

البحث الرابع

رقم البحث في قائمة الأبحاث الكلية (25)

عنوان البحث باللغة الإنجليزية:

Title:

Syntheses and Molecular Docking Analysis of Some New Thiazole and Thiazine Derivatives as Three Armed Molecules with a Triazine Ring as a Core Component: A Search for anti-Obesity Agents

اسم المجلة المنشور بها البحث وسنة النشر

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Abstract:

A number of new three-armed heterocycles as thiazoles and thiazines linked to triazine moiety was prepared starting from cyanuric chloride and thiosemicarbazide which gave the target compound 1. The reaction of the tris-thiosemicarbazide with a variety of hydrazonoyl halides afforded thiazole derivatives. In addition, a thiazole derivative could be prepared from the reaction of the target compound 1 with DMAD. Moreover, thiazine derivatives were synthesized from compound 1 through its interaction with benzyldinmalonitrile. In this work, the molecular docking analysis of thirteen compounds against FTO (Fat mass and Obesity-Associated) protein is carried out to investigate the mode of their molecular interactions. Furthermore, in silico ADMET predictions for the new compounds were calculated with the objective to gain an insight into their pharmacokinetic, safety, and drug-likeness profile. The new compounds could be promising

chemical scaffolds for the development of future anti-obesity drug candidates.

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