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اللغة الانجليزية: (١)

Design, Synthesis, Biological Evaluation and Molecular Docking of Some Novel Benzopyrane-2-one Derivatives as Potential Selective Beta-1 Adrenergic Blockers

Background:

Hypertension is a widely prevalent and major risk factor for cardiovascular diseases (heart attacks, strokes, and congestive heart failure) and renal failure. It is considered one of the leading causes of morbidity and mortality worldwide. Benzopyrane-2-one (coumarin) is considered an attractive scaffold and was used to design numerous vasodilators. Nebivolol, a selective Beta-1 blocker, was used for the treatment of hypertension and chronic heart failure. Being a benzopyran derivative, nebivolol inspired the discovery of potential selective beta-1 adrenergic blockers with improved pharmacological profiles with higher potency and fewer side effects.

Aim of study:

The objective of the present study was to synthesize some novel benzopyrane-2-one derivatives as potential selective beta-1 blockers

Methods:

Fifteen novel benzopyrane-2-one derivatives have been synthesized and confirmed by spectral and elemental analysis. Introduction of hydrophobic / hydrogen bond acceptor / hydrogen bond donor / polar moieties at 3,4,7,8-positions in synthetic benzopyran-2-one aimed to improve the physicochemical properties and to study the binding mode of the new compounds on the β1-adrenergic receptor as well as assessing its pharmacological activity. Biological evaluation of the synthesized compounds is in progress. Molecular docking techniques of the target compounds against beta-1 adrenergic receptor exhibited binding pattern similar to that of the co-crystallized ligand using MOE program.