

The Influence of Ligands Molecular Structure on the Antibacterial Activity of Some Metal Complexes

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Abstract : In last decade, metal-organic complexes have captured intensive attention because of their wide range of biological activities such as antibacterial, antifungal, anticancerous, antimicrobial and antiHIV. 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 view of our studies, we reasoned that benzimidazoles complexed to metal ions could act as a potent antibacterial agents. Thus, we have bioassayed the inhibitory potency of benzimidazoles and their metal salts (Co or Ni) against Gram negative bacteria *Escherichia coli*. In order to validate our in vitro study, we performed in silico studies using molecular docking software's. The investigated compounds and their metal complexes (Co, Ni) showed good antibacterial activity against *Escherichia coli*. In silico docking studies of the synthesized compounds suggested that complexed benzimidazoles have a greater binding affinity and enhanced antibacterial activity in comparison with noncomplexed ligands. In view of their enhanced inhibitory properties we propose that the studied complexes can be used as potential pharmaceuticals. This study is financially supported by COST action CM1306 and the project No. 114-451-347/2015-02, financially supported by the Provincial Secretariat for Science and Technological Development of Vojvodina.

Keywords : benzimidazoles, complexes, antibacterial, *Escherichia coli*, metal

Conference Title : ICBB 2016 : International Conference on Biochemistry and Biotechnology

Conference Location : Kuala Lumpur, Malaysia

Conference Dates : February 11-12, 2016