

## The coordination site investigation of bioactive coumarin Schiff base complexes with Cu ions

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Schiff bases as well as coumarin derivatives are known for having a broad spectrum of biological activity. They form stable complexes with transition metal ions often showing an increase in biological activity, what makes them perfect as potential pharmacological agents. The potential of pharmacological action depends on the chemical structure, therefore, the binding mechanism between copper ions and organic ligands in biologically active Schiff base complexes with 7-hydroxycoumarin derivatives has been studied.

To get structural information about non-crystalline coumarin Schiff base complexes with copper ions the multi-approach methodology has been applied. Using the XAS (X-ray absorption spectroscopy) technique the local atomic environment around the specific element can be described. EXAFS and XANES spectra have been measured at the XAFS beamline (Elettra-Sincrotrone Trieste, Italy). As a support for structural characterization, several spectroscopic as well as analytical techniques, i.e. FTIR and UV-VIS spectroscopy, elemental analysis, DFT calculations, have been applied.

Combination of mentioned experimental methods enabled to obtain information about coordination site of studied complexes. The metal to ligand ratio was determined and the oxygen atoms of deprotonated hydroxyl group has been identified as possible active site in coordination process. By comparison of the experimental data with the reference oxides spectra oxidation state of copper ions has been found. With EXAFS analysis a local atomic environment of copper ions have been determined i.e. the number and type of neighboring atoms, as well as their average distance to Cu ion have been found.

Based on the results of the EXAFS analysis an initial structural model was built. XANES analysis and DFT calculations allowed to refine the initial model. The final three-dimensional molecular structure model of the studied complexes has been proposed.

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