Design and Performance of a Person-portable Two-dimensional Tandem Mass Spectrometer for Machine-Learning Enhanced Identification of Threats

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Abstract

There is an urgent need for high sensitivity chemical detectors for untargeted threat detection. The proliferation of novel, cheap synthetic drugs of high toxicity has made clear that current detection solutions are insufficient when new chemical variants, often of higher toxicity than the original threat molecule, can be created easily and at low cost and then distributed worldwide. Fentanyls and nitazenes are two classes of synthetic opioid narcotics that have proliferated over the last decade, causing tens of thousands of overdose deaths every year since 2017 and showing little sign of abating despite intensified public health efforts and greater attention from law enforcement. Other chemical threats such as chemical warfare agents continue to see sporadic usage against civilian populations. A prominent 21st century example was the use of sarin gas in an August 2013 attack in Ghauta, Syria, killing more than 1,000 people and injuring thousands more. These instances highlight the need not only for highly sensitive, selective, and broadly applicable chemical detectors, but also the desire for more advanced software and algorithms so that existing tools are more adaptable to existing and emerging threats.

Current fieldable and man-portable mass spectrometers, both GC-MS and direct sampling MS (DSMS) systems, rely on comparison of experimental data acquired in the field to libraries of spectra onboard the instrument via cosine similarity scoring or similar 'dot product' algorithms.

While accurate, reliable, and computationally inexpensive (allowing the process to be run onboard the instrument in real time), this 'gold standard' approach fails to identify or even classify near-neighbor variants of molecules in the library, although hybrids of cosine similarity scoring can partially address this issue. Moreover, the onboard libraries become out-of-date quickly as new chemical threats emerge, and so the libraries must be updated periodically, allowing nefarious actors to stay 'ahead of the curve' by continually introducing novel threat analogs that evade existing libraries. For systems in the field, regularly updating the target libraries is often impractical or impossible (e.g. for systems that are deployed on the battlefield).

Teledyne FLIR has developed a person-portable (~33 lb) direct sampling mass spectrometer with novel two-dimensional tandem mass spectrometry (2D MS/MS) capabilities. 2D MS/MS is an untargeted analysis technique that yields rich mass spectra consisting of three dimensions of information (precursor m/z, fragment m/z, and abundance). When 2D MS/MS as an untargeted survey scan is combined with data-dependent acquisition (which we refer to as 'intelligent' DDA, or iDDA), the MS achieves low false positives compared to the traditional DDA approach while more intelligently acquiring MS/MS spectra. The system is further enhanced with library-less chemical identification and/or classification capabilities through novel machine learning algorithms. This presentation will highlight the design and capabilities of the MS, the novel algorithmic approaches being applied to the 2D data to achieve library-less identification of threats, and the vision for the future of the 2D MS/MS platform.

Biography - Dalton Snyder

Dalton Snyder is currently the Research & Development Manager for the Teledyne FLIR West Lafayette (IN) site, driving the development of compact, person-portable mass spectrometers for CBRNE threat detection. Prior to his tenure at Teledyne FLIR he obtained his PhD from Graham Cooks' lab at Purdue University, where he specialized in ion trap miniaturization and novel scanning methodology. He then was a postdoctoral research associate in Vicki Wysocki's laboratory focusing on instrumentation development for native mass spectrometry, culminating in the first commercialization of a surface-induced dissociation cell.

Keywords

Mass spectrometry, Miniature mass spectrometer, Portable mass spectrometer, 2D MS/MS, Machine learning, Ambient ionization