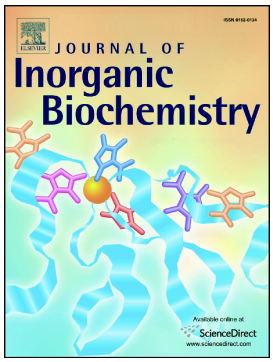

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Manganese coordination compounds of mefenamic acid: *in vitro* screening and *in silico* prediction of biological activity

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Abstract

The *in vitro* and *in silico* biological properties of two manganese complexes with the non-steroidal anti-inflammatory drug mefenamic acid (Hmef) in the presence or absence of salicylaldoxime (H_2sao), i.e. [$Mn_6(O)_2(mef)_2(sao)_6(CH_3OH)_4$] **1**, and [$Mn(mef)_2(CH_3OH)_4$] **2**, respectively, are presented in the present contribution. More specifically, the *in vitro* biological activity of the complexes was investigated by studying their affinity to calf-thymus DNA (by diverse spectroscopic and physicochemical techniques) and their binding towards bovine (BSA) or human serum albumin (HSA) by fluorescence emission spectroscopy. Molecular docking simulations on the crystal structure of HSA and DNA, exploring *in silico* the ability of the complexes to bind to these macromolecules, were also employed in order to explain the described *in vitro* activity of the compounds. Furthermore, *in silico* predictive tools have been employed to study the properties of the most active complex **2** to act as anticancer agent, in continuation of the previously reported cytotoxic activity. It is adopted *in silico* studies on a multitude of proteins involved in cancer growth, as well as prediction of drug-induced changes of gene expression profile, protein- and mRNA-based prediction results, prediction of sites of metabolism, quantitative prediction of antitarget interaction profiles etc.

Keywords: Bioinorganic chemistry; DNA; manganese compounds; albumins; *in silico* predictive tools

1 Introduction

Mefenamic acid (Hmef, Figure 1(A)) is a non-steroidal anti-inflammatory drug (NSAID) that belongs to the anthralinic acid derivatives [1]. Hmef is mainly used as an analgesic and

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