Rapid Quality Assurance Screening for Comprehensive Two-Dimensional Chromatography Stephen E. Reichenbach^{1,2} Qingping Tao¹, Trevor S. Janke¹ ¹GC Image, LLC; ²University of Nebraska – Lincoln reich@cse.unl.edu; www.gcimage.com

Motivation & Goals

Comprehensive two-dimensional chromatography, including both GCxGC and LCxLC, produces large, information-rich data for difficult chemical analyses. Quality assurance is especially important for complex and sophisticated analyses in challenging applications . A new informatics framework and associated tools support rapid and effective quality assurance.

QA Rapid Screen[™] guides users through a sequence of tightly integrated visualizations that highlight pertinent aspects of the data analysis.



Software for Multidimensional Chromatography

QA Rapid Screen

During screening, the analyst can confirm acceptable results, make notes, reprocess data, reject unacceptable results, and generate reports. The workflow also can be used for side-by-side visualizations for comparative analyses.

QA Configuration

Select the features of interest, e.g., peaks or areas. Here, the selected regions are potential metabolomic biomarkers with large Fisher Ratios differentiating samples from two variants of Arabidopsis plant.

- Select the attributes of interest, e.g., retention times, SNR, and the best match from the NIST MS
- 3. Set the QA Criteria, e.g., a GC Image CLIC expression that constrains MS match factor and qualifier ion ratio. Here, the criterion is that the TIC in the region is within the expected range for this strain.
- **Configure the QA Rapid Screen** 4. for visualization. (See next panel.)

QA Rapid Screen can be configured The views are tightly integrated so to show many views, including, as shown below: TIC Image View, SIC Image View, MS View, Navigator View, and 1D Slice View.

that changing the focus feature in the Blob/Area Table changes all of the views to show the new focus feature.



In QA Rapid Screen mode, users can

Results of QA Screening can be included as a sub-report in the GC Image Summary Report. Fields in the Blob/Area Table can be color coded for clear visual cues.

Library.



1. GC Image Investigator[™] identified peaks for registration and potential biomarkers.

Start

Close

2. Attributes of interest are selected blob/area properties to be shown in the Blob/Area Tables.

Blob Table Configuration		×	Review Configurations				x
Blob Table Configuration Invisible Features Adjusted Time I Adjusted Time II Amount Amount Percent Amount Source Area (pixel count) BlobID Capacity Factor I Capacity Factor II Center I Center II	Visible Features Review Status Compound Name Retention I Retention II Percent Response aCLIC aCLIC Result		Review Configurations Selected Configuration Chromatogram Review Spectral Review	Name: Spectral Review Views Features Spectral Included Blob/Area Features: Co Colorize Blob/Area Columns: Co Add Remove aCLIC Result Typ Value	nfigure Minimum e: Percent -	Midpoint Percent -	Maximum Percent 100
Characteristic Ions Characteristic Ions Response Chemical Structure Object CLIC Constellation Name Add All Rem	nove All System Default Cancel			Colo	r:	Save	Default vert Default

employ GC Image tools to examine and/or reprocess data. Users can confirm results, make notes, or reject unacceptable results in the **Blob/Area Table.**

Comparative Analyses

In a dual-monitor setup, QA Rapid Screen can be used for compoundby-compound feature comparisons. With QA Rapid Screen, comparative analyses can be conducted quickly to confirm similarities or differences.



Blob Table						
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Review Status	Compound Name	Retention I (min)	Retention II (sec)	Percent Response	aCLIC	aCLIC Result
	(18)	36.58	2.26	2.76	Percent_Response	1.00
	(14)	71.29	3.17	1.6	(Percent_Response	1.00
	(16)	43.39	2.28	1.0	(Percent_Response	1.00
	(20)	71.29	1.87	0.38	(Percent_Response	1.00
	(80)	33.09	3.11	0.1	(Percent_Response	1.00
	(66)	71.46	2.15	0.24	(Percent_Response	1.00
	(30)	95.71	1.70	0.0	(Percent_Response	1.00
	(78)	62.32	4.96	0.04	(Percent_Response	1.00
	(92)	64.15	1.72	0.14	(Percent_Response	0.00
	(157)	65.65	3.35	0.12	Percent_Response	0.00









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