AbstractID: 1346 Title: Computational modeling of radiation interaction and chemistry with a 167-base pair segment of DNA and comparison with experimental results

Introduction: One of the most confounding issues in the treatment of cancer is that two patients with the same diagnosis respond differently to the same treatment. The ultimate goal of this research effort is to better understand why this occurs. As a first step, the study presented here is performed to develop a system of computer codes to model the complex reactions between ionizing radiation and DNA. Methods: A mathematical atomistic model of a 167 base-pair B-DNA molecule was constructed using commercially available software packages. The probability of each possible fate of an •OH approaching to this 167 base-pair molecule was determined by implementing the "near-approach" DNA-radiation chemistry computational model described by Aydogan et al. (Radiat Res 157(1), 38-44, 2002) and compiled into an outcomes database. The secondary electron spectrum generated at depth in tissue by a Co-60 beam was modeled using the code MCNP 4.B. Two microdosimetry codes, OREC and RADLYS, originally developed at Oak Ridge National Laboratory, were adapted for this research. Attack sites were logged and single strand break (ssb) and double strand break (dsb) rates were calculated. Results: D_{0ssb} was found to be equal to 69.9Gy. Results of this study compare well with available experimental data.