OpenMSI Arrayed Analysis Toolkit: Analyzing Spatially Defined Samples Using Mass Spectrometry Imaging - DTU Orbit (30/09/2019)

Mass spectrometry imaging (MSI) has primarily been applied in localizing biomolecules within biological matrices. Although well-suited, the application of MSI for comparing thousands of spatially defined spotted samples has been limited. One reason for this is a lack of suitable and accessible data processing tools for the analysis of large arrayed MSI sample sets. The OpenMSI Arrayed Analysis Toolkit (OMAAT) is a software package that addresses the challenges of analyzing spatially defined samples in MSI data sets. OMAAT is written in Python and is integrated with OpenMSI (http://openmsiniersc.gov), a platform for storing, sharing, and analyzing MSI data. By using a web-based python notebook (Jupyter), OMAAT is accessible to anyone without programming experience yet allows experienced users to leverage all features. OMAAT was evaluated by analyzing an MSI data set of a high-throughput glycoside hydrolase activity screen comprising 384 samples arrayed onto a NIMS surface at a 450 pm spacing, decreasing analysis time >100-fold while maintaining robust spot-finding. The utility of OMAAT was demonstrated for screening metabolic activities of different sized soil particles, including hydrolysis of sugars, revealing a pattern of size dependent activities. These results introduce OMAAT as an effective toolkit for analyzing spatially defined samples in MSI. OMAAT runs on all major operating systems, and the source code can be obtained from the following GitHub repository: https://github.com/biorack/omaat.

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