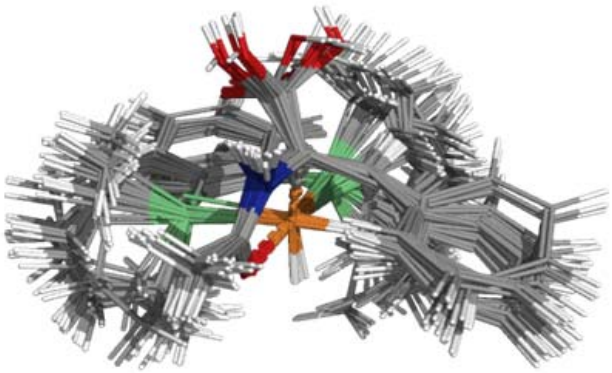
PREDICTING REACTION SELECTIVITY

Per-Ola Norrby

Data Science & Modelling, Pharmaceutical Sciences, R&D,
AstraZeneca, Gothenburg, Sweden

Detailed knowledge of reaction mechanism will in principle allow prediction of the various possible outcomes, the reaction selectivity. Reactions are usually explored using quantum chemical methods such as DFT. However, such methods are too slow to allow a full exploration of all possible reaction paths for conformationally complex molecules. We explore more efficient and more accurate methods, combining features from different levels of quantum mechanics, combined with rapid molecular mechanics methods as well as with machine learning from available data. Here, I will exemplify such approaches for regioselectivity predictions, and then focus on accurate predictions of stereoselectivity using our in-house method Q2MM.



Conformational sampling of a TS for asymmetric hydrogenation