

PAHONTU, Elena, USATAIA, Irina, GRAUR, Vasiliu et al. Synthesis, characterization, crystal structure of novel Cu (II), Co (III), Fe (III) and Cr (III) complexes with 2-hydroxybenzaldehyde-4-allyl-S-methylisothiosemicarbazone: Antimicrobial, antioxidant and in vitro antiproliferative activity. In: Applied Organometallic Chemistry .2018. ISSN 0268-2605.

2-Hydroxybenzaldehyde-4-allyl-S-methylisothiosemicarbazone and Cu (II), Co (III), Fe (III) and Cr (III) complexes were synthesized and characterized. The new obtained compounds were investigated by elemental analysis, magnetic susceptibility measurements, molar electric conductivity, IR, ^1H NMR, ^{13}C NMR, UV–Vis spectroscopy. In addition, the structure of the ligand and six complexes has been determined by single-crystal X-ray diffraction analysis. The Cu atom in complex **3** is penta-coordinated in a distorted square–pyramidal coordination geometry, while the metals in complexes **5–9** are in a distorted octahedral environment. For all compounds the antimicrobial activity was studied on a series of standard strains, such as *Staphylococcus aureus*, *Escherichia coli*, *Enterococcus faecalis*, *Salmonella abony* and *Candida albicans*. The *in vitro* antiproliferative activity of the ligand and complexes was screened on human leukemia HL-60 cells, human cervical epithelial HeLa cells, human epithelial pancreatic adenocarcinoma BxPC-3 cells, human muscle rhabdomyosarcoma spindle and large multinucleated RD cells. The primary screening on a wider series of cancer cells showed that copper coordination compound **2** manifests high activity towards HeLa, BxPC-3 and RD cancer cells, which is three–six times higher than the activity of doxorubicin. The selectivity index that is the ratio between the IC_{50} value for the normal MDCK cells and IC_{50} values for the cancer cells varies in the range 2.44–21.17. This index is 5.5–11 times higher for the copper coordination compound **2** than for the doxorubicin. Cr (III), Fe (III) and Co (III) coordination compounds **6–9** manifest high antioxidant activity towards ABTS^{*+} that exceeds 47–67 times the activity of Trolox.