SEMINARIUM RENTGENOWSKIE

Dnia 14.01.2020 r. o godz. 10.30, w sali D Instytutu Fizyki PAN, odbędzie się seminarium rtg., na którym **mgr Diana Kalinowska z SL-1 IF PAN,** wygłosi referat na temat:

“Local atomic environment of Cu and Ag ions of new bioactive 1,5-disubstituted tetrazole complexes investigated using multi–technique approach methodology”

Summary:

Although the quality of healthcare has increased with the invention of antibiotics, nowadays the antimicrobial resistance remains a global and critical healthcare issue. WHO reports about the growing threat of bacterial infections, that may become the top cause of mortality in the world within the next three decades. Greater effort is required in research and development of the novel class of compounds effective against pathogens [1, 2]. Tetrazole derivatives are a potential in this field of research. Their wide range of biological activity and polynitrogen planar structure make them perfect template aimed at the development of new bioactive compounds [3–9].

Structural characterization of new, bioactive 1,5-disubstituted tetrazole-derivative complexes with Cu and Ag ions will be presented. The studies have been carried out for compounds in a form of solvates with growth cell culture medium as a solvent. It simulate living environment of the cells and is commonly used for various biological assays. Solvent molecules may modify the surrounding of metal ion and enhance the activity of a compound. Since the potential of pharmacological action depends on the chemical structure, there is an interest in detailed investigation of complex’s molecular structure.

Due to fact that diffraction methods are inapplicable in case of compounds in form of solution, methodology developed in our laboratory has been used. It assumes using the X–ray absorption spectroscopy (XAS), which provides information about the local atomic order around the specific element regardless of their form or state. With support of laboratory based techniques (e.g. FTIR spectroscopy, elemental analysis) and DFT calculations applying methodology made it possible to propose the three-dimensional models of the analyzed compounds.

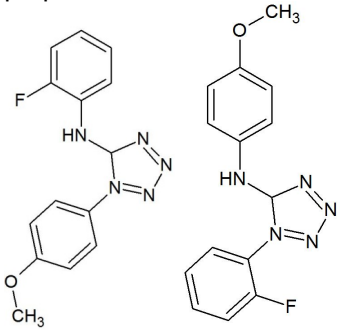

Figure 1. Schematic structure of two tautomeric forms of 1,5–substituted tetrazole-derivative ligand used as ligands in coordination reaction.

[1] A. Bielenica, et al., *Eur. J. Med. Chem.* **101** (2015) 111.
[2] J. Stefańska, et al., *Polish Journal of Microbiology* **65** (2016) 451.
[3] D. Szulczyk, et al., *Eur. J. Med. Chem.* **156** (2018) 631.
[4] M. Staniszewska, et al., *Eur. J. Med. Chem.* **145** (2018) 124.
[5] C. X. Wei, et al., *Molecules* **20** (2015) 5528.
[6] A. Qian, et al., *Bioorganic & Medicinal Chemistry Letters* **28** (2018) 344.
[7] V. A. Ostrovskii, et al., *Russ. Chem. Bull.* **61** (2012) 768.
[8] L. L. Dai, et al., *Med. Chem. Comm.* 6 (2015) 147.
[9] R. Sribalan, et al., *J. Mol. Struct.* 1175 (2018) 577.
[10] M. T. Klepka, et al., Chemical Physics Letters **691** (2018) 190.
[11] M.T. Klepka, et al., *Radiat. Phys. Chem.* (2018) https://doi.org/10.1016/j.radphyschem.2018.11.001

Prof. dr hab. Krystyna Jabłońska