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

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Data produced by comprehensive two-dimensional chromatography is rich with information, but extracting and evaluating this information from multiple varying chromatograms can be a complicated challenge. Two new interactive tools provide rapid visual feedback that greatly accelerates the process of determining optimal settings for blob/peak detection and analyte pattern matching.

Data Processing Challenges

Experimental Samples

- Multiple runs of a single sample of roasted cocoa from Ecuador.
- Analyzed at the Università degli Studi di Torino, Italy.

Instrumentation (collected using two different systems)

1. Reverse-inject differential flow modulator (Agilent): Agilent 7890B GC unit coupled to an Agilent 5977A fast quadrupole MS detector with modulation of 3 seconds and sampling rate of 35Hz. (Non-optimized configuration.)
2. Thermal modulator (Zoex): Agilent 6890 unit coupled to an Agilent 5975C MS detector with modulation of 3 seconds and sampling rate of 29 Hz.

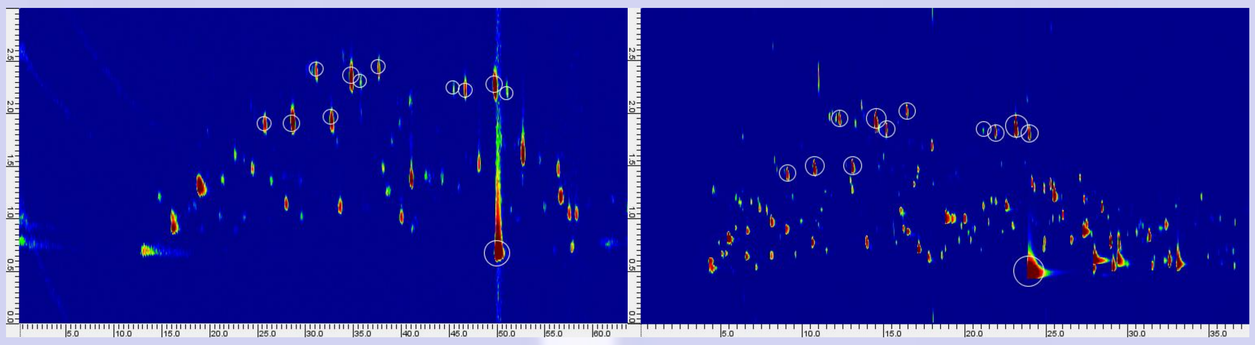

***Figure 1**: GCxGC chromatograms from flow modulation (left) and thermal modulation (right) have significant differences in retention times and peak dimensions.*

Challenge

Detect and match peaks and other chromatographic features in complex GCxGC chromatograms with significant differences in retention times and peak dimensions.

Interactive Blob Detection

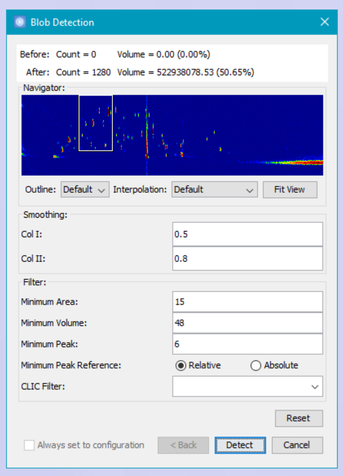

***Figure 2**: Initial detection settings.*

Interactive Blob Detection allows users to refine blob detection parameters through interactive experimentation using advanced filters with a large set of blob properties. This tool allows optimization of targeted and untargeted detection, for example to minimize false detections, exclude peaks in regions with bleed or solvent front, etc.

Initial settings apply smoothing and threshold filters for area, volume, and peak intensity.

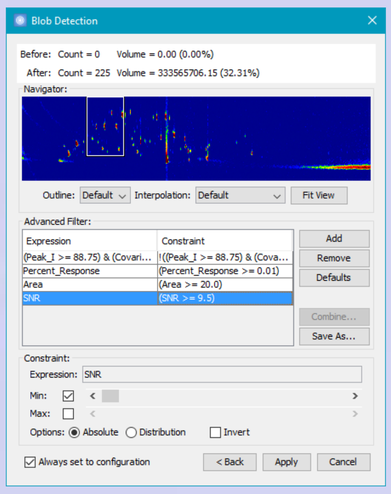

***Figure 3**: Advanced filters, e.g., SNR, Area, Percent Response, and combination.*

Advanced filters are created and parameterized to accept or reject blobs. The filters, e.g., as Shown in Figure 3, use various properties such as peak shape, SNR, retention times, etc. to refine blob/peak detection. Changes to the filters are applied immediately in the Image view, providing direct feedback. The Filters can be saved and reused.

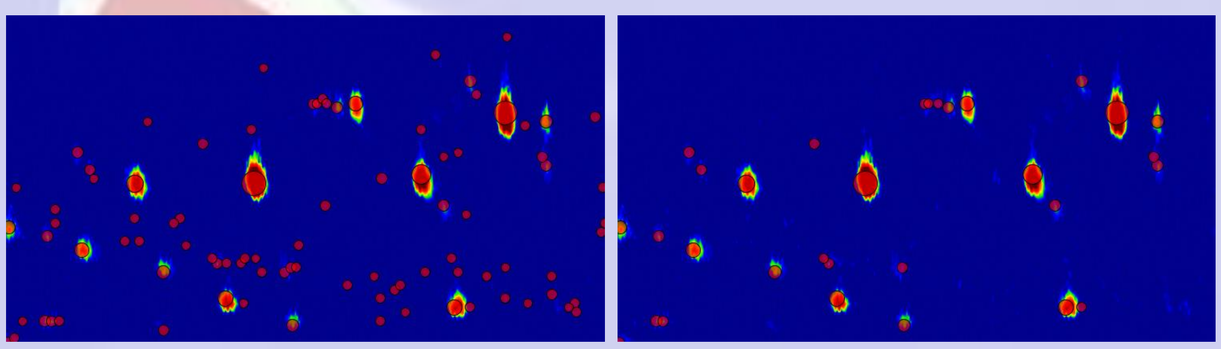

***Figure 4**: Flow-modulated chromatogram with blobs (indicated with bubble highlights) before and after advanced filtering.*

The new interactive user interface allows the user to experiment with the detection settings and fine-tune the recognition of blob peaks. The combination of smoothing options and customizable filters can optimize the trade-off between false detections and missed peaks.

Interactive Template Matching

This example illustrates matching a peak template created for the flow-modulated chromatograms to the thermal-modulated chromatograms. The template includes *Match Factor* QCLICs to match the mass spectra.

GC Image's interactive template-matching UI is used to edit matches and See changes in the Image view. For this data, the chromatogram is severely misaligned, so a quick start is to manually set a few matches. With just a few matches, a template transform function is fit for alignment.

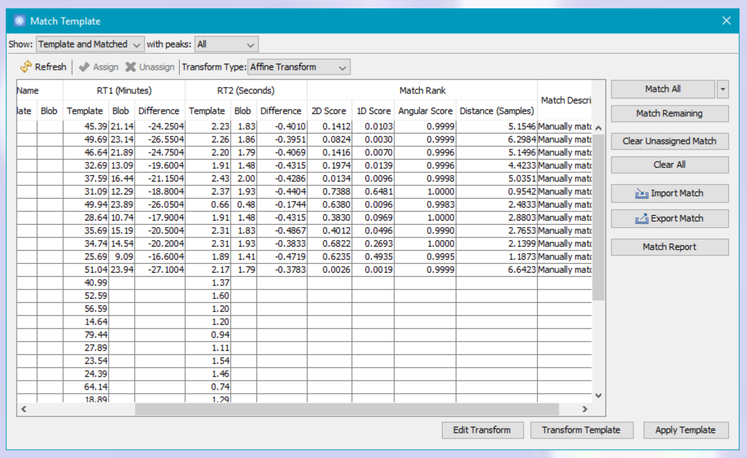

***Figure 5**: Interactive Template Matching UI with several matched peaks.*

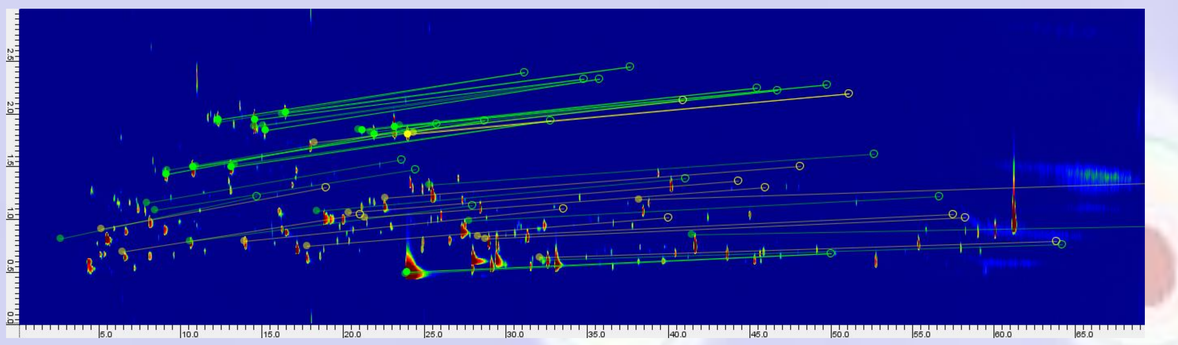

***Figure 6**: Image view showing template peaks along with transformed positions and matches. An affine transform is used in this case.*

Changes to template matches update the image view and refine the template transform. *Match Remaining* matches other peaks with the refined transform. In this way, using both automated and manual matching, the desired template transform and matching is obtained.

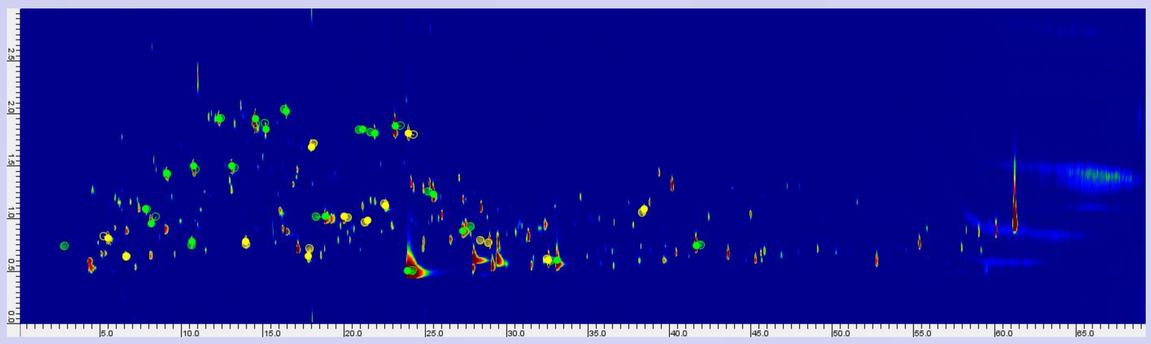

***Figure 7**: Image view after matching peaks and applying the template transform.*

University of Nebraska Lincoln

GC IMAGE
Software for Multidimensional Chromatography

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