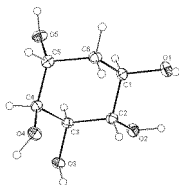


W0219

A New Biological Insight for the Organic Compounds $C_6H_{12}O_5$, Hamilton Napolitano¹, Ademir Camargo¹, Jahyr Theodoro², Marcelo Castillo² & Javier Ellena², ¹Ciências Exatas e Tecnológicas, UEG & ²Instituto de Física de São Carlos, USP.

Leishmaniasis is a tropical disease caused by a protozoal parasite of the order Kinetoplastid. Looking for new bioactive substances, 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 quercitol 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 R_1 -values of 0.033. The molecules are joined in crystal structure through five twice classical O–H...O hydrogen bonds linking the atoms O4–H4...O5ⁱ [$i = -x+3, 0.5+y, -z+1$], O5–H5...O2ⁱⁱ [$ii = x, y, 1+z$], O2–H2...O4ⁱⁱⁱ [$iii = x+2, y-0.5, -z$], 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 nature of the hydrogen bonds O1–H1...O3^{iv} and O3–H3...O1^v observed in the crystal structure was theoretically investigated using the Kohn-Sham density functional theory (DFT).

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