Structural Insights of a Potential Inhibition Against Leishmania Major

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Leishmaniasis is a tropical disease caused by a protozoal parasite of the order Kinetoplastid. According to the World Health Organization reports, 88 countries are affected, with 12 million infected people and approximately 350 million people at risk. The need for new drugs for the treatment of leishmaniasis infections comes from a lack of safe drugs and the serious secondary effects observed in available chemotherapy. Looking for new bioactive substances [1], potentially useful against leishmaniasis, we used both PRTase adenine phosphoribosyltransferase from L. tarentolae and parasite L. major as a model system to screen the inhibitory capacity of one small molecule compound from Brazilian plant. The data collection was performed using Enraf Nonius KappaCCD at room temperature. The structure was analyzed from 1425 reflections with $I > 2\sigma(I)$ and refined to R1-values of 0.033 [1]. The molecules are joined in crystal structure through five twice classical O–H…O hydrogen bonds linking the atoms O4–H4...$O5^{i}$ [i = -x+3, 0.5+y, -z+1], O5–H5...$O2^{ii}$ [ii = x, y, 1+z], O2–H2...$O4^{iii}$ [iii = x+2, y-0.5, -z], O1–H1...$O3^{iv}$ [iv = x-1, y, z] and O3–H3...$O1^{v}$ [v = -x+2, 0.5+y, -z] with distances between donor and acceptor of 2.707(1), 2.808(1), 2.780(1), 2.736(1) and 2.843(2) Å, respectively. The theoretical analysis of occupancy factor for the hydrogen atoms of two last ones is consistent to crystallographic model.

[1] Napolitano H.B., Silva M., Ellena J., Rocha W.C., Vieira P.C., Thiemann O.H., Oliva G., *Acta Cryst.*, 2003, **E59**, o1503-o1505.

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