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Houk-Jung Organic Colloquium

NaviCat: Computational Tools to Navigate Molecular Catalyst Landscape

Abstract: Over the last few years, we have worked on an assortment of computational and digital tools aimed at accelerating the through exploration and optimization of homogeneous catalyst landscapes. These interoperable tools are assembled into the NaviCat (Navigating Catalysis) platform, which includes: volcanic, an automated generator of volcano plots and activity/selectivity maps; NaviCatGA, a genetic algorithm-based catalyst optimizer; and additional pipelines that generate structures, create catalyst libraries as well as statistical models and representations specifically developed to accelerate the exploration process. The complementary nature of these tools will be demonstrated through optimizing the catalytic activity and selectivity of both prototypical classes of reactions and challenging organic processes. Overall, the NaviCat platform aims to expand upon original data-driven tools and broaden their application in the field of computational homogeneous catalysis.

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