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In silico evaluation of the stability and antibacterial activity of some cobalt complexes

Ana-Cristiane DRAGOMIR,[1] Alina Ramona BUZATU,[2] Oana-Raluca POP[*],[3] Mihaiela ANDONI,[3] Doru BUZATU,[4] and Marilena MOTOC[2]

[1]*Doctoral School, Department of Biochemistry and Pharmacology, Faculty of Medicine, Victor Babeş University of Medicine and Pharmacy, 2 Eftimie Murgu Square, 300041 Timisoara, Romania*
[2]*Discipline of Biochemistry, Department of Biochemistry and Pharmacology, Faculty of Medicine, Victor Babeş University of Medicine and Pharmacy, 2 Eftimie Murgu Square, 300041 Timisoara, Romania*
[3]*Faculty of Pharmacy, University of Medicine and Pharmacy "Victor Babeş" Timisoara, Eftimie Murgu Square 2, 300041 Timişoara, Romania*
[4]*National Institute for Research and Development in Electrochemistry and Condensed Matter, Dr. A. Paunescu Podeanu Street 144, 300569, Timisoara, Romania*

Abstract. The properties and stability of six octahedral cobalt(II) complexes were evaluated by means of DFT computations. Three types of ligands were assigned: heterocycles like 1,3-thiazole and 1,2,4-thiadiazole (unsubstituted, and substituted with amine and hydrazine groups, respectively), water molecules and chlorine. The results suggest that the major influence on the chemical properties of the complexes is given by the substituents, and only in a small extent by the heterocycle type. Taking into account the major health issue of the antibiotic resistance, the design of new compounds with antibacterial properties has attracted an increased interest. In this regard, the antibacterial activity of the proposed cobalt complexes has been evaluated by means of molecular docking. Three receptors have been employed, namely *S. aureus* tyrosyl-tRNA, *E. coli* DNA polymerase II, and Methicillin-resistant *S. aureus*, a panthetonate synthetase. The results show that the best results have been obtained for the complexes where the heterocycle is substituted with hydrazine group, followed by the amino-substituted ones.

***Keywords*:** cobalt complex; thiazole; thiadiazole; antibacterial activity; molecular docking.

[*] Corresponding author. *E-mail address:* pop.raluca@umft.ro (Oana-Raluca Pop)