Department of Chemistry and Biochemistry

Organic/Inorganic Seminar Series presents

Leah Frye, Ph.D.

Schrödinger Pharmaceuticals

Vice President, Drug Discovery Group

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Seminar: 2:30–3:30 pm, 331 KLA ❖ Coffee reception @ 2:00 pm, 377 KLA

"Computational Chemistry-Driven Drug Discovery: Structure to Man"

ABSTRACT: The development of drugs is a long, arduous and costly endeavor. Clearly, approaches that increase the efficiency and probability of success in the overall process should ultimately reduce costs and shorten the time to market. In the past few decades, it has become clear that computational methods can greatly facilitate the development of small molecule drugs. This talk will introduce the drug discovery process and discuss how structure-based computational approaches are utilized in the pharmaceutical industry. Computational methods for identifying lead compounds and their optimization to clinical candidates will be presented. Two real world examples will be provided that demonstrate the overall process, including one that resulted in the initiation of a clinical study in April of 2015.

**** Hosted by Vickie DeRose ****