

DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE
SEMINAR SERIES
SPRING 2023

WEDNESDAY, APRIL 12, 2023
TIERNAN HALL – LECT. HALL 2
1:00PM-2:20PM

GUEST SPEAKER

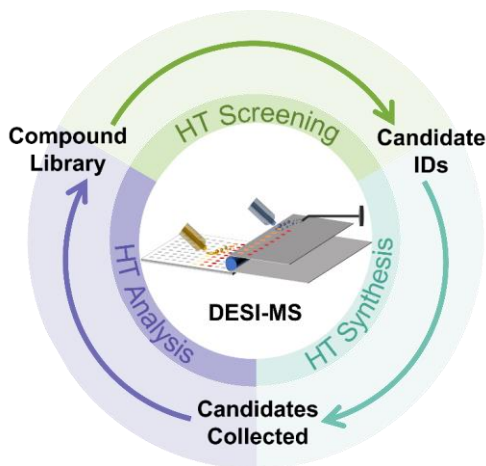
Dr. Graham Cooks
Distinguished Professor at Purdue University and
Fellow, National Academy of Sciences and National Academy of Inventors
Purdue University
West Lafayette, IN

TOPIC

Mass Spectrometry for Chemical Synthesis and Analysis

ABSTRACT

This talk will describe a new approach to **Drug Discovery using DESI-MS** for reaction screening, small scale synthesis and bioassays. DESI (desorption electrospray ionization) is an ionization method that uses solvent droplets to sample and ionization compounds at atmospheric pressure. It can be used for **molecular imaging or for diagnostics**, including intrasurgical diagnostics. Here we apply it with high throughput robotics to perform reaction screening (e.g. 6,144 reaction mixtures in ca. 1 hr) sampling reaction mixtures at rates of one mixture/sec. **Accelerated reactions** occur on the secondary droplets generated in DESI as they move towards the mass spectrometer so that reaction products are recorded by MS. The droplets can, alternatively, be deposited on a collector surface for small-scale (low ng amounts) **high-throughput synthesis**. The resulting reaction products are then used in bioassays, so that DESI-MS performs the full cycle of reaction optimization, small scale synthesis and biological testing. Examples discussed will include (i) synthesis and then bioassays after late stage functionalization of opioid agonists and antagonists, the bioactivity of which is determined in competitive binding assays and (ii) screening of compound libraries for inhibition of **enzymatic activity** of a sulfotransferase relevant to prostate cancer. Work supported by **NIH NCATS 1UG3TR004139**



BIO

R. Graham Cooks Distinguished Professor at Purdue University and Fellow, National Academy of Sciences and National Academy of Inventors, is a recipient of the Dreyfus Prize. He has served as major professor to 150 PhD students. Research interests include 1) ambient ionization and tandem mass spectrometry analysis of complex mixtures, 2) mass spectrometry in cancer diagnostics and 3) high-throughput synthesis and analysis techniques. Prof. Cooks has published over 1500 research articles, ranks among the most cited chemists worldwide. Several start up companies have emerged from his laboratory.

Seminar Coordinator:

Dr. Genoa Warner – grw4@njit.edu
Dr. Lijie Zhang - lijie.zhang@njit.edu