DIGITAL DISCOVERY OF METAL-ORGANIC CAGES FOR NEXT-GENERATION THERAPIES

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The project focuses on the design and optimization of metal–organic cages (MOCs) as advanced nanocarriers for drug delivery. Thanks to their tunable architecture and physicochemical properties, MOCs are particularly promising for the selective transport of drugs. The objective is to develop a computational platform that integrates molecular modeling and machine learning (ML) to efficiently and reliably explore vast chemical spaces, overcoming the traditional trial-and-error approach and generating MOCs with target properties defined "by design." The structural and physicochemical properties, along with the drug-complexation abilities of specific drug classes across a wide set of MOCs, will converge in the construction of a FAIR database, which will be made accessible at the end of the project. This database will serve both as a guide for informed design and as a training set for ML and deep learning algorithms, enabling the prediction of properties of MOCs relevant to user-defined needs.

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