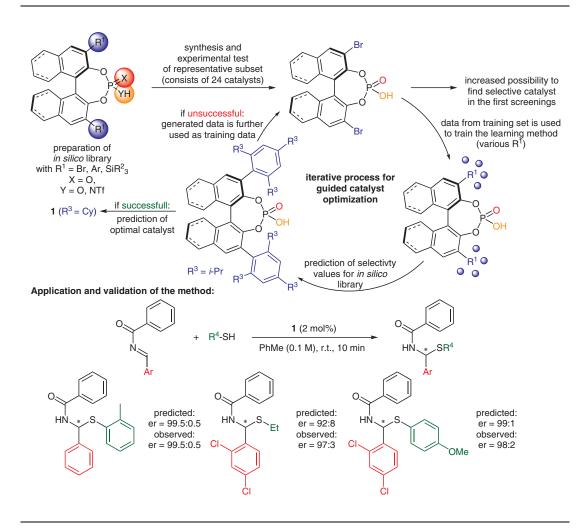
A. F. ZAHRT, J. J. HENLE, B. T. ROSE, Y. WANG, W. T. DARROW, S. E. DENMARK* (UNIVERSITY OF ILLINOIS, URBANA, USA)

Prediction of Higher-Selectivity Catalysts by Computer-Driven Workflow and Machine Learning *Science* **2019**, 363, DOI: 10.1126/science.aau5631.

Application of Chemoinformatics in Asymmetric Catalysis



Significance: Denmark and co-workers report a computer-driven workflow and a machine-learning method that is capable of predicting the enantio-induction of a range of chiral phosphoric acids in *N*,*S*-acetal formation. The mathematical model is based on a new descriptor introduced by the authors, i.e. the average steric occupancy, which considers the variability of catalyst conformations and describes points in a 3D space in which a given catalyst resides. The mathematical model is iteratively trained with experimental data, leading to a system that can predict selectivities for catalysts that have not been experimentally tested.

Comment: The concept of model-driven method development has far-reaching implications in and beyond the chemical community. However, computer-driven workflows have hitherto not proven capable of predicting experimental results beyond data collected empirically. By describing the population of a catalyst and its conformers in space, a key factor in asymmetric induction, Denmark and co-workers have successfully expanded the utility of such processes, permitting accurate predictions outside the range of the training set. We look forward to the implementation of such a model in systems with greater complexity and in providing solutions to actual problems.

SYNFACTS Contributors: Benjamin List, Joyce A. A. Grimm Synfacts 2019, 15(04), 0419 Published online: 19.03.2019 **DOI:** 10.1055/s-0037-1612338; **Reg-No.:** B01519SF

Organo- and Biocatalysis

Key words

chiral phosphoric acids catalyst design chemoinformatics acetals artificial intelligence

