The Schistosomiasis is a disease caused by a parasitic worm of the genus Schistosoma and affects almost 210 million people in the world. The main treatment is the praziquantel, but are too many side effects. One alternative is the 2(3H)-Furanone,dihydro-3-(hydroxyphenylmethyl)-4-[1-methyl-1H-imidazol-4-yl)methyl]-[3S-[3a(R*),4b]] (Epiisopiloturine). An alkaloid extracted from leaves of Pilocarpus microphyllus, a typical Brazilian plant, which was recently described as a potential drug against Schistosomiasis. [1] Here we investigate the electronic and magnetic hyperfine properties of the copper(II) and zinc(II) complexes of Epiisopiloturine and its changes in the biological activity. Due to the high sensibility of the properties, we use the Gaussian09 and ORCA computational codes in the framework of the Kohn-Sham Density Functional Theory. [2] These two softwares take into account different exchange correlation functionals, basis set, relativistic and spin-orbit effects. The initial geometry of our complexes were obtained from the determined crystallographic X-Ray. The results for EPR and NMR parameters, calculated using these strategies, are in have a good agreement with the experimental results. This work is still in progress. We acknowledge CAPES, INEO, LCCA, CENAPAD/SP and FAPESP.
