CONFORMATIONAL CHARACTERISTICS DECISIVE FOR THEIR BIOLOGICAL ACTION OF ORGANOTIN METALLOTHERAPEUTICS

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This study involves the structure elucidation and conformational analysis of three metallotherapeutics organotin (IV) derivatives of cholic acid (CAH) with the formulae $R_3Sn(CA)$ (R= Ph- (**1**), *n*-Bu- (**2**)) and $R_2Sn(CA)_2$ (R= Me- (**3**). The structure of compounds (**1-3**) was determined;using a combination of homonuclear and heteronuclear 2D NMR spectroscopy. Semi-empirical quantum mechanic computations PM6, based on the Neglect of Diatomic Differential Overlap (NDDO), contributed to the estimate of an optimized conformation. The geometry of compounds found are: Triangular dipyramid for (**1**), tetrahedral geometry for (**2**) and octahedral geometry for (**3**). Biological activity of these compounds is related with the conformation of atoms which endue the metal of Sn. Having received all the necessary information about the structure and conformation of the moleculesand obtaining *in vitro* results it was deemed necessary to perform *in silico* studies, about the binding of compounds with receptor 1A52 of ER-α (Estrogen receptor alpha ligand) hormone to provide a plausible explanation and proceed to a rational design of new molecules. Following at figure is depicted the binding of compound 2 with the receptor 1A52.