البحث الخامس

رقم البحث فى قائمة الأبحاث الكلية (26)

عنوان البحث باللغة الإنجليزية:

Title:

Cyanauric Chloride as a key precursor and a core component for Three-Armed Triazolopyrimidines: Recent finding about SARs and docking analyses

اسم المجلة المنشور بها البحث وسنة النشر

Results in Chemistry, 7, 2024, 101337

Abstract:

The s-triazine trichloride is a reactive compound and can be used as key intermediate for delivering polysubstituted triazines specially the three-armed ones. Therefore, this compound is utilized here for the synthesis of multi-armed triazines bearing various heterocyclic moieties. A group of novel heterocycles with three arms as pryrimidines and fused triazoles linked to triazine core component are prepared from the s-trichlorotriazine and aminothiouracil which gave the title compound with three pyrimidinthione arms. The combination of the tris-pyrimidinthione with versatile hydrazonoyl halides in basic medium afforded novel triazoles fused to pyrimidine ring. The structures of the prepared compounds are characterized by analytical and spectroscopic tools. For discovering new antibiotics scaffolds, the synthesized three-armed 1,2,4-triazoles were considered and the most recent findings about triazole derivatives' structure-activity relationships (SARs) is included in this article. One promising issue

about the results of the docking analyses of some of our synthesized compounds' about the binding modes is that its binding scores against various amino acids of the selected protein (PDB Code–3TTZ) is effective. In docking study **7d** (−10.1 kcal/mol) was also displayed highest docking score.

اسماء المشاركون:

Mohamed G. Badrey, Sobhi M. Gomha , Magdi E.A. Zaki, Basant Farag, Ahmed A.M. El-Reedy