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Design, synthesis, biological evaluation and molecular docking study of novel benzopyran and benzochromene derivatives as anti-Alzheimer's agents

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Abstract

A series of molecules was synthesised and evaluated as dual inhibitors of acetylcholinesterase (AChE) and butyrylcholinesterase (BChE). To further explore the multifunctional properties of the newly prepared derivatives, their antioxidant activities were also tested. The results showed that most of these compounds could effectively inhibit cholinesterases. In particular, a compound derived from eugenol showed the best AChE /BChE inhibitory activity with IC_{50} values <3.125 µM and 22.26 µM, respectively. These compounds further showed different levels of antioxidant activities. Indeed, the same compound showed effective inhibition against all the studied methods (β-carotene, ABTS, Phenanthroline and CUPRAC).

The *in-silico* approach also revealed that all tested compounds had a high affinity towards AChE and their Scoring values were lower than those of ACh and Galantamine. This may be due to the presence of both functional and substituent groups as well as heteroatoms in the heterocycles. The results obtained in this project may provide a new starting point for the further development of multifunctional agents for the treatment of Alzheimer's disease.

Keywords: Alzheimer’s disease, Benzopyran and benzochromene derivatives, Inhibitors of cholinesterases, Antioxidant activity, Molecular docking.