XXI Brazilian Meeting on Inorganic Chemistry
X Brazilian Meeting on Rare Earths
III Workshop on Theoretical Bioinorganic Chemistry
Belo Horizonte, September 12 - 15th 2024

Essential metal Zn(II) naphthoquinone complex as new potential metallodrugs

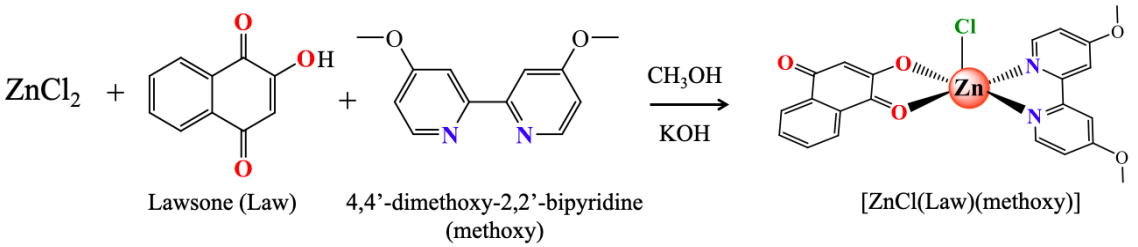
Mariana P. Viana [1*], Pedro H. O. Santiago[2], Javier A. Ellena[2], Katia M. Oliveira[1]

[1]Institute of Chemistry, University of Brasília, Brasília - DF, Brazil
[2]Institute of Physics of São Carlos, University of São Paulo, São Carlos - SP, Brazil
**E-mail: marianapaivaviana@gmail.com*

Thematic Area: Biological Inorganic Chemistry

Keywords: zinc complexes, naphthoquinone, biological activities.

Studies on the synthesis of complexes derived from molecules that present biological activity are promising in the area of bioinorganics as an alternative in the search for new anticancer drugs. Lawsone (2-hydroxy-1,4-naphthoquinone) is a naturally occurring compound derived from the leaves of the Henna plant, belonging to the class of naphthoquinones. This substance exhibits a wide range of biological properties, including antiviral, antibacterial, antiparasitic and anticancer potential[1]. In addition to the biological properties of the ligand, the metal center also plays a fundamental role. Among the different types of metals, zinc is of particular interest for developing new compounds with biological properties due to its essential role in the body, potentially resulting in compounds with lower toxicity[2]. In this work, a new metal complex was synthesized containing lawsone (law) as the ligand, Zn(II) as metal center, and 4,4'-dimethoxy-2,2'-bipyridine (methoxy) as the co-ligand, with the general formula [ZnCl(law)(methoxy)] (Scheme 1). The complex was characterized by melting point, molar conductivity, elemental analysis, infrared and UV-Vis absorption spectroscopy, NMR (1D e 2D), x-ray crystallography. The interaction of the complex with bovine serum albumin (BSA) protein and CT-DNA was analyzed by fluorescence quenching. The binding constant (Kb) values of the complex with BSA are in the order of magnitude of 10^4 - 10^5 mol^{-1} L. Additionally, negative values for ΔHº and positive values of ΔSº were obtained, indicating that the interaction between the complex and BSA is of an electrostatic nature. The complex's potential interaction with CT-DNA via minor groove binding and intercalation was explored through displacement assays employing Hoechst 33258 and thiazole orange (TO), and it was possible to observe the prevalence of interaction through the grooves of CT-DNA. In this sense, the complex show potential in the development of new anticancer drugs.



Scheme 1. Synthetic route used to obtain Zn(II) complex with lawsone.

Acknowledgments: CNPq, FAPDF (Proc. 00193-00002088/2023-42)

References

[1] Wellington, K. W. Understanding cancer and the anticancer activities of naphthoquinones –a review. RSC Adv., 5(26), 20309–20338 (2015).
[2] Pellei, M., Del Bello, F., Porchia, M., & Santini, C., Coordination Chemistry Reviews, 445, 214088 (2021).