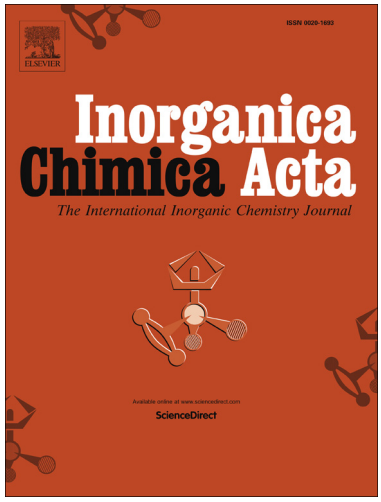

Research paper

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Structural Investigations, Anti-Leishmanial, Antibacterial and Docking Studies Of New Pentavalent Antimony Carboxylates

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Abstract: In order to investigate the new drug candidates for healthy and risk free treatment of parasitic diseases like leishmaniasis, a series of new bioactive pentavalent antimonials (**LS-1** to **LS-8**) of the type $[SbR_3(OOCR')_2]$ (R = $-C_6H_5$, $-(C_6H_4)CH_3$ and R′ = $-(C_6H_4)NO_2$, $-(C_6H_4)Br$, $CH(C_6H_5)_2$, $CH_2CH(C_3H_7)NHSO_2C_6H_5$) were synthesized. All the antimonials have been characterized using melting points, elemental analysis, and multinuclear (^1H and ^{13}C) NMR spectroscopy. In addition two compounds (**LS-3** and **LS-5**) were also studied by X-ray crystallography and showed trigonal-bipyramidal geometry around antimony. The leishmanicidal activity was assessed against the Leishmania tropica promastigote parasite. It was observed that IC_{50} of the antimonials was many fold superior as compared with the standard antimonial drug used. Antibacterial assay along with docking study proved that the synthesized compounds are highly effective against various human pathogens.

Keywords: Leishmanicidal; antimonial compounds; antibacterial; X-ray crystallography; Molecular docking