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Extending dynamic range for untargeted ion mobility-MS workflows

July 2018

A.B. Pena
S.H. Payne

U.S. DEPARTMENT OF ENERGY

Prepared for the U.S. Department of Energy
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Agilent CRADA 367 Final Report

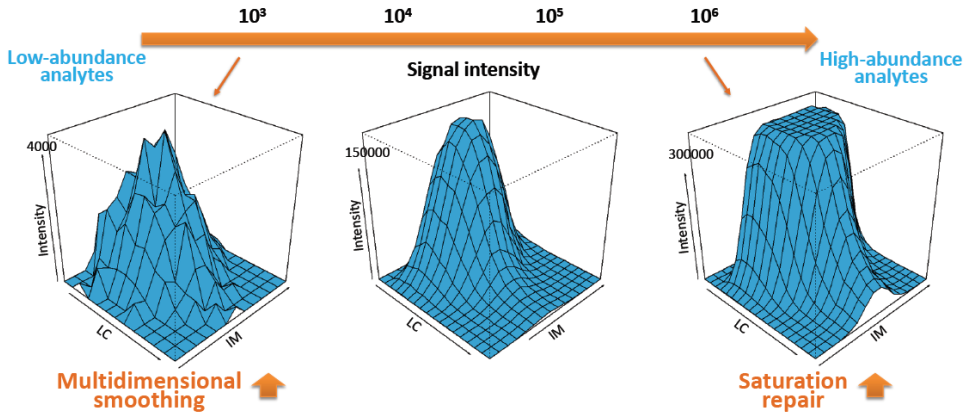
Samuel Payne and Aivett Bilbao

Extending dynamic range for untargeted ion mobility-MS workflows

Preprocessing and identification algorithms can boost the quality and reproducibility of results in untargeted ion mobility (IM)-MS workflows. For this CRADA we developed two methods for pre-processing to improve the quality of Agilent .d metabolomics data: i) a new saturation repair preprocessing method and ii) multi-dimensional smoothing.

To apply saturation repair, for each ion found to exceed a defined intensity level (given the MS instrumentation), the undistorted isotopic distribution is recovered from spectra at later elution or drift time, i.e., from the tail of the peak where the intensity returns below the saturation level. The most intense isotopic peak for which saturation does not occur is utilized as reference to reconstruct the time profile of the saturated ones based on the recovered isotopic ratios. The algorithm was implemented in C# and generates new raw data files in the original Agilent MassHunter format.

Multi-dimensional smoothing is used to improve the signal of low intensity peaks. The developed software tools were integrated to process IMS-MS data. To minimize the effects of low ion statistics (e.g., jagged profiles), several smoothing kernels were evaluated: Gaussian, Savitzky-Golay, moving average and weighted moving average. Among those, moving average smoothing provided the best results for retrieving low-abundance features and merging at least 40% more of the features with split profiles. Smoothing increased by a factor of 2.5 the number of high quality features (quality score = 80; a 0-100 scale considering signal-to-noise, number of isotopic ions and m/z stability).



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