Database of metal-phosphine complexes and its application to the prediction of the catalytic abilities using machine learning

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In recent years, in silico screening using machine learning (ML) has attracted attention in the development of new catalysts and is expected to improve development efficiency. However, experimental data on catalytic abilities are generally scarce, and the number of features applicable to catalysts with different skeletons is limited, making it difficult to construct ML models. To address these challenges, we propose a novel strategy for metal complex catalysts that utilizes the reaction energies and activation barriers of elementary reactions as features of catalysts. To validate our strategy, we constructed ML models predicting the catalytic abilities of the Pd-catalyzed reductive conversion of acyl fluoride. According to the previous research, this catalytic reaction afforded two products, which were obtained via the pathways with and without decarbonylation, respectively, and their yields depended on the phosphine ligands. The results of ML models indicated that the features of reaction energies, as well as activation barriers, are effective for predicting the yield of product with decarbonylation and not for another.