SYNTHESIS, SPECTRAL CHARACTERIZATION, α–GLUCOSIDASE INHIBITION AND TD/DFT STUDY OF THE Ni(II) COMPLEXES

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ABSTRACT

The Ni(II) complex of 6–methylpyridine–2–carboxylic acid and its mixed ligand complex with 22'-bipyridiyl were synthesized and characterized by XRD, LC-MS/MS, FT–IR and UV–Vis spectroscopies. The α–glucosidase inhibition activity of the synthesized complexes were determined by IC_{50} values. The optimized molecular structure and vibrational frequencies were obtained by using Density Functional Theory (DFT)/HSEh1PBE/6–311G(d,p)/LanL2DZ level. In order to investigate electronic spectral properties, TD–DFT calculations in ethanol solvent and gas phase were fulfilled. The NLO parameters and FMO energies of complexes were calculated by using HSEh1PBE/6–311G(d,p) level. Finally, to show interactions of the binding site of the target protein (the template structure S. cerevisiae isomaltase), the docking study of complexes were performed.

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