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Importance of 5-(5-nitrohetroaryl-2-y1)-1,3,4-Thiadiazole scaffolds for development of potential leishmanicidal agents

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Parasitic diseases are a major problem in tropical and subtropical regions of the world such as malaria and leishmaniasis. These diseases are the cause of considerable mortality and morbidity annually. No vaccines to prevent infections are available. In the other hand, parasitic drug resistances have restricted the use of available drugs for treatment of malaria and leishmaniasis. Actually, Identification and development of new, cheap, efficient, and safe compounds as drug candidates for the treatment of these diseases are imperative from pharmaceutical point of view. Therefore, a range of creative strategies are required to achieve new lead compounds. The aims of our studies were to synthesis and assess anti-parasitic property of 5-(5-nitrohetero aryl-2-yl)-1,3,4-thiadiazoles with different substituents at the 2-position of thiadiazole ring. It was notable that the bioresponses and physicochemical properties of the molecules depended on the type of these substituents. In these studies, MLR and ANN models were used for the prediction of the antileishmanial activity of some thiadiazole derivatives. Both of them were successful in predicting the antileishmal activity. Also, molecular modeling and docking studies were conducted based on DNA topoisomerase I as a target enzyme. The results suggested that hydrogen bonding and hydrophobic interactions of ligands with the active site of *Leishmania major* topoisomerase IB were responsible for their potent anti-leishmanial activity. Therefore, these results can be used for drug design and development of new and selective leishmania topoisomerase inhibitors.

Biography

Azar Tahghighi has completed her PhD from Tabriz University of Medical Science of Iran. She is a Medicinal Chemist, Assistant Professor and a Member of research team focusing on drug and insecticide discovery at MVRG in Pasteur Institute of Iran. She has published more than 15 papers in reputed journals and is serving as a Reviewer for some journals.

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