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Modeling the radiobiological effects of gold nanoparticles in proton therapy of glioblastomas

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Several studies show that the combination of high-Z nanoparticles and external radiotherapy leads to an increased radiation effect in tumoral cells without an increase of the patient dose. However, it is not yet clear how the sequence of physical, chemical, and biological mechanisms contributes to the observed synergic effect.
The objective of this work is to develop simulation tools that allow the analysis and interpretation of radiobiology studies with multifunctional nanoparticles (NPs). To do that, we will develop realistic simulations of the irradiation of monolayer (2D) and spheroid (3D) human glioblastomas multiforme (GBM) cell cultures, taking into consideration different concentrations and cellular and subcellular distributions of the gold nanoparticles (AuNPs).
The simulations will be implemented based on TOPAS [1] software more specifically the extension TOPASn-Bio [2] that includes models of the physical and chemical processes induced by radiation at the DNA scale. These must describe the laboratory experimental conditions of irradiation with X-rays, Co-60 sources and with proton beams considering the cell lines morphology and 2D and 3D cell culture scenarios. The construction of the computational cell models will be developed based on confocal microscopy images of the biological samples.
Based on the simulations, the dose distributions at the subcellular scale will be obtained, as well as the temporal distribution of the reactive oxygen species (ROS) induced by the different irradiation conditions, AuNPs distribution, and concentrations. The microdosimetric distributions in cells will be used to predict cell survival fractions, using standard mathematical models of the biological effects of radiation as Local Effect Model (LEM) [3], Nanodosimetric Oxidative Stress (NanOx) [4] and Microdosimetric Kinetic Model (MKM) [4].
The results obtained in the simulations will be compared with the biological in vitro and in vivo experimental results, which will include evaluation of cell viability and survival. Moreover, the simulated ROS yields will be also compared with the experimentally determined values.

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