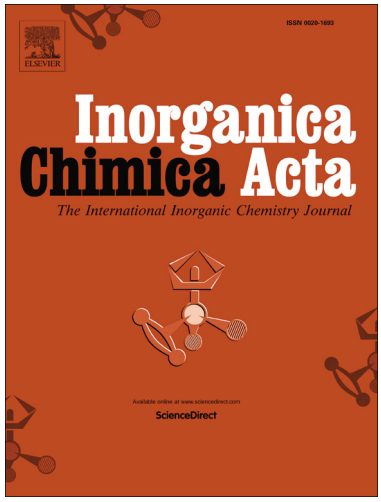

Research paper

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Complexation of trichlorosalicylic acids by alkaline and first row transition metals as a switch for their antibacterial activity

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Abstract:

3,5,6-trichlorosalicylic acid (TCSA) does not show a good antibacterial activity. In contrast, here metal complexes with TCSA have shown better antibacterial activity for selected bacterial strains with a good degree of selectivity. Amongst the eight synthesized essential metal complexes complexed with TCSA, Mn(II)-TCSA and Ni(II)-TCSA have been found to be more effective with MIC range 20-50 µg/L as compared to control (chloramphenicol). The activity of an individual complex against different microbes was not found to be identical, indicating the usage of an individual metal chelate against a targeted bacterial strain. Further, the protein (BSA) binding constant of TCSA and its metal complexes were determined and ordered as Ca(II)-TCSA > Cu(II)-TCSA > Mg(II)-TCSA >> Mn(II)-TCSA >> Zn(II)-TCSA >>> Ni(II)-TCSA >>> Co(II)-TCSA > Fe(II)-TCSA > TCSA. The present study has confirmed enhanced antibacterial activities and binding constants for metal chelates of TCSA as compared to free TCSA, which seems directly related with the antioxidant activities of these complexes. Further, bearing the ambiguity related to the structural characterization of the metal complexed with TCSA ligands, DFT calculations have been used as the tool to unravel the right environment around the metals, studying basically the relative stability of square planar and octahedral metal complexes with TCSA.

Keywords: Trichlorosalicylic acid, divalent essential metal complexes, antibacterial activity, DFT calculation, BSA protein binding.