

# Complementary use of various X-ray sources to study metal-based complexes in biological systems.

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Many metal complexes are widely known for their activity in biological systems. In addition to the compounds occurring naturally in the human body, metal ions are also required for their role as pharmaceuticals as well as diagnostic agents. Due to the increasing number of cancer cases in the world, research into new anti-tumor drugs containing metal ions is particularly important. Therefore, our research is focused on interaction of metal-complexes with cell constituents and their potential anti-tumor activity.

Herein I will present our results of studies of platinum and copper complexes utilizing X-ray spectroscopy with laboratory and synchrotron X-ray sources. Proposed methodology of research, called *atomic telemetry*, can be used to obtain information about chemical structure of studied metal complexes, hydrolysis as well as interaction mechanism with other biomolecules. This approach was successfully implemented in the studies of cisplatin [1], novel platinum drugs [2,3] and copper complexes with phenanthroline [4]. Moreover, the methodology of time-resolved studies of DNA damage formation was proposed [5], which can be used on pulse X-ray sources, and give us the information about dynamics of the studied interactions.

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1. E. Lipiec, J. Czapla, J. Szlachetko, Y. Kayser, W. Kwiatek, B. Wood, G. B. Deacon, Jacinto Sá, Novel in situ methodology to observe the interactions of chemotherapeutical Pt drugs with DNA under physiological conditions, *Dalton Trans* 43 (2014) 13839–13844
2. J. Czapla-Masztafiak, J. J. Nogueira, E. Lipiec, W. M. Kwiatek, B. R. Wood, G. B. Deacon, Y. Kayser, D. L. A. Fernandes, M. V. Pavliuk, J. Szlachetko, L. Gonzalez, J. Sa, *Direct Determination of Metal Complexes' Interaction with DNA by Atomic Telemetry and Multiscale Molecular Dynamics*, *J Phys Chem Lett*, 8 (2017), 805–811
3. J. Czapla-Masztafiak, A. Kubas, Y. Kayser, D.LA Fernandes, W. M Kwiatek, E. Lipiec, G. B Deacon, K. Al-Jorani, B. R Wood, J. Szlachetko, J. Sa, *Mechanism of hydrolysis of a platinum (IV) complex discovered by atomic telemetry*, *J Inorg Chem*, 187 (2018), 56-61
4. W. Stańczyk, J. Czapla-Masztafiak, *The use of the X-ray absorption spectroscopy laboratory setup in the examination of copper(II) compounds for biomedical applications*, under review
5. J. Czapla-Masztafiak, J. Szlachetko, C.J. Milne, E. Lipiec, J. Sá, T.J. Penfold, T. Huthwelker, C. Borca, R. Abela, W.M. Kwiatek, *Investigating DNA radiation damage using X-ray Absorption Spectroscopy (XAS)*, *Biophys J*, 110 (2016), 1304-1311