

In Silico Design of Organometallic Complexes as Potential Antibacterial Agents

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Abstract : The complexes of transition metals with various organic ligands have been extensively studied as models of some important pharmaceutical molecules. It was found that biological properties of different substituted organic molecules are improved when they are complexed by different metals. Therefore, it is of great importance for the development of coordination chemistry to explore the assembly of functional organic ligands with metal ion and to investigate the relationship between the structure and property. In the present work, we have bioassayed the antibacterial potency of benzimidazoles and their metal salts (Cu or Zn) against yeast *Sarcina lutea*. In order to validate our in vitro study, we performed in silico studies using molecular docking software. The investigated compounds and their metal complexes (Cu, Zn) showed good to moderate inhibitory activity against *Sarcina lutea*. In silico docking studies of the synthesized compounds suggested that complexed benzimidazoles have a greater binding affinity and improved antibacterial activity in comparison with non-complexed ligands. These results are part of the CMST COST Action No. 1105 "Functional metal complexes that bind to biomolecules".

Keywords : organometallic complexes, benzimidazoles, chemometric design, *Sarcina lutea*

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