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A combined *in-vitro* and *in-silico* studies of macrocyclic complexes of Tin(II) with potent anti-cancer, anti-inflammatory and anti-microbial properties

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The combined use of both molecular docking and *in vitro* studies has become a productive trend. Both methods provide valuable information for determining the structure and dynamics of the biomacromolecular complexes. Moreover, they have proved to be perfectly complementary techniques. In particular, their combination is widely used in drug discovery research. The rich diversity of macrocyclic compounds provides exciting prospects for the design of novel therapeutic agents with unique mechanisms of action. From such a viewpoint, a new class of bioactivable tetradentate macrocycles of tin(II) have been derived from diammines and dicarboxylic acids.The newly synthesized scaffold displayed promising pharmacological property and cytotoxic activity. The compounds have been comprehensively characterized by elemental analysis, molecular weight determinations, infrared spectroscopy and multinuclear NMR spectroscopy and tested for antimicrobial, anti-inflammatory and anticancer activity. The various physico-chemical data indicate that the complexes have octahedral geometry. The coherence of the results obtained from the docking simulations and characterizations enables us to reliably distinguish the preferable structures.In studies of the cytotoxicity, the complex exhibited significant activity against a panel of cancer cell lines.The compounds have also exhibited noteworthy anti-inflammatory activity. The obtained results clearly indicate that the tin(II) complexes behave as very effective anti-inflammatory agents and could prove to be useful for the treatment of difficult to treat inflammatory diseases. The anti-microbial efficiency of the complexes was also examined by *in vitro* method against various pathogenic bacterial and fungal strains. The metal complexes were found to possess efficient antimicrobial properties compared to starting materials and most of these complexes could turn out to be excellent models for the design of effective antibiotic drug substances.

Biography

Ekta Rawat is a research scholar at Department of Chemistry at Kurukshetra University, India. Her research interests have been focusing on pharmacogical and anticancer properties of macrocyclic and supramolecular frameworks. She has been awarded with Young Scientist Award and Best Paper Presentation Award at National conferences organised by reputed Universities of India. She has co-authored eight papers in journals of international repute and one book chapter. She has steadily presented papers in various international and domestic conferences. She has been awarded with the Fellowship by University Grants Commission; India in 2013. Moreover, she is also working on Major Research Project funded by UGC, India on organometallic compounds in cancer therapy. She is also a life member of Indian Science Congress Association, Kolkata, India. One of her paper has been selected in 3rd Annual International Conference on Chemistry 2015 at Athens, Greece. Her paper has also been selected for oral presentation under young researcher forum at 5th World Congress on Cancer Therapy during September 28-30, 2015 at Atlanta, USA.

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