CANCER PREVENTION & RESEARCH
INSTITUTE OF TEXAS

Award ID:
RP140478

Project Title:
Computational Chemistry Determination of DNA Damage Mechanisms in Proton Cancer Therapy To Optimize Its Clinical Use

Award Mechanism:
High Impact/High Risk

Principal Investigator:
Morales, Jorge

Entity:
Texas Tech University

Lay Summary:

Proton cancer therapy (PCT) uses high-energy proton projectiles to kill cancerous tumors with minimum damage on healthy tissues and without the side effects of X-Ray therapy. PCT is effective on non-spread cancers in the eyes, head, neck, lungs, prostate, and breast. The healing action of the protons results from their damage on cellular DNA. Because of their high rate of division and reduced ability to repair damaged DNA, cancerous cells are much more vulnerable to DNA attacks than normal cells and are killed at a higher rate. However, the mechanisms of DNA damage in PCT remain mostly unknown. That has prevented a rational design of PCT that can maximize its therapeutic power, minimize its side effects, and guide the construction of PCT equipment. The poor characterization of the PCT processes is due to the fact that even the most advanced experimental and clinical techniques cannot completely reveal the microscopic details of PCT, especially without risking human subjects. Inspired by the research of the 2013 Chemistry Nobel Laureates, we propose the computer simulation of PCT chemical reactions by using novel quantum-dynamics models. Thus, dangerous PCT reactions that cannot be tested in the human body will be innocuously run on computers. The proposed quantum-dynamics models have been created by the Principal Investigator following the electron nuclear dynamics theory and are implemented in his powerful computer code PACE. PACE will elucidate three essential types of PCT reactions: (1) The fragmentation of cellular water by colliding protons into harmful electrons, radicals, and ions; (2) the damage on DNA by the colliding protons; and (3) the damage on DNA by the electrons formed in (1). These simulations will bring about a unique way to understand and control PCT that at very low cost will drastically improve the treatment of cancer patients without risking human subjects.