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Experimental and Numerical Investigation of Polydopamine Nanoparticles for Enhanced Photothermal Cancer Therapy

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ABSTRACT

Photothermal therapies are considered to be a safe and promising choice for small, localized superficial tumors. During photothermal therapies, near-infrared light generates heat and selectively destroys the tumorous tissue. However, achieving precise control over the tissue heating confined only to the localized zone remains a challenge. Any deviation from the intended heating can lead to over-ablation, resulting in significant damage to the surrounding healthy tissue and critical structures, or under-ablation, which increases the chances of tumor recurrences. To overcome these challenges, administering nanoparticles within a target tumor has been proven to generate more precise heating and minimize damage to the surrounding healthy tissues, thereby increasing the overall efficacy of the procedure. The use of metallic nanoparticles (e.g., silver, gold) to enhance photothermal effects has received significant attention over the past decade. However, this approach introduces concerns regarding material toxicity and patient risk. Polymer-based nanomaterials, with their biocompatible and biodegradable properties, offer a promising alternative to address these complications, warranting further exploration. This study aims to investigate the potential of polymer-based nanoparticles composed of polydopamine (PDA) to enhance the effectiveness of photothermal therapies for cancer treatment. PDA nanoparticles are melanin-like structures synthesized through the oxidation of 3,4-dihydroxy-L-phenylalanine (DOPA) in an alkaline aqueous environment with oxygen, and their size can be easily controlled by adjusting the solution's pH. In this study, the influence of various concentrations of spherical PDA nanoparticles (1000, 400, 200, 100, 50, and 25 μg/mL) was explored through in vitro photothermal experiments. The temperature profile of the samples during 808 nm laser irradiation with an intensity of 1.4 W/cm^2 was captured with a thermal camera. A concentration-dependent relationship was identified, and the highest PDA concentration of 1000 μg/mL led to the largest temperature change of 19.4 °C. Furthermore, a finite element-based computational model was developed to quantify spatio-temporal thermal dynamics across different PDA nanoparticle concentrations. The absorption cross-sections of individual PDA nanoparticles were derived using Maxwell's equations and extrapolated to different concentrations. The computational absorption spectrum was compared to experimental data obtained using a spectrophotometer, highlighting reasonable agreement. Beer-Lambert's law was then applied to model the heat transfer within the nanoparticle suspension utilizing a Gaussian laser profile across different concentrations. The model was validated against experimental in vitro photothermal data of maximum attained temperature, and a parametric sensitivity analysis was conducted to assess the impact of laser power and nanoparticle size on the efficacy of nanoparticle-assisted photothermal therapy. Both experimental and computational results highlight the significance of nanoparticle concentration, size, and laser power in improving the photothermal response of polymer-based nanoparticles. The optimal nanoparticle parameters generating enhanced photothermal effects have also been identified based on parametric sensitivity analysis. This study offers valuable insights into the future advancements and clinical translation of precision photothermal therapy, benefiting millions affected by cancer.

Keywords: Thermal ablation, cancer treatment, polydopamine nanoparticles, photothermal therapy, heat transfer, computational modeling.

Conflict of Interest: The authors declare that they have no conflict of interest.