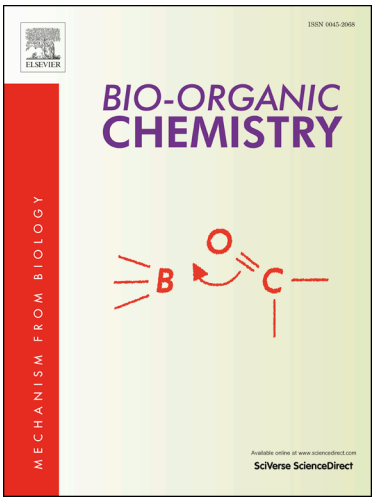

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PII: S0045-2068(18)30680-1
DOI: https://doi.org/10.1016/j.bioorg.2018.09.032
Reference: YBIOO 2529

To appear in: *Bioorganic Chemistry*

Received Date: 10 July 2018
Revised Date: 19 September 2018
Accepted Date: 21 September 2018

Please cite this article as: I. Okon Isaac, M. al-Rashida, S. Ur Rahman, R.D. Alharthy, A. Asari, A. Hameed, K. Mohammed Khan, J. Iqbal, Acridine-based (Thio)semicarbazones and Hydrazones: Synthesis, *In Vi*tro Urease Inhibition, Molecular Docking and *In-Silico* ADME Evaluation, *Bioorganic Chemistry* (2018), doi: https://doi.org/10.1016/j.bioorg.2018.09.032

Acridine-based (Thio)semicarbazones and Hydrazones: Synthesis, *In Vitro* Urease Inhibition, Molecular Docking and *In-Silico* ADME Evaluation

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Abstract: Urease is a bacterial enzyme that is responsible for virulence of various pathogenic bacteria such as *Staphylococcus aureus, Proteus mirabilis, Klebsiella pneumoniae, Ureaplasma urealyticum, Helicobacter pylori* and *Mycobacterium tuberculosis*. Increased urease activity aids in survival and colonization of pathogenic bacteria causing several disorders especially gastric ulceration. Hence, urease inhibitors are used for treatment of such diseases. In search of new molecules with better urease inhibitory activity, herein we report a series of acridine derived (thio)semicarbazones (**4a-4e**, **6a-6l**) that were found to be active against urease enzyme. Molecular docking studies were carried out to better comprehend the preferential mode of binding of these compounds against urease enzyme. Docking against urease from pathogenic bacterium *S. pasteurii* was also carried out with favorable results. *In silico* ADME evaluation was done to determine drug likeness of synthesized compounds.

Keywords: (Thio)semicarbazones, Urease inhibition, pathogenic bacteria, acridine, *In silico* ADME

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