

VIRTUAL SCREENING BY MOLECULAR DOCKING OF MIXED DEHYDROACETIC ACID COMPLEXES

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Code CCP11

Abstract

Dehydroacetic acid (DHA) is a rapidly growing area of research due to the important role it has played in the development of coordination chemistry [1]. The latter has attracted the attention of many research teams around the world, both at the academic and industrial levels. This can be mainly associated with the importance and diversity of applications of this type of compound [2, 3]. A recent literature study reveals that the reactions of DHA and its derivatives with different reagents such as metal ions can provide versatile routes for the synthesis of a wide variety of biologically active compounds [4, 5]. In our work, two transition metal complexes formed with mixed ligands are synthesized and characterized. To compare the effect of metal ions on some biological activities, a theoretical virtual screening study was performed to explain the inhibitory potential of our complexes using an automated software [6]. The results obtained show that the nature of the metal ion plays an important role in the binding affinity of the selected complexes-targets by comparing the binding energy and the inhibition constant of the two coordination compounds.

Keywords: DHA, metal complexes, mixed ligands, biological activities, virtual screening.

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