



Einladung zum Wilhelm-Ostwald-Institutskolloquium

Am **Mittwoch, dem 04.03.2020, 16:15 Uhr**, spricht

Prof. W. Scott Hopkins, PhD

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im Raum 429, Technikum Analytikum, Linnéstr. 3, 04103 Leipzig

zum Thema:

Determining Physicochemical Properties with Differential Mobility

Abstract

Differential Mobility Spectrometry (DMS) is an analytical technique that is often used to separate isomeric, conformeric, and even tautomeric species based upon their subtly different interactions with a gas-phase environment. By using DMS to assess the interaction propensities between drug molecules and solvent vapor, we have identified correlations between drug microsolvation and several condensed phase drug properties. Our measurements, which can be conducted in seconds using only nanograms of sample, and supporting electronic structure calculations provide insight regarding the subtle effects of geometric and electronic structure on *in vitro* drug properties. By introducing machine learning techniques, we have developed highly accurate models for assessing a suite of molecular properties including pKa, solubility, collision cross section, Log D, and cell permeability.

In this seminar, I will discuss our most recent results – which includes the introduction of trapped ion spectroscopy – and I will provide a perspective for future directions in this research.