# Theoretical studies of a new iron(III) complex containing sulfadiazine with antitoxoplasma activity

Vagner M. de Assis[1,2]*, Nathália F. B. de Azeredo[3], Christiane Fernandes[3], Adolfo Horn Jr[3], Sergio de P. Machado[2]

*[1]Instituto Federal Fluminense, Campus Cabo Frio, RJ, Brazil, [2] Departamento de Química Inorgânica, Instituto de Química, UFRJ, Rio de Janeiro, RJ, Brazil, [3] Laboratório de Ciências Químicas, UENF, Campos dos Goytacazes, RJ, Brazil*

*e-mail: vagnerassis@gmail.com

New metallopharmacs to treat toxoplasmosis are needed due to several factors, such as high daily dose and side effects related to the current treatment (pyrimethamine and sulfadiazine)[1,2]. Herein we present the theoretical study of a new binuclear iron(III) complex: [(Cl)(SDZ)Fe(III)(μ-BPClNOL)$_2$Fe(III)(SDZ)(Cl)].2H$_2$O **1**, which has been investigated in the treatment of Toxoplasmosis. Complex **1** was obtained by the reaction between the known compound [Fe(HBPClNOL)Cl$_2$].H$_2$O[3] and sodium sulfadiazine (NaSDZ). Subsequently, complex **1** was characterized by a variety of physic-chemical methods. ESI(+)-MS results suggest the presence of mononuclear and binuclear cationic complexes in solution So, in order to deduce the correct structure, computational chemistry was used to predict the geometry of complex **1** and analyze the frontier orbitals. Thus, all calculations were performed in Gaussian 09W software using density functional theory (DFT) with B3LYP functional and LANL2DZ basis set. The harmonic vibrations were also calculated in order to characterize the stationary point. The results show that a binuclear structure is correct, due to the comparison between the theoretical and experimental IR spectra. Therefore, this proposal can be discarded, since the theoretical spectrum binuclear has similarities with the experimental spectrum. Theoretical studies of this binuclear compound allowed us to infer about the multiplicity of the complex, this data was obtained by optimization calculations of different multiplicities and indicated the the lowest energy was the singlet. Other important data obtained in this study is related to the frontier orbitals, HOMO and LUMO, which are directly related to the reactivity of complex **1**. The LUMO has the contribution of orbitals from the sulfadiazine molecule, especially the pyrimidine group, as well as one orbital dz$^2$ from the Fe centre and the dxy orbital from another Fe centre, the p-orbitals of chloride ions coordinated to the metal centre and the p-orbitals from the oxygen atoms of sulfadiazine. Taking part in the HOMO, we can mention the d-orbitals of the metal centre linked to the aliphatic nitrogen atom of the ligand H$_2$BPClNOL, the p-orbitals of the bridge phenolate oxygen atoms and the p orbitals of atoms from the sulfadiazine coordinated. Also the hardness of complex **1** was calculated: -41.16784 kJ mol$^{-1}$.

1- Caumes, E.; Bocquet, H.; Guermonprez, G., Rogeaux, O.; Bricaire, F.; Katlama, C.; Gentilini, M.. Clin Infect Dis, **1995**, 21(3), 656-658.
2- Montoya J.G.; Liesenfeld, O. The Lancet, **2004**, 363, 1965–1976.
3- Silva, G.C.; Parilha, G.L.; Carvalho, N.M.F.; Drago, V.; Fernandes, C.; Horn Jr., A.; Antunes, O.A.C.; Catal. Today, **2008**, 133–135, 684–688.

CAPES, CNPq, FAPERJ.