

INTERACTIVE TOOLS FOR OPTIMIZING BLOB DETECTION AND TEMPLATE MATCHING FOR COMPREHENSIVE TWO-DIMENSIONAL CHROMATOGRAPHY

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Comprehensive two-dimensional chromatography is a powerful technique for highly effective chemical separations of complex mixtures, so GCxGC, LCxLC, and other two-dimensional techniques are increasingly popular. The data produced by comprehensive two-dimensional chromatography is rich with chemical information, but extracting that information from large complex datasets is challenging even for well-designed and executed analytical methods. The data analysis problems are even more difficult when the more complex instrument settings and conditions involving two columns are suboptimal. Regardless of the quality of data, it is important to optimize processing of that data in critical operations.

Two new interactive tools that provide rapid visual feedback greatly accelerate the process of determining optimal settings for:

- blob/peak detection and
- analyte pattern matching.

Blob/peak detection is essential for accurate quantification and analyte pattern matching is the basis for effective compound identification and cross-sample analyte comparisons.

Interactive blob/peak detection implements controls in two highly visual steps. The first step allows analysts to adjust the level of smoothing, to suppress noise, in the watershed blob detection algorithm. This setting is especially important for detecting trace analytes. The second step allows analysts to construct sophisticated peak detection filters using CLIC, a language for chemical expressions, involving peak shape, size, geometry, and statistical characteristics. Each filter is implemented with an interactive slider to adjust the minimum and/or maximum thresholds. So, for example, filters for flat shapes can be used to reject streaks.

Interactive template matching provides controls and visual feedback to align a previously recorded pattern of peaks (and other features) with the same pattern of peaks (and other features) in a new chromatogram. The controls allow selection of the template transformation model (including higher-order transformations) and configuration of the parameters and thresholds for automated matching. Transformations can be applied globally or limited to a specified region. The transformed template and matches are presented in the image view and shown in a table with sortable matching-quality metrics for each matched peak. The views in the image and table have synchronized selections with automatic image zoom to focus on a selected match. The interface allows manual assignment/unassignment of matches with recomputations of the transformation model parameters.