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Predicting highly enantioselective catalysts using tunable fragment descriptors

Nobuya Tsuji[1†]*, Pavel Sidorov[1†]*, Chendan Zhu[2], Yuuya Nagata[1], Timur Gimadiev[1], Alexandre Varnek[1, 3]*, and Benjamin List[1, 2]*

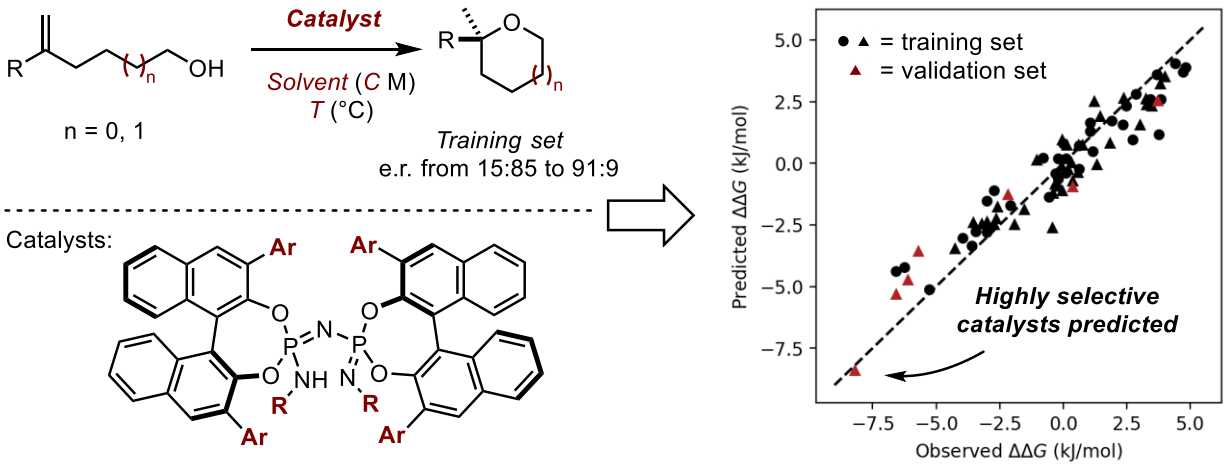
[1]WPI-ICReDD, Hokkaido University, Sapporo 001-0021, Japan

[2]Max-Planck-Institut für Kohlenforschung, D-45470 Mülheim an der Ruhr, Germany

[3]Laboratory of Chemoinformatics, University of Strasbourg, 67081 Strasbourg, France

E-mail: tsuji@icredd.hokudai.ac.jp, [†]Equal contribution.

Catalyst optimization processes typically rely on inductive and qualitative assumption of chemists based on screening data. While machine learning models using molecular properties or calculated 3D structures enable quantitative data evaluation, costly quantum chemical calculations are often required. In contrast, readily available binary fingerprint descriptors are time- and cost-efficient, but their predictive performance remains insufficient.[1] In this presentation, we describe a machine learning model based on fragment descriptors, which are fine-tuned for asymmetric catalysis and represent cyclic or polyaromatic hydrocarbons, enabling robust and efficient virtual screening. Using training data with only moderate selectivities, we designed theoretically and validated experimentally new catalysts showing higher selectivities in a previously unaddressed transformation.[2]



Reference

1. Review: Zahrt, A. F.; Athavale, S. V.; Denmark, S. E. *Chem. Rev.* **2020**, *120*, 1620-1689.
2. Tsuji, N.; Sidorov, P.; Zhu, C.; Nagata, Y.; Gimadiev, T.; Varnek, A.; List, B. *ChemRxiv*, **2022**. DOI: 10.26434/chemrxiv-2022-bsmdl

Nobuya Tsuji
Max-Planck-Institut für Kohlenforschung (Ph.D., 2018).
Postdoctoral Researcher, University of California, Berkeley (2019).
Specially appointed assistant professor, WPI-ICReDD, Hokkaido university (2020-).
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