



Synthesis, Characterization and Biological Activity of 3-aryl-6-(4-fluorobenzyl)-7*H*-thiazolo[3,2-*b*]-1,2,4-triazin-7-one Derivatives as Novel Acetylcholinesterase Inhibitors

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SUMMARY. Acetylcholinesterase (AChE) inhibitors play an important role in the treatment of Alzheimer's disease. To study the effect of the presence of a fluoro group on inhibitory activity against AChE, a series of 3-aryl-6-(4-fluorobenzyl)-7*H*-thiazolo[3,2-*b*]-1,2,4-triazin-7-one derivatives have been synthesized, in which a hydrogen atom has been substituted by a fluorine in the aromatic nucleus of 6-aryl-methyl-3-phenyl-7*H*-thiazolo[3,2-*b*]-1,2,4-triazin-7-one derivatives, a series of compounds previously reported by us to have inhibitory activity against acetylcholinesterase. From the molecular docking studies, it was found that, in general, a key hydrogen bond of target compounds to the OH of Tyr341 and a close contact with relevant residues in the catalytic site are prerequisites for high inhibitory activity.

KEY WORDS: Acetylcholinesterase inhibitor, Docking, Fluorine substitution, Heterocycle, Synthesis, 7*H*-thiazolo[3,2-*b*]-1,2,4-triazin-7-one derivatives.

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