البحث الثالث

رقم البحث فى قائمة الأبحاث الكلية (24)

عنوان البحث باللغة الإنجليزية:

Title:

Evaluation of the Binding Relationship of the RdRp Enzyme to Novel Thiazole/Acid Hydrazone Hybrids Obtainable through Green Synthetic Procedure

اسم المجلة المنشور بها البحث وسنة النشر

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Abstract:

The viral RNA-dependent RNA polymerase (RdRp) complex is used by SARS-CoV-2 for genome replication and transcription, making RdRp an interesting target for developing the antiviral treatment. Hence the current work is concerned with the green synthesis, characterization and docking study with the RdRp enzyme of the series of novel and diverse hydrazones and pyrazoles. 4-Methyl-2-(2-(1-phenylethylidene)hydrazineyl)thiazole-5-carbohydrazide was prepared and then condensed with different carbonyl compounds (aldehydes and ketones either carbocyclic aromatic or heterocyclic) afforded the corresponding hydrazide-hydrazones. The combination of the acid hydrazide with bifunctional reagents such as acetylacetone, β-ketoesters (ethyl acetoacetate and ethyl benzoylacetate) resulted in the formation of pyrazole derivatives. The synthesized compounds were all obtained through grinding method using drops of AcOH. Various analytical and spectral analyses were used to determine the structures of the prepared compounds. Molecular Operating Environment (MOE®) version 2014.09 was used to estimate interactions between the

prepared thiazole/hydrazone hybrids and RdRp obtained from the protein data bank (PDB: 7bv2) using enzyme-ligand docking for all synthesized derivatives and Remdesivir as a reference. Docking results with the RdRp enzyme revealed that the majority of the investigated drugs bind well to the enzyme via various types of interactions in comparison with the reference drug.

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