Natural Compounds	Binding Energy	H.bind
Ephedrine	-4.66	3
Quercetin	-5.44	5
Catechin	-5.34	4
Resveratrol	-5.01	3

The results showed that ephedrine formed hydrogen bonds with key β2-AR residues, aligning with previous findings. Quercetin exhibited strong binding interactions, reinforcing its potential as a natural inhibitor. Catechin and resveratrol also demonstrated stabilizing interactions, though their binding affinities were lower than quercetin.

CONCLUSION

These findings suggest that natural compounds could serve as safer and more effective alternatives to synthetic drugs in targeting GPCR-related diseases. The use of molecular docking further highlights their potential in drug discovery and the development of bio-inspired therapeutic strategies.





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