



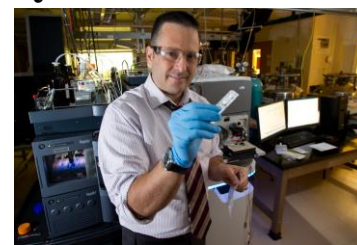
## Department of Chemistry & Biochemistry Seminar

Friday, March 12<sup>th</sup>, 2021

1:30pm – 2:45pm

**Zoom ID: 960 452 0800**

**Password: Cascade**



### *“New Developments in Mass Spectrometry-based Metabolomics”*

**Speaker:** *Dr. Facundo M. Fernandez, Georgia Institute of Technology*

**Abstract:** The highly dynamic nature of metabolites and their abundances makes metabolomics a powerful endpoint of the ‘omics’ cascade, yielding a molecular profile that is closest to the physiological phenotype. Metabolomic profiles are therefore sensitive to subtle perturbations observed in early disease stages or disease progression, which may be difficult to detect at the proteome or transcriptome levels. Human diseases are multi-factorial in nature, and studying small parts of their associated molecular changes is generally insufficient for understanding the full spectrum of disease phenotypes.

The metabolome is the total collection of biologically-active small molecules with molecular weights lower than about ~1.5 kDa in an organism. This includes endogenous molecules that are biosynthesized by metabolic networks in “primary metabolism”, specialized “secondary metabolite” signaling or defense molecules, molecules derived from diet or environmental exposures (the exposome), and molecules derived from the biosynthetic interactions with associated microbes (the microbiome). Metabolomics can either be “targeted” to a set of known compounds, for example certain lipids, or “non-targeted”, which attempts to detect and relatively quantify as many metabolites as possible.

The vast chemical diversity of the metabolome (lipids, sugars, amino acids, etc.), and its wide dynamic range (mM to fM) implies that no single analytical method can adequately profile all metabolites in one metabolomics experiment. Along these lines, the “fusion” of mass spectrometry (MS) and nuclear magnetic resonance spectroscopy (NMR) is emerging as one of the most powerful avenues to increase metabolome coverage. Nested separations that work in a time frame compatible with mass spectrometry, such as those performed by ion mobility, are also playing a key analytical role in metabolomics as a way of increasing peak capacity, and identifying metabolites through ion mobility collision cross section measurements. Further, localization of metabolites at the tissue level with imaging mass spectrometry experiments, allows linking their abundance with changes observed in biofluids. In this seminar, I will highlight progress along these various fronts, with emphasis on the detection, screening and treatment of complex diseases such as prostate and ovarian cancer, cystic fibrosis and traumatic brain injury.

**Biography:** Prof. Facundo M. Fernández was born in Buenos Aires, Argentina. He received his MSc in Chemistry from the College of Exact and Natural Sciences, Buenos Aires University in 1995 and his PhD in Analytical Chemistry from the same University, in 1999. In August 2000, he joined the research group of Prof. Richard N. Zare in the Department of Chemistry at Stanford University. His work focused on several aspects of Hadamard transform time-of-flight mass spectrometry with an emphasis on coupling this technique to capillary-format separation methods. In 2002, he joined the group of Prof. Vicki Wysocki in the Department of Chemistry at the University of Arizona, to develop novel tandem mass spectrometers for gas-phase peptide ion studies. In 2004 he joined the School of Chemistry and Biochemistry at the Georgia Institute of Technology where he currently holds the position of Vasser-Woolley endowed Professor in Bioanalytical Chemistry and Associate Chair. He is the author of over 180 peer-reviewed publications and numerous invited presentations at international conferences. He has received several awards, including the NSF CAREER award, the CETL/BP Teaching award, the Ron A. Hites best paper award from the American Society for Mass Spectrometry, and the Beynon award from Rapid Communications in Mass Spectrometry, among others. He serves on the editorial board of the Journal of the American Society for Mass Spectrometry (JASMS) and The Analyst, and in 2020 he started serving as an Associate editor for JASMS. His current research interests include the field of metabolomics and the development of new ionization methods and ion mobility tools for probing composition and structure in complex molecular mixtures.