

PHOTOFRAGMENTATION OF THE RADIATION THERAPY ENHANCERS: CAN WE MAKE BETTER ONES?

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Abstract. In this progress report, we show the results of two mass spectrometric experiments performed on a set of nitroimidazole-based radiosensitizers, medications that enhance radiation damage to the cancerous cells (Itälä et al. 2019 and 2020, Rockwell et al. 2009). We have incorporated a heavy element (Br and/or I) into the structure to introduce an additional function to the radiosensitizer. The idea here is that heavy element absorption hotspot locally enhances the radiation dose by generating secondary X-rays, photo- and Auger electrons, while the other part of the molecule produces sensitization-relevant species upon fragmentation (radicals originating from nitro group). Potentially it could increase the positive outcome from the radiation therapy, minimizing negative effects on normal cells. It is often difficult to interpret the results of clinical trials in the context of fundamental physical and chemical processes. Therefore, fundamental investigations on isolated molecules are crucial to determine directly the relationship between the structure of the radiosensitizer and its fragmentation outcome after X-rays absorption. We compare the results with non-halogenated references to evaluate the differences in the fragmentation dynamics using such methods as photoelectron-photoion-photoion coincidence (performed at MAX IV, FinEstBeAMS beamline) and near edge X-ray absorption mass spectrometry (performed at BESSY II, UES2_PGM beamline).

References

- Itälä, E.; Myllynen, H.; Niskanen, J.; González-Vázquez, J.; Wang, Y.; Ha, D. T.; Denifl, S.; Kuk, E. 2019, *J. Phys. Chem. A*, **123** (14), 3074–3079.
Itälä, E.; Niskanen, J.; Pihlava, L.; Kuk, E. 2020, *J. Phys. Chem. A*, **124** (27), 5555–5562.
Rockwell, S.; Dobrucki, I. T.; Kim, E. Y.; Marrison, S. T.; Vu, V. T. 2009, *Curr. Mol. Med.*, **9** (4), 442–458.