AUTOMATED VISUALIZATION, EXPLORATION AND MATERIAL SEGMENTATION OF ION-MOBILITY MASS SPECTROMETRY IMAGING DATA

Scott Trinkle, Bindesh Shrestha, Richard Chapman
Waters Corporation, Milford, MA

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INTRODUCTION

Ion mobility (IM) provides additional separation of analytes from mass spectrometry imaging (MSI) data based on size, shape, and charge for isomer and isobar differentiation. When combined, these methods produce large amounts of multi-dimensional data, leading to the need for more powerful statistical techniques and software packages in order to guide and streamline data interpretation. The Waters™ MSI Analyte Browser and MSI Segmentation MicroApps have been updated to use unsupervised machine learning to automate the exploration, analysis, and visualization of these IM-MSI datasets.

HIGHLIGHTS

- Compatible with processed analyte text files from Waters HDI™ software, or custom .csv text files from processed data containing (x,y) coordinates intensities at each peak-picked m/z-drift time pair

- Performs automated object detection and pixel segmentation using UMAP and HDBSCAN, resulting in a list of pixel IDs with corresponding average m/z-drift time plots

- Clusters individual analyte images into groups for visualization of patterns across the m/z-drift time plot as well as average ion images within each cluster

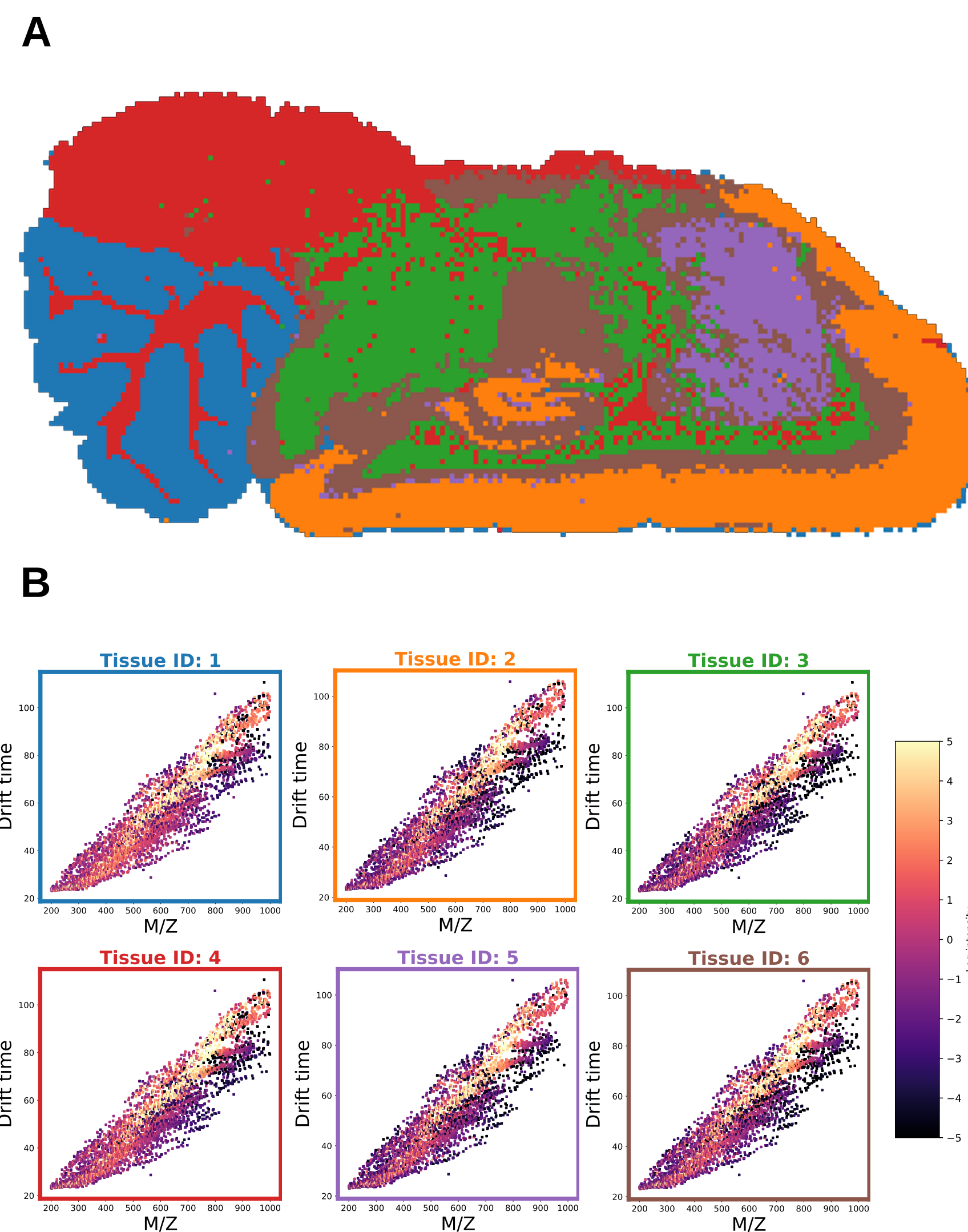- Outputs all results to .csv for downstream processing of raw data

Figure 1. Pixel segmentation results for a rat brain sample. A: Segmentation map, showing clusters of pixels grouped together based on their m/z and drift time spectra. B: Average m/z-drift time plots for each cluster from 1A, with color corresponding to average log-intensity for all pixels within each tissue ID group.
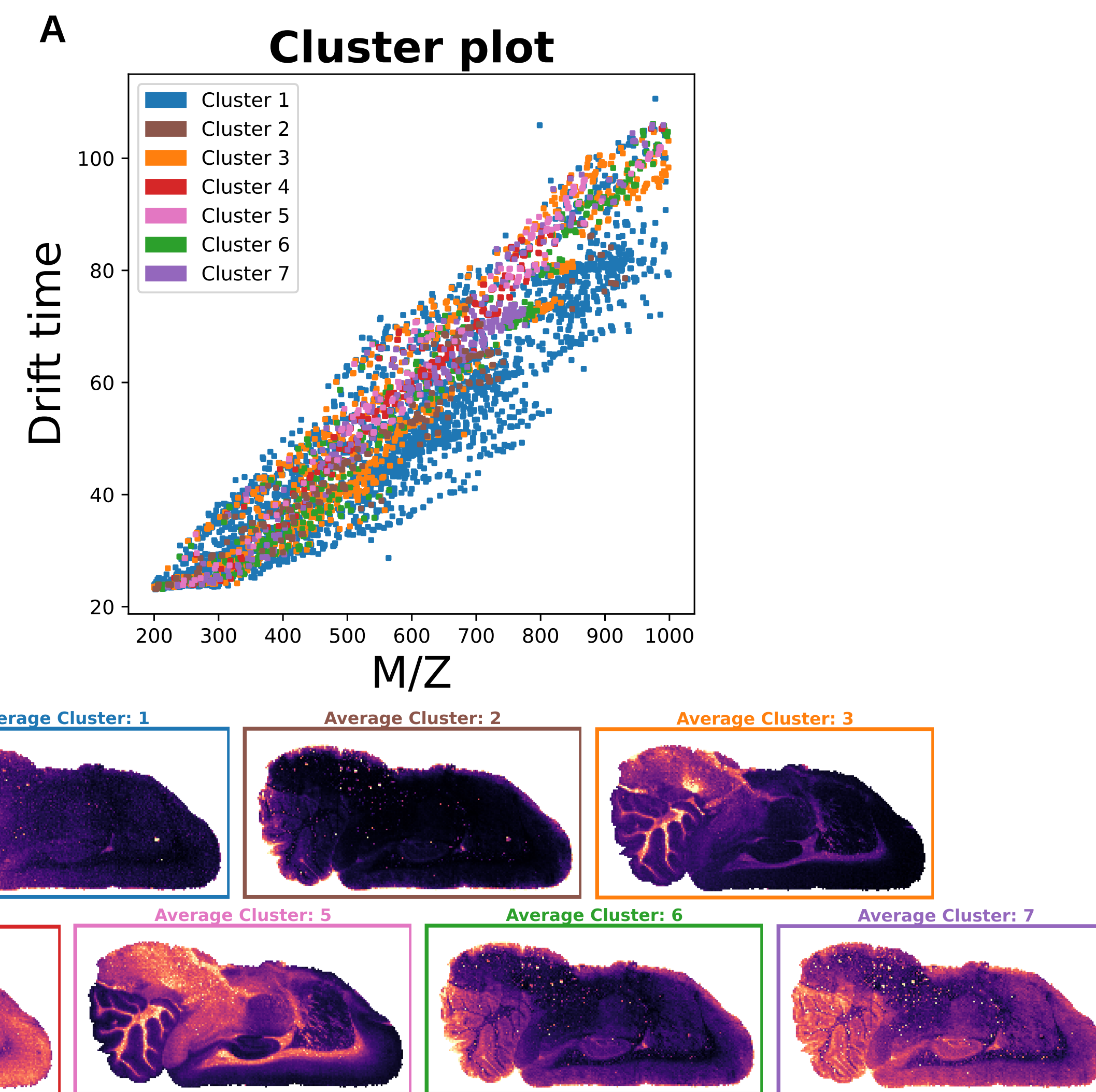
RESULTS

Figure 2. Analyte image clustering for a rat brain sample. A: M/z-drift time plot across entire dataset. Each point represents a single ion image, with color and label corresponding to cluster results where the images are grouped together based on having similar spatial distributions. B: Average representative cluster images for each of the groups from 2A. These results help determine spatial colocalization of potential analytes of interest across both m/z and drift time.