Rapid Quality Assurance Screening
for Comprehensive Two-Dimensional Chromatography

Stephen E. Reichenbach,[1,2] Qingping Tao,[1] Trevor S. Janke[1]
[1]GC Image, LLC; [2]University of Nebraska – Lincoln
reich@cse.unl.edu; www.gcimage.com

GC IMAGE
Software for Multidimensional Chromatography

UNIVERSITY OF NEBRASKA Lincoln

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. 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.
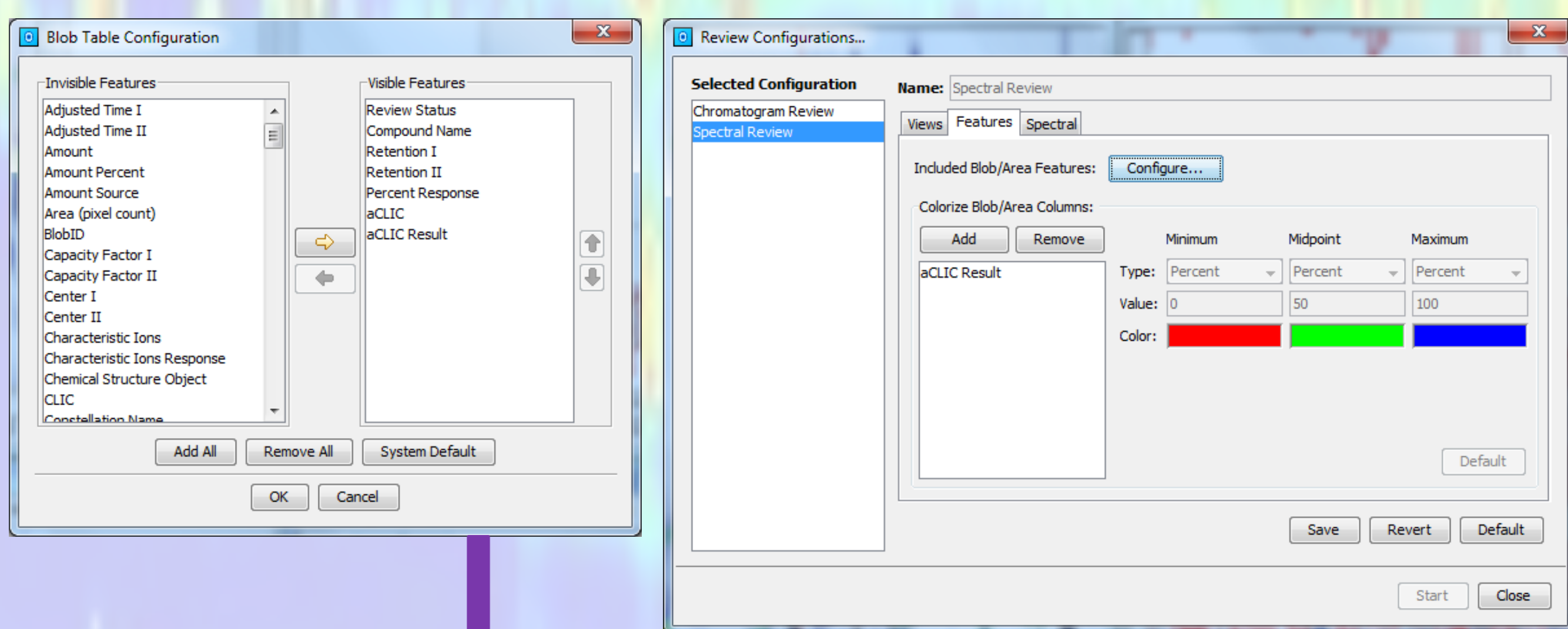
QA Configuration

1. **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.
2. **Select the attributes of interest,** e.g., retention times, SNR, and the best match from the NIST MS Library.
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.
4. **Configure the QA Rapid Screen** for visualization. (See next panel.)
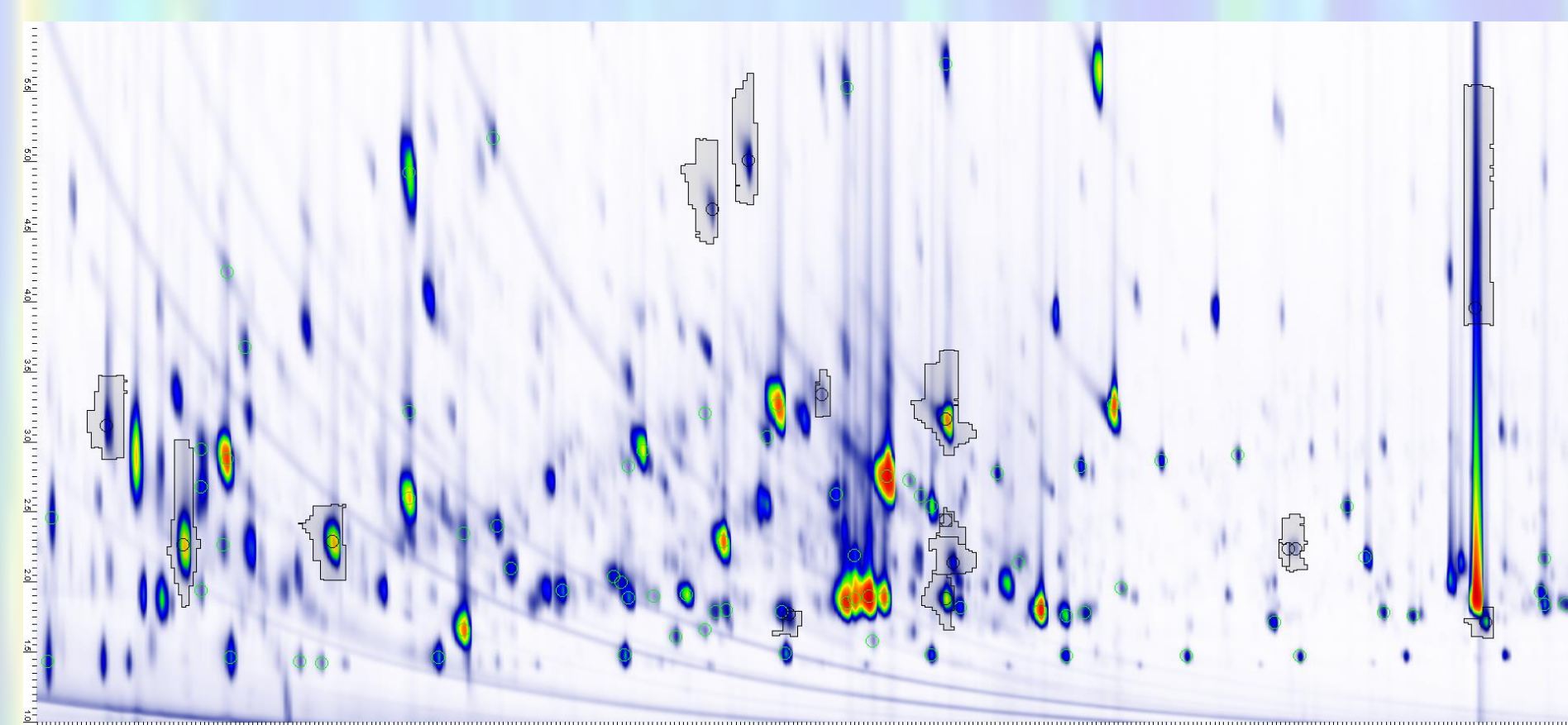
1. GC Image Investigator™ identified peaks for registration and potential biomarkers.
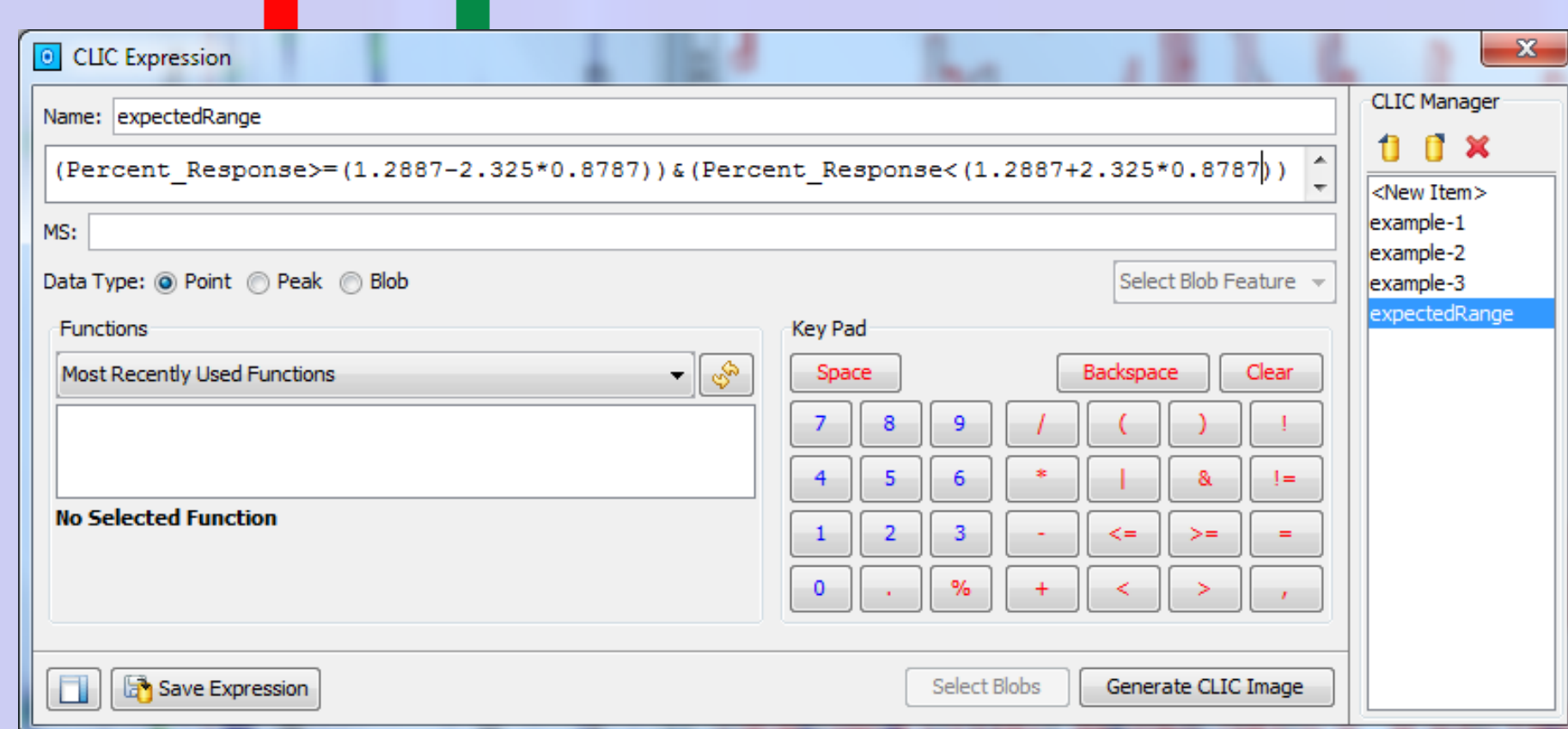
2. Attributes of interest are selected blob/area properties to be shown in the Blob/Area Tables.

3A. QA Criteria in CLIC expression.

3B. QA Criteria evaluation result.

QA Rapid Screen

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

The views are tightly integrated so that changing the focus feature in the Blob/Area Table changes all of the views to show the new focus feature.
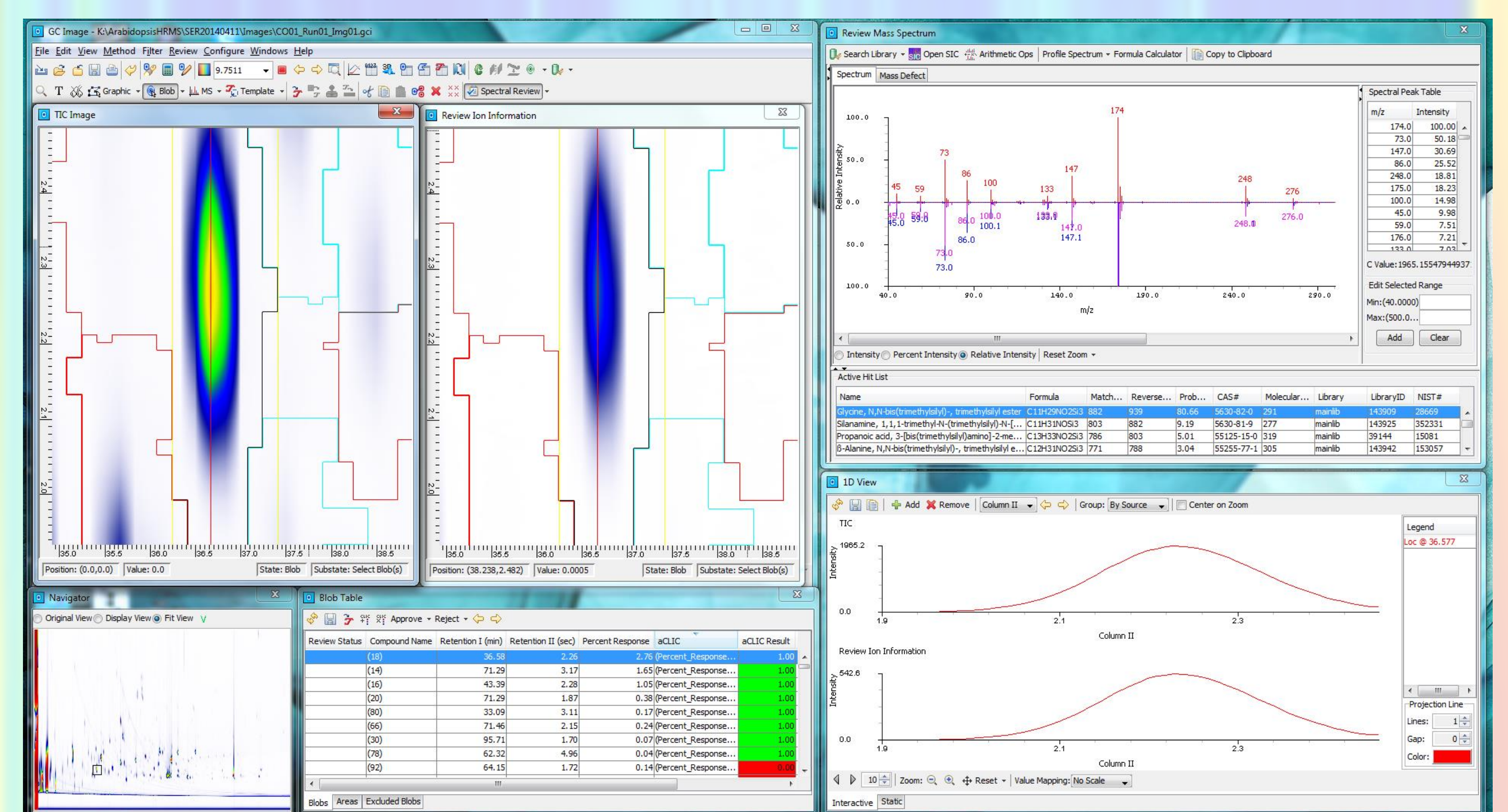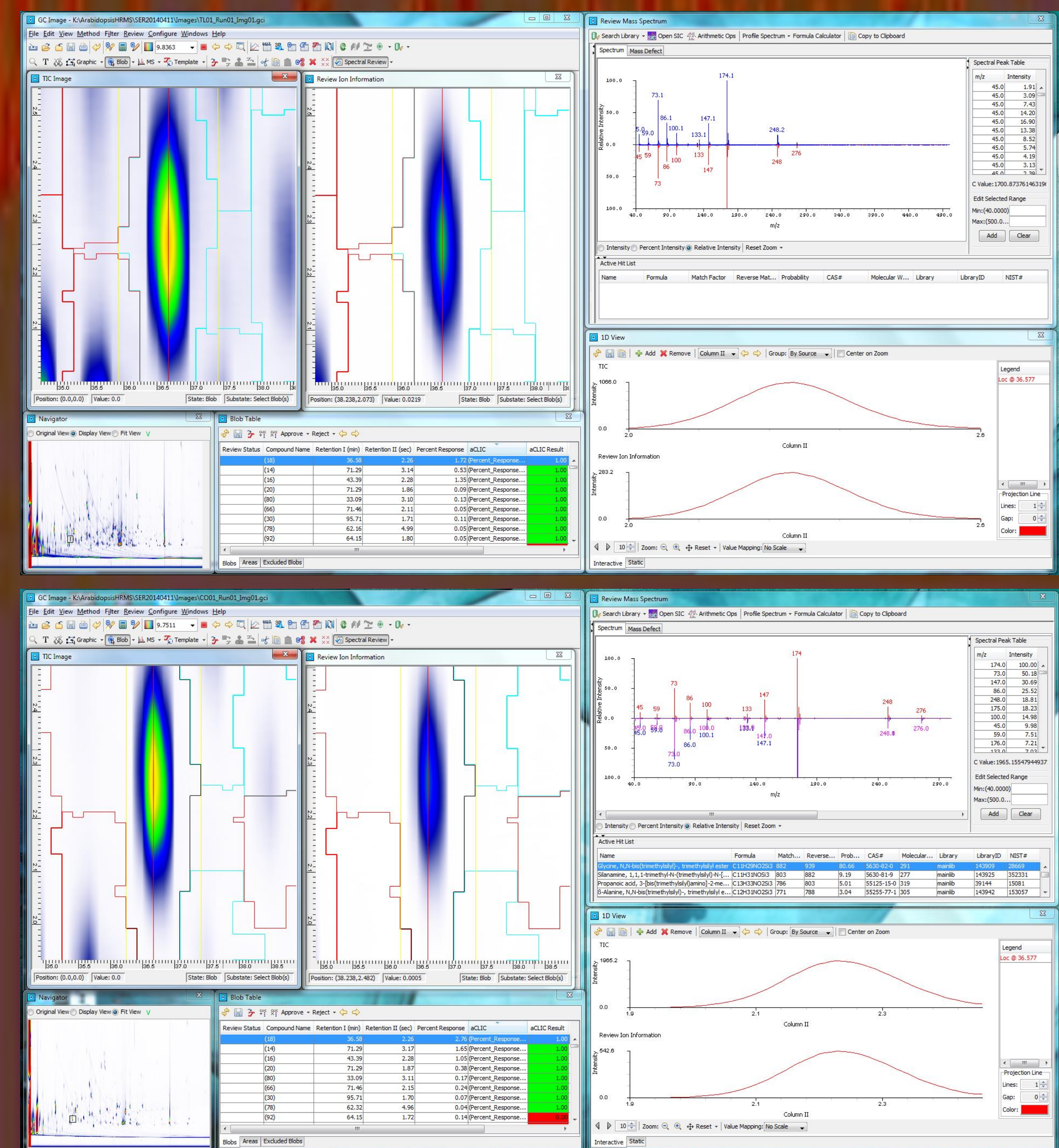
In QA Rapid Screen mode, users can employ GC Image tools to examine and/or reprocess data. Users can confirm results, make notes, or reject unacceptable results in the Blob/Area Table.

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.

Comparative Analyses

In a dual-monitor setup, QA Rapid Screen can be used for compound-by-compound feature comparisons.

With QA Rapid Screen, comparative analyses can be conducted quickly to confirm similarities or differences.

Code: 7881c7