

The Summer Undergraduate Research Fellowship (SURF) Symposium

2 August 2018

Purdue University, West Lafayette, Indiana, USA

# Mass Spectrometry Image Creator (MSIC): Ion Mobility / Mass Spectrometry Imaging Workflow in Python

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## ABSTRACT

Mass spectrometry (MS) is a powerful characterization technique that enables identification of compounds in complex mixtures. Acquiring mass spectra in a spatially-resolved manner (i.e. over a grid), allows the data to be used to generate images that show the spatial distribution and relative intensities of every compound in a sample. These images can be used to monitor and identify biomarkers, explore the metabolism of compounds within tissues, and much more. However, the limitations of mass spectrometry can result in ambiguous compound identifications. Another characterization tool, ion mobility spectrometry (IM) can be integrated into existing MS routines to address this problem; measuring an ion mobility spectrum along with a mass spectrum over the grid results in more accurate compound identification in imaging experiments. While many software solutions exist for visualizing MS data, none of them support ion mobility. Thus, we have developed a novel program to incorporate this new dimension of data called Mass Spectrometry Image Creator (MSIC). Using existing software within a Python shell, MSIC creates images from raw IM-MS data through a semi-automated and batch-capable pipeline. Additionally, it includes several post-processing tools for further analysis and error correction.

## KEYWORDS

Mass Spectrometry Imaging, Nano-DESI, Ion Mobility, Skyline, Python, Data Visualization, Lipidomics, Mass Profiler