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Multiple-Scale Computational Studies of Redox-Controlled Supramolecular Co-Assembly Nanoplat form: Toward Immunochemotherapy-Driven Antitumor Augment

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1. Abstract

Programmed cell death protein 1 (PD1)/programmed death ligand 1 (PD-L1) blockades provide an effective and safe therapeutic option in the field of refractory cancer therapy. However, not more than 30% response rate of most cancers seriously impedes their therapeutic efficacy. Previous investigations have proved the effectiveness of combining chemotherapy with immunotherapy for unsatisfactory response to anti-PD1. However, there is a lack of methodologies promoting researchers to rationalize co-delivery system of chemotherapeutic agents and PD-1 inhibitors in order to enhance the immunochemotherapeutic efficiency in difficult-to-treated tumors. Herein, chemotherapeutic agent (Doxorubicin, DOX)/small molecular PD-1 inhibitor (BMS-202)-citronellol conjugates were designed using disulfide bond. This novel dual-prodrug supramolecular co-assembly modality is developed to serve as a model co-delivery nanoplatform for immunochemotherapeutic synergistic cancer therapy. Using multiple scale computational studies including density functional theory (DFT) calculation, atomistic molecular dynamics (MD) simulations and dissipative particle dynamics (DPD) simulations, we greatly observed the structure change of PD-1 protein upon BMS-202 binding. Original analyses of assembly/release of supramolecular co-assembly nanoplatform revealed a distinct pattern between both bonds (disulfide bond and carbon-carbon bond), which can be associated to the bond angle/energy differences. As we know, this work confirmed the ability of computational simulation investigations for the first time to design the *in silico* promising nanomedicine for clinical immunochemotherapy-driven cancer therapy.

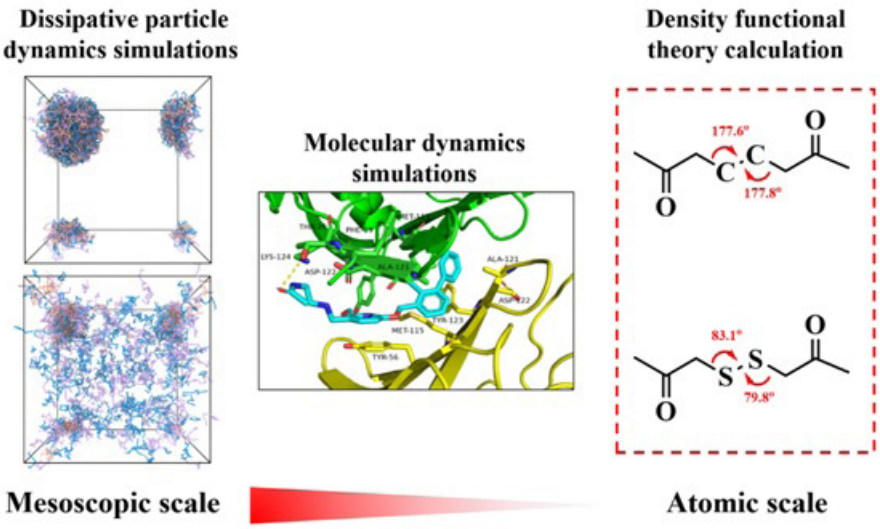

Figure 1: Schematic representation multiple-scale computational studies of redox-controlled supramolecular co-assembly nanoplatform for anti-tumor immunochemotherapy.