SPRING 2022 CHEMISTRY SEMINAR SERIES

DR. TIMOTHY A. RHODES

Materials & Biophysical Characterization Analytical Research & Development

Merck & Co., Inc. Rahway, NJ

HOST: DR. GALOPPINI

ALL THOSE INTERESTED ARE WELCOME TO ATTEND

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"Predicting Pharmaceutical Product Performance through Modeling, Machine Learning and Statistics"

Friday, February 11, 2022, 11:30 AM

Life Science Center II, Room 130

Abstract: The delivery of novel pharmaceuticals to address unmet medical needs to patients is a long and arduous path, historically on the order of 10 years from target identification to commercial launch. In the case of some therapeutic areas, such as cholesterol lowering therapeutics, the impact of these time scales on human health is not always readily obvious. In oncology, long development times can have a stark impact literally measured in lives lost. We have also seen firsthand in the last few years how advances in the development of vaccines and the associated diagnostics can dramatically alter global morbidity numbers. Therefore, any advances we can make that shorten development timescales not only has financial benefits but also can have profound benefits to global human health.

This talk will focus on advances in modeling, machine learning and the application of statistics to challenges in developing pharmaceutical products. Our group is focused on advancing novel computational approaches, in concert with experimentation, that can help us forecast product performance over long time-scales, typically physical and chemical stability, or drug release rates, or extrapolating across compositional space or across scales. These concepts will be illustrated through a few examples ranging from machine deep learning applications applied to 3D XRCT imaging of small molecule formulations and coarse grain modeling applied to protein therapeutics in understanding protein aggregation risk. These examples will illustrate how experimental measurements on fresh samples can be used in conjunction with modeling to predict macroscopic behaviors at longer time scale or, in contrast, modeling can be applied to predict experimental observables at later times.

We view the seamless integration of modeling and statistical approaches as becoming an integral part of any robust experimental plan. Today, we need to have a close collaboration between colleagues to achieve this as the skillsets don't generally reside within any one individual.

Biographical sketch: As Senior Principal Scientist in the Materials and Biophysical Characterization organization, Tim is responsible for managing the development of predictive models and tools to drive faster and better decision making. The efforts comprise challenges in both small and large molecule and span both formulation process and composition and influencing compound selection coming into the development space from discovery labs. This current focus is a natural evolution of Tim's prior role in developing and supporting high throughput automation where large datasets were being generated but efforts largely stopped at providing empirical guidance to formulation project teams.

Tim earned a B.S. in chemistry from New York University and a Ph.D. in organic chemistry from the University of Texas at Austin. Prior to joining Merck in 1999, he conducted post-doctoral research at the NSF Center for Photoinduced Charge Transfer Studies at the University of Rochester. His group's current focus includes applications of machine deep learning and coarse grain modeling to drive a deeper understanding of our materials performance during formulation development, spanning both small and large molecule formulation challenges.