

# Richard F. Heck Lectureship

In person/ zoom <https://udel.zoom.us/j/99759540951>

101 BRL

Wednesday, March 22, 2023, 4pm

## *Data Science Meets Organic Chemistry*



**Matthew Sigman Ph.D.**  
University of Utah

The optimization of catalytic reactions for organic synthesis is difficult as the interplay between the ligand, 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 interrupt why a certain set of conditions are required for a particular reaction. Therefore, we have aimed to develop several data science-based tools that assist the rapid analysis of structure function relationships to reveal the underlying reasons for improved performance of substrates and catalysts. 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 reaction optimization with a focus on new case studies in bio and organo-catalytic processes.

Light refreshments served in Brown  
Lab Lobby at 3:45



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