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A Study on the Nanoscale Metal-Organic Frameworks(NMOFs) for the Treatment of Pancreatic Ductal Adenocarcinoma (PDAC) JI YOON KOH, RICHARD KYUNG, Choice Research Group — Due to increased surface area, porosity, and functionality, Metal-organic-frameworks (MOFs) have potential to be effective in cancer diagnosis and treatment. This project examines new effective targeted nanoparticle molecules for Pancreatic Cancer Therapy (PCT). Metalorganic frameworks (MOFs), also called coordination polymers or coordination networks, are hybrid materials formed by metals ions and bridging ligands, typically under mild conditions. Due to limitless combinations of metals and ligands, physicochemical properties of MOFs can be tuned for specific applications. NMOFs can be used as delivery vehicles for imaging agents and drug molecules, possessing potential advantages over existing nanocarriers. When linked to appropriate cell-targeting molecules, the NMOFs can be selectively and efficiently delivered to tumors to allow for early diagnosis and effective treatment of pancreatic cancer. In this paper, open-source molecular editing program with an auto-optimization feature that determines the theoretical values of the structures atomic properties is used to model the NMOFs. It allows users to build virtually any molecule with the optimized geometry according to the various force field options.

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