We model molecular toxicity pathways to understand how chemicals affect biological systems and develop methods that systematize the analysis of large amounts of high-throughput data to predict their toxic effects. These tools facilitate countermeasure development and provide diagnostics for toxic exposure. In this talk, I will present an approach to identify organ-specific injury signatures associated with toxic insults. Modules, or gene groups associated with specific adverse outcomes, offer a source of potential diagnostic biomarkers. We explore unbiased systems approaches to identify toxicity modules for specific histopathologies of liver and kidney injuries. We aim at identifying molecular toxicity pathways associated with such injuries (e.g., fibrosis and necrosis); developing and validating biomarkers in animal models; examining \textit{in vitro–in vivo} correlations; and studying specific chemical exposures in detail. I will also present an \textit{in silico} modeling platform for Adsorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) endpoints. We develop \textit{in silico} models, which enable rapid high-throughput screening for different ADMET assay endpoints, and are thereby suitable for pre-clinical evaluation of drugs and countermeasures. To enable prioritization of drug candidates, we develop computational tools, for example, which rapidly screen compounds to assess AMES mutagenicity, hERG for cardiac toxicities, drug efflux via P-glycoproteins, and drug metabolism via cytochrome P450 enzymes.

\textbf{BIO}

Dr. Patric Schyman is a scientist at the Biotechnology HPC Software and Application Institute (BHSAI) in Frederick, Maryland. He received his postdoctoral training in computational chemistry under Prof. William Jorgensen at Yale University under Prof. Sason Shaik at The Hebrew University in Jerusalem, Israel. Dr. Schyman received his Ph.D. in Physical Chemistry at Stockholm University in 2008 and his M.Sc. in Physics at Uppsala University in 2003. Dr. Schyman’s research interests involve developing chemoinformatics- and bioinformatics-based models to identify pharmacokinetic and toxicity properties of drug-like molecules and military-relevant chemicals.

\textbf{Patric Schyman, Ph.D.}
Research Scientist
Biotechnology HPC Software Applications Inst. (BHSAI)

\textbf{Friday, April 27, 2018}
SEH B1220
2:00-3:00 pm
Refreshments will be served at 1:45 p.m.