Developing Data Science Tools for Synthetic Chemists

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The optimization of catalytic reactions for organic synthesis can be challenging as the interplay between the catalyst structure, reaction conditions, and substrates involved is a complex multidimensional problem. In other words, it is difficult to ascertain the pattern within the noise to offer a complete picture of how to optimize and/or interpret why a certain set of conditions are required for a particular reaction. Therefore, we have aimed to develop several data science and machine learning tools that assist in designing the proper experiments to facilitate the analysis of structure function relationships while also providing platforms for reaction optimization. Specifically, we have used new methods to develop descriptors for complex molecular architectures as well as data science methods to discern how these catalysts interact with a range of substrate types. This lecture will outline how we have put into practice a workflow that integrates data science tools, physical organic chemistry, and experiments with a focus on new case studies on a broad array of chemical processes.

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Sigman Biography: Matt Sigman was born in Los Angeles, California in 1970. He received a B.S. in chemistry from Sonoma State University in 1992 before obtaining his Ph.D. at Washington State University with Professor Bruce Eaton in 1996 in organometallic chemistry. He then moved to Harvard University to complete an NIH funded postdoctoral stint with Professor Eric Jacobsen. In 1999, he joined the faculty of the University of Utah where his research group has focused on the development of new synthetic methodology with an underlying interest in reaction mechanism. His research integrates the study/development of new chemical reactions with the invention of new data science approaches to reaction interrogation and optimization. He currently holds the rank of Distinguished Professor.

Sigman's research efforts have been recognized by several awards including the Pfizer Award for Creativity in Organic Chemistry (2004), the Camille and Henry Dreyfus Teacher Scholar Award (2004), the Arthur C. Cope Scholar Award (2010), the University of Utah Distinguished Research Award (2011) and ACS Award for Creative Work in Synthetic Organic Chemistry (2017). Additionally, he has been recognized for outstanding teaching at the University of Utah as highlighted by being named the University of Utah Distinguished Honors Professor (2008), the Robert W. Parry Award (2009) and Distinguished Teaching Award (2022).