

## ION PEAK DETECTION FOR COMPREHENSIVE MULTIDIMENSIONAL CHROMATOGRAPHY

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Mass spectrometry adds an additional dimension to comprehensive multidimensional chromatography. With mass spectrometry, each analyte may generate many multidimensional ion peaks. The additional mass-spectral dimension and proliferation of ion peaks pose additional complexity for data analysis, including analyte peak detection. The drain algorithm, which adapts the watershed algorithm for highly effective peak detection with comprehensive two-dimensional chromatography, can be extended to detect multidimensional peaks across the mass-spectral range. Ion peak detection presents several challenges, especially with high-resolution mass-spectrometry (HRMS) data. In HRMS data, the peak mass-to-charge ( $m/z$ ) ratio of the same ion of the same analyte can vary slightly in individual spectra, especially for centroided spectra. The drain algorithm can be employed to collect slightly varying spectral peaks into the same ion peak. After spectral peaks are collected into multidimensional ion peaks, those ion peaks must be collected into multi-spectral analyte peaks. Our research explores temporal proximity and peak-shape metrics for collecting ion peaks into analyte peaks.

For co-eluting analyte peaks, the ion peak collections provide useful initialization states for iterative, numerical analyte peak unmixing, e.g., deconvolution with Parallel Factor Analysis (PARAFAC) or PARAFAC2. Results are demonstrated for ion peak detection in comprehensive two-dimensional chromatography with both nominal-mass and HRMS data.