OCCI Lecture

Speaker: Prof. Lars Konermann
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Title: A Journey Through Protein Mass Spectrometry: Enzyme Mechanisms, MD Simulations and "Supercharged" Proteins

Date, Time and Place: Friday, March 3, 10 am, TB342

Electrospray ionization (ESI) allows the production of desolvated ions from proteins and protein complexes in solution. Analysis of these gaseous biomolecules by mass spectrometry reveals the nature of protein interaction partners. Ion mobility spectrometry and various dissociation experiments provide additional insights. This presentation will focus on two research directions that are being pursued in the Konermann laboratory. At the very "fundamental" end of the spectrum, we conduct experiments and molecular dynamics simulations to uncover the ESI mechanism, and for understanding how proteins respond to the transition from solution into the gas phase. Our work also has a more "applied" side, where hydrogen/deuterium exchange techniques are being used to decipher the inner workings of proteins in solution. This presentation will highlight recent experiments on ATP synthase, the world's smallest rotational motor, as well as studies on the relationship between enzyme function and dynamics.

Selected Publications:

"Load-dependent destabilization of the γ-rotor shaft in F_0F_1 ATP synthase revealed by H/D-exchange mass spectrometry" S. Vahidi, Y. Bi, S. D. Dunn, and L. Konermann *PNAS 113*, 2412 (2016).

"Evidence for Allosteric Enzyme Regulation via Changes in Conformational Dynamics: An H/D Exchange Investigation of Dihydrodipicolinate Synthase" M. A. Sowole, S. Simpson, Y. V. Skovpen, D. R. J. Palmer, and L. Konermann *Biochemistry 55*, 5413 (2016).

"Collision-Induced Dissociation of Electrosprayed Protein Complexes: An All-Atom Molecular Dynamics Model with Mobile Protons" V. Popa, D. Trecroce, R. G. McAllister, and L. Konermann *J. Phys. Chem. B*, *120* 5114 (2016).

"Mechanism of Protein Supercharging by Sulfolane and m-NBA: Molecular Dynamics Simulations of the Electrospray Process" H. Metwally, R. G. McAllister, V. Popa, and L. Konermann *Anal. Chem. 88*, 5345 (2016).

"Release of Native-Like Gaseous Proteins from Electrospray Droplets via The Charged Residue Mechanism: Insights from Molecular Dynamics Simulations" R. G. McAllister, H. Metwally, Y. Sun, and L. Konermann *JACS 137*, 12667 (2015).