Design of Metal Organic Frameworks and their application in anti-cancer drugs by machine learning

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This study explores metal–organic frameworks (MOFs) as advanced carriers for anticancer drug delivery, leveraging their high porosity, stability, and biocompatibility. By integrating machine learning (ML) with experimental and computational analyses, a predictive framework was developed to optimize MOF design and accurately model drug-release behavior. Various ML algorithms were evaluated to predict MOF functionality and guide the rational design of customized delivery systems. The results demonstrate that ML-assisted MOF engineering enables precise control over drug release, supporting optimized dosing strategies and personalized cancer treatment. Overall, this work highlights the strong synergy between materials science and machine learning in advancing next-generation drug delivery technologies.

Keywords:
Metal-Organic Frameworks (MOFs), Drug delivery Systems, Machine learning(ML)

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