Navigating homogeneous catalyst landscapes

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Homogeneous transition metal catalysts are highly active and selective. However, the design of new catalysts for specific asymmetric transformations is challenging due to the endless possibilities in ligand design. Based on Sabatier's principle, molecular volcano plots are a key tool to identify the most promising catalyst for a given transformation and guide experimental efforts in the right direction. Here, we will detail the latest generation of molecular volcano plots, including explicit microkinetic modeling, and combine them with generative models and machine learning algorithms to navigate the landscape of homogeneous catalysts. Furthermore, in the NaviCat platform, we build interoperable open source tools to share these methodologies with the broader computational catalysis community.

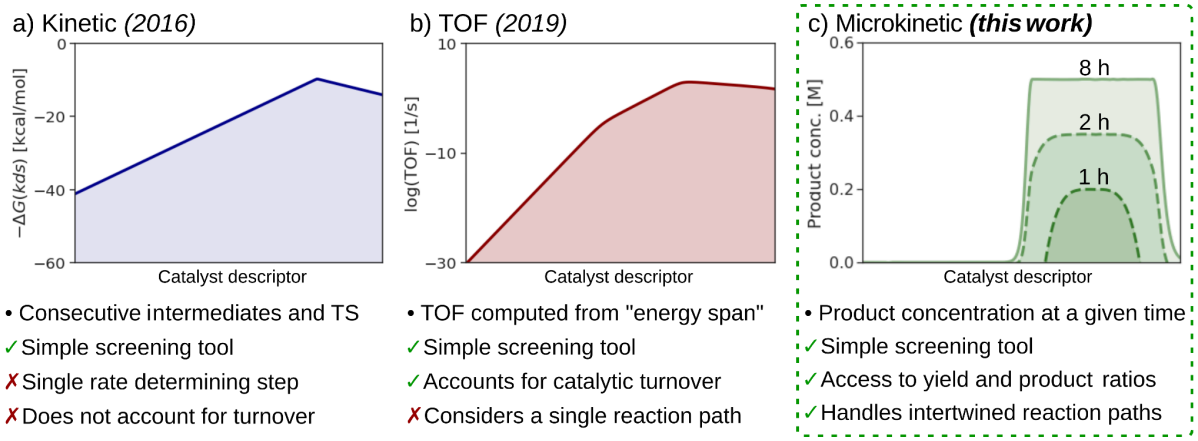

Fig. 1. Generations of molecular volcano plots.