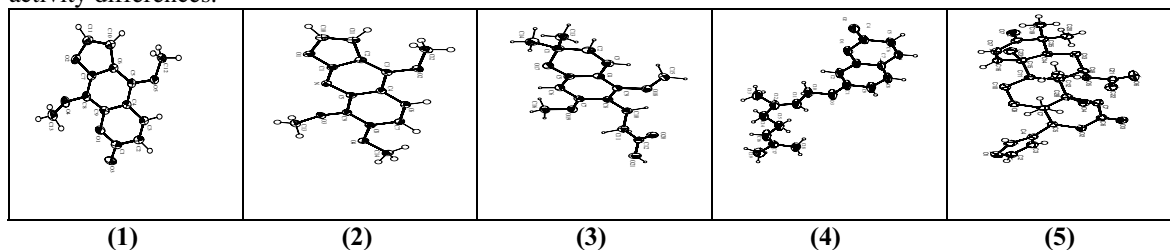


A New Structural Insight from inhibition against *Leishmania major* promastigotes. H.B. Napolitano¹, M. Silva¹, J. Ellena¹, W.C. Rocha², P.C. Vieira², B.D.G. Rodrigues², A.L.C. Almeida², G. Oliva¹ & O. H. Thiemann², ¹Inst. de Física de São Carlos, USP & ²Depto. de Química, UFSCar.

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, 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 several small molecule compounds from Brazilian plants. The data collections of selected inhibitors (1), (2), (3), (4) and (5) were performed using Enraf Nonius KappaCCD at 115 K. These structures were analyzed from 2450 (1), 2672 (2), 2666 (3), 1579 (4) and 8436 (5) reflections with $I > 2_{\sigma}(I)$ and refined to R1-values of 0.044 (1), 0.038 (2), 0.033 (3), 0.089 (4) and 0.054 (5). The structural difference among these compounds seems to be consistent with the observed inhibitory activity differences.



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