

Protein and Peptide studies in Medicinal Chemistry of Neglected Diseases
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Aims and Scope:

Neglected Diseases are those that affect almost exclusively poor and powerless people living in rural parts of low-income countries [1]. They sometimes attract other labels, such as tropical diseases or poverty-related diseases. Neglected diseases include leishmaniasis (kalazar), onchocerciasis, Chagas disease, leprosy, tuberculosis, schistosomiasis, lymphatic filariasis, African trypanosomiasis (sleeping sickness), malaria and dengue [2]. Some neglected diseases are life-threatening, while others result in high morbidity and severe disabilities [1, 3].

Several free ligand databases are widely available today. Virtual structure-based screening has become prominent in drug discovery. Using homology of peptides, crystallographic or modeled protein structures, molecular docking is often employed to screen compound libraries and to predict the conformation of a protein-ligand complex and calculate its affinity energy. Targeting these interactions with small molecule inhibitors as well as searches for new targets is of increased interest for therapeutic purposes of these tropical infections [4].

The objective for this thematic issue is to report recent studies about different approaches using proteins and peptides in medicinal chemistry applied to drug discovery for neglected diseases, that comprises synthesis, semi-synthesis, searches for new targets, natural products, evaluation of biological activities, and/or theoretical approaches as structure-based approaches, SAR, QSAR, docking and several cheminformatics methods. These efforts that involve several studies to aid the discovery of new legends to treatment or cure of these diseases.

References:

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3- Scotti, L.; Ferreira, E.I.; da Silva, M.S.; Scotti, M.T. Chemometric Studies on Natural Products as Potential Inhibitors of the NADH Oxidase from *Trypanosoma cruzi* Using the VolSurf Approach. *Molecules* **2010**, *15* (10), 7363-7377.

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