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

Blob Detection	×						
Before: Count = 0 Volume = 0.00) (0.00%)						
After: Count = 1280 Volume = 5229 Navigator:	938078.53 (50.65%)						
Outline: Default \lor Interpolation:	Default v Fit View						
Smoothing:							
Col I:	0.5						
Col II:	0.8						
Filter:							
Minimum Area:	15						
Minimum Volume:	48						
Minimum Peak:	6						
Minimum Peak Reference:	Relative Absolute						

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.

Blob Detection									
Before: Count = 0	Volume = 0.00 (0.00%)								

Interactive Template Matching

This example illustrates matching a peak template created for the flowmodulated 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

Match Template												×			
how:	Templ	ate and Mat	tched	with peaks	s: All	~]								
Ş	Refres	h 🛛 🛷 Assi	ign 🗙	Unassign T	Transform T	ype: A	ffine Transfo	rm 🗸							
Nam	e	RT1 (Minutes)			RT2 (Seconds)			Match Rank			Match Danai		Match All	Ŧ	
late	Blob	Template	Blob	Difference	Template	Blob	Difference	2D Score	1D Score	Angular Score	Distance (Samples)	Match Descri		Match Remaining	
		45.39	21.14	-24.2504	2.23	1.83	-0.4010	0.1412	0.0103	0.9999	5.1546	Manually mate			
		49.69	23.14	-26.5504	2.26	1.86	-0.3951	0.0824	0.0030	0.9999	6.2984	Manually mate		Clear Unassigned Match	
		46.64	21.89	-24.7504	2.20	1.79	-0.4069	0.1416	0.0070	0.9996	5.1496	Manually mate			
		32.69	13.09	-19.6004	1.91	1.48	-0.4315	0.1974	0.0139	0.9996	4.4233	Manually mate		Clear All	
		37.59	16.44	-21.1504	2.43	2.00	-0.4286	0.0134	0.0096	0.9998	5.0351	Manually mate			
		31.09	12.29	-18.8004	2.37	1.93	-0.4404	0.7388	0.6481	1.0000	0.9542	Manually mate		🚵 Import Match	
		49.94	23.89	-26.0504	0.66	0.48	-0.1744	0.6380	0.0096	0.9983	2.4833	Manually mate			
		28.64	10.74	-17.9004	1.91	1.48	-0.4315	0.3830	0.0969	1.0000	2.8803	Manually mate		🛃 Export Match	
		35.69	15.19	-20.5004	2.31	1.83	-0.4867	0.4012	0.0496	0.9990	2.7653	Manually mate			
		34.74	14.54	-20.2004	2.31	1.93	-0.3833	0.6822	0.2693	1.0000	2.1399	Manually mate		Match Report	
		25.69	9.09	-16.6004	1.89	1.41	-0.4719	0.6235	0.4935	0.9995	1.1873	Manually mate			-
		51.04	23.94	-27.1004	2.17	1.79	-0.3783	0.0026	0.0019	0.9999	6.6423	Manually mate			
		40.00			1.07										



Figure 2: Initial

detection settings.

Initial settings apply smoothing and threshold filters for area, volume, and

peak intensity.

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



Figure 4: Flow-modulated chromatogram with blobs (indicated with bubble)

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



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

just a few matches, a template transform function is fit for alignment.



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.

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.



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





