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<u>Entitled</u>

DESIGN, SYNTHESIS AND CHARACTERIZATION OF ZINC AND GOLD-BASED METAL-ORGANIC FRAMEWORKS AND COMPLEXES FOR THE DETECTION AND TREATMENT OF CANCER

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<u>Abstract</u>

The early detection of cancer plays a pivotal role in improving patient outcomes, emphasizing the urgent need for highly sensitive and selective biosensing platforms. Metal-Organic Frameworks (MOFs) have emerged as promising candidates in this domain due to their tunable properties, large surface area, and high porosity. Herein, the utilization of zinc-based MOF as a sophisticated biosensing platform tailored for the precise detection of the HER2 cancer biomarker is presented. HER2, a critical protein marker in breast cancer diagnostics and treatment, demands highly selective and accurate detection methods for effective patient management. Simple hydrothermal synthesis methodology has been adopted to synthetize zinc-based MOF while the structural properties of this MOF are thoroughly examined to elucidate its inherent advantages in biosensing applications. Based on the tunability of MOF, functionalization strategies and surface engineering were employed to enhance the specificity of zinc-based MOF towards HER2. Additionally, incorporating advanced fluorescent ligand provides a robust fluorescent-based assay for the sensitive detection of HER2. To comprehend the interaction between the protein and zinc-based MOF, a computational docking was operated. Cancer treatment has long been a challenging endeavor, prompting researchers to explore innovative approaches. One promising avenue involves the use of organic-inorganic hybrid structures, which offer unique advantages in targeting cancer cells. Herein, investigating the efficacy of employing such hybrid structures in cancer treatment, particularly focusing on their performance in Fenton reaction and chemodynamic therapy (CDT) was implemented. Utilizing organic-inorganic hybrid nanostructures including MOFs, Coordination Polymers (CPs) and organic/inorganic complex as anticancer agents have shown promise as efficacy in combating cancer. The influence of small size on activity is examined, elucidating how nano-scale dimensions enhance therapeutic outcomes by facilitating cellular uptake and targeted delivery. Furthermore, the selection of biocompatible inorganic elements such as gold and zinc has demonstrated significant efficacy in cancer treatment while ensuring safety towards normal cells. On the other hand, the choice of organic ligands is explored, highlighting its fundamental role in modulating the reactivity and selectivity of hybrid structures in cancer treatment. Through a comprehensive analysis of experimental data, valuable insights into optimizing the design of organicinorganic hybrid structures for enhanced efficacy in cancer therapy have been revealed, thereby contributing to the advancement of precision medicine and personalized treatment approaches.

Keywords: Zinc-MOF, MOF, Biosensing, Fluorescence, HER2, Cancer, Coordination Polymer, Gold Complex, Nanoparticles, Chemodynamic Therapy (CDT).