

# What's New in GC Image R2.5

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## GC Image, Release 2.5

- For many years, GC Image has made an annual release with new features.
- Our projected release schedule for Release 2.5 (R2.5):
  - Distributors' Test Version in late June, 2014
  - Users' Test Version in late July, 2014
  - Commercial Version in August or September, 2014
- These slides describe some of the new features and improvements.

## Outline

- QA Rapid Screen
- HRMS
- Data Processing
- Template Transformations
- Image Investigator
- 3D Modeling & Visualization
- Slice Reports & MW Distribution Averages
- Other Improvements

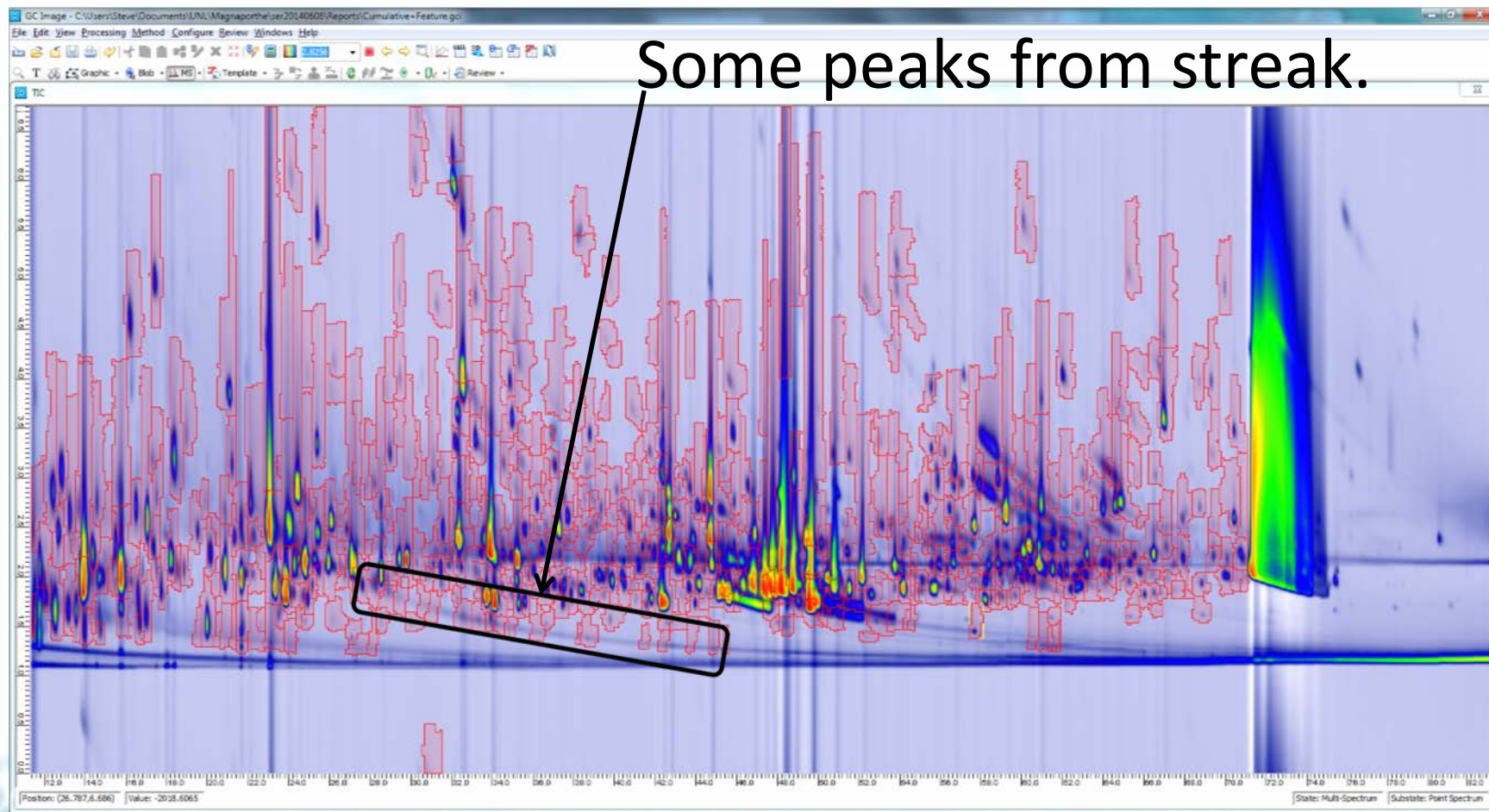
## QA Rapid Screen

- QA Rapid Screen™ allows users to quickly review analytical results.
  - Presents multiple integrated views of a blob or area of interest
  - Allows streamlined navigation from blob to blob (or area to area), with optional status update or reprocessing

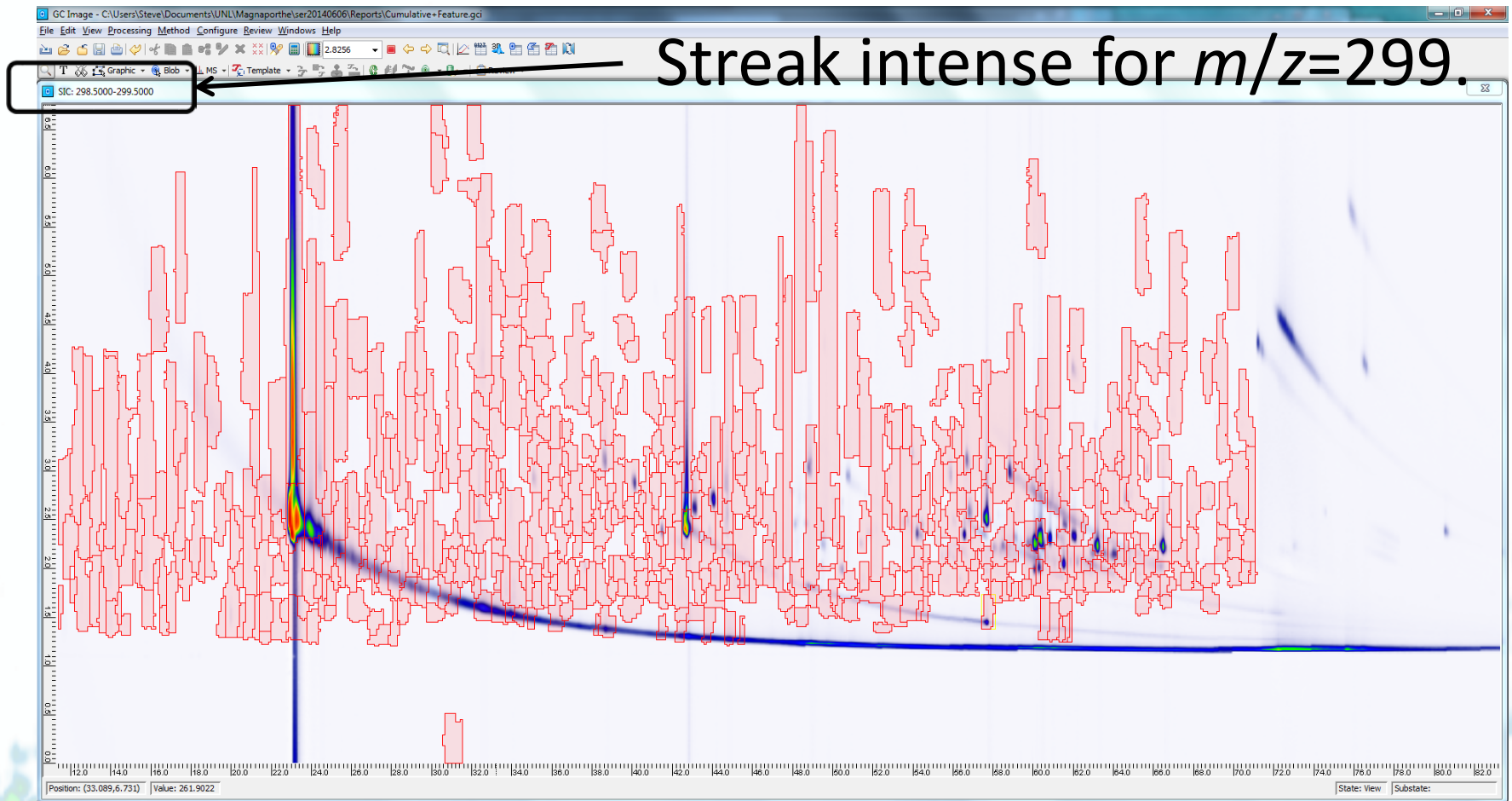
## QA Rapid Screen

1. User configures QA Perspective:
  - Visualization configuration
  - Attributes of interest, including optional QA criteria
2. User starts QA Rapid Screen.
3. User selects blob (or area) of interest from sorted blob/area table to:
  - View analysis
  - Optional update, e.g., set status, reprocess data, etc.

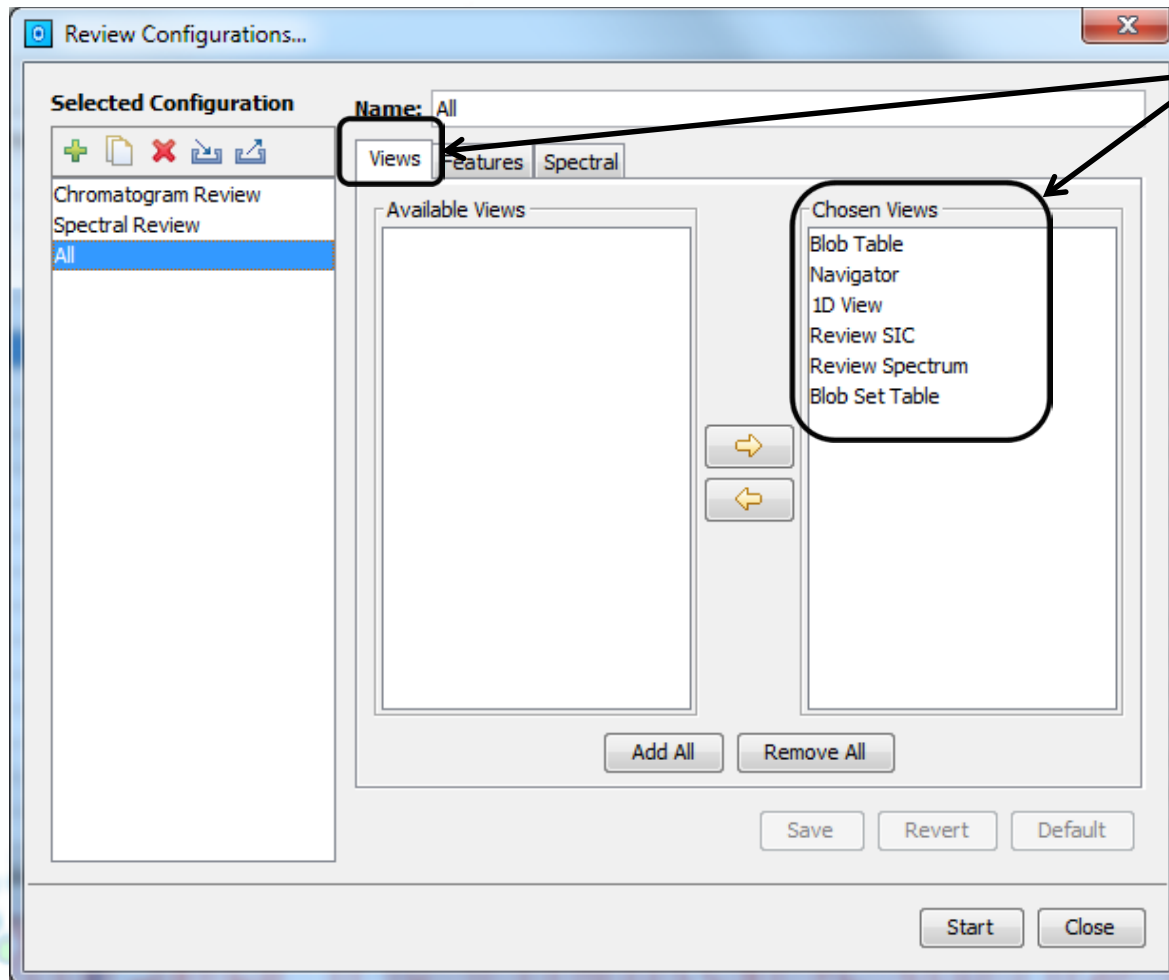
## QA Rapid Screen - Example



## QA Rapid Screen - Example



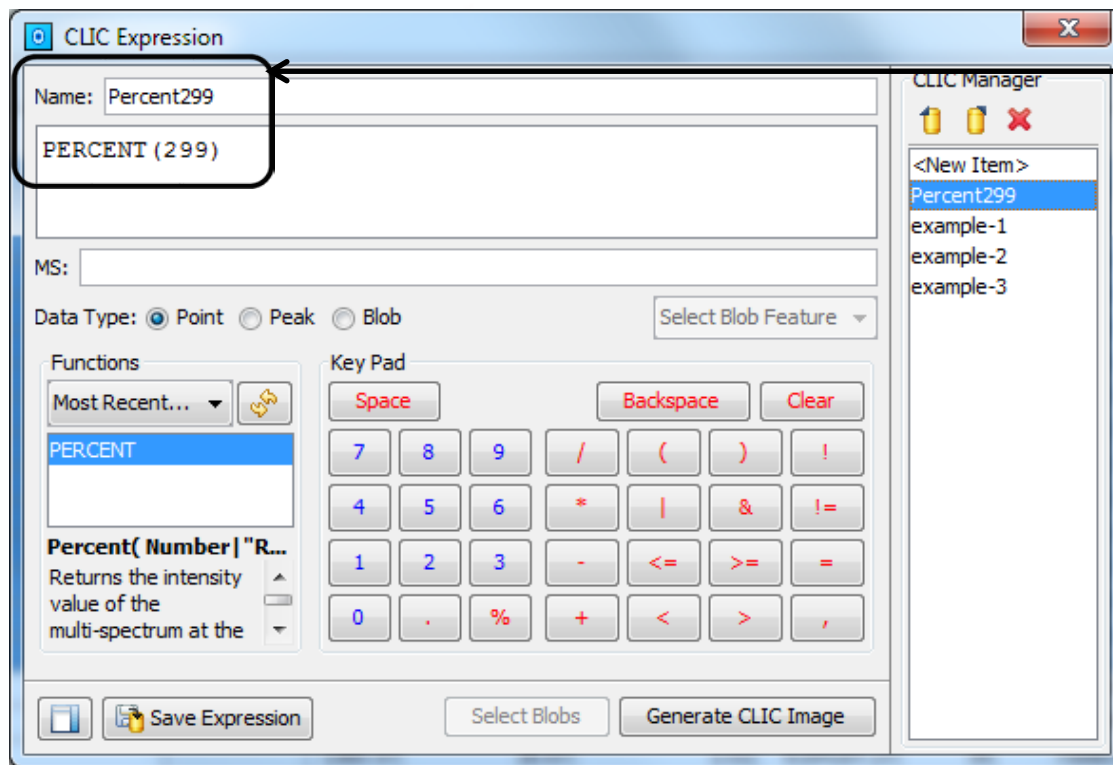
## QA Rapid Screen - Example



Select views for named QA configuration, which can be saved and reused. Also, arrange layout of views (to be shown).

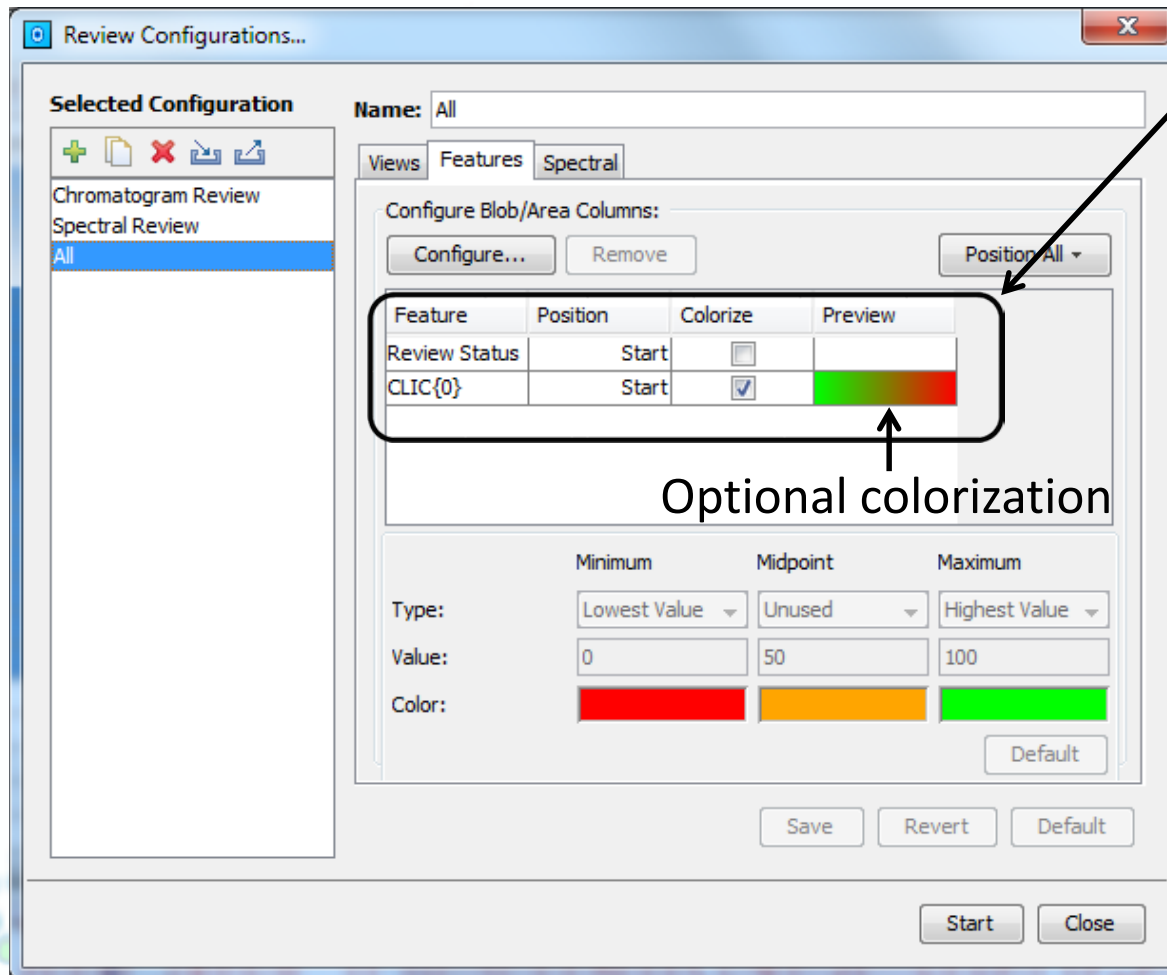


## QA Rapid Screen - Example



Optional criterion to order peaks for review. Here, the CLIC expression is the percent of ion 299 for the spectrum.

## QA Rapid Screen



Select extra blob attributes for review, here with CLIC to order blobs for review. Blob table fields also are displayed.

## QA Rapid Screen - Example

The screenshot displays the GC Image software interface with several panels:

- TIC:** Total Ion Chromatogram showing a complex signal with multiple peaks.
- Review: SIC:** Selected Ion Chromatogram for peak 299, showing a single sharp peak.
- Review: Peak spectrum for Blob 520:** Mass spectrum plot with intensity vs. m/z, showing a base peak at m/z 299 and other smaller peaks at 73, 147, 191, 211, 263, and 314.
- Blob Table:** A table listing detected blobs. A red box highlights the row for BlobID 299, which is selected. An arrow points from the text overlay to this row.
- ID View:** A chromatogram showing the intensity profile of the selected blob (Blob 299) over time, with a green line representing the TIC and a red line representing the Review SIC.
- Navigator:** A small thumbnail view of the chromatogram.
- Blob Set Table:** A table listing the included blobs for the selected blob.

**Selecting a blob or area synchronously updates all views to visualize selected object.**

## QA Rapid Screen - Example

The screenshot displays the GC Image software interface with several key windows:

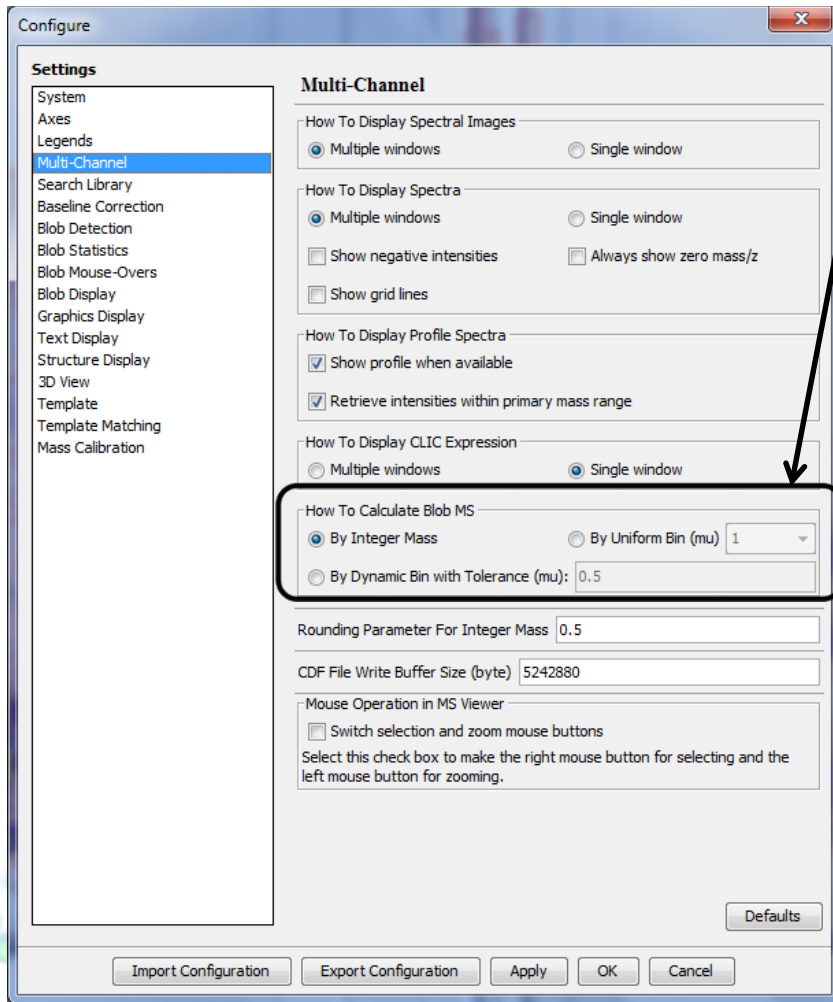
- TIC (Total Ion Chromatogram):** Shows a 2D heatmap of the chromatogram with a red box highlighting a specific region.
- Review: SIC: 72.5000-73.5000:** A zoomed-in view of the selected region from the TIC.
- Review: Peak spectrum for Blob 255 - Peak Value: 20127671.6837:** A mass spectrum plot showing intensity versus m/z. The base peak is at m/z 73. Other significant peaks are labeled at m/z 147, 299, and 357.
- Blob Table:** A table listing detected blobs with columns for Review Status, CLIC1-Percent, Blob ID, Compound Name, Group Name, LRI, Retention I (min), Retention II (sec), Peak Value, Area, Volume, and Percent Response. The row for Blob 255 is highlighted in blue.
- ID View:** A chromatogram plot showing intensity versus time. A red line represents the TIC and a green line represents the Review SIC. The peak at 57.625 minutes is highlighted.
- Navigator:** A small window showing a thumbnail of the chromatogram.
- Blob Set Table:** A table showing the results of the blob set analysis, including columns for ID, Name, Type, # of Blobs, # of Included Blobs, Volume (Total), Included Volume (Total), and Percent.

**Ordering by attribute (with color) allows easy navigation. Can update or reprocess objects.**

# HRMS - Blob/Area Integrated Spectra

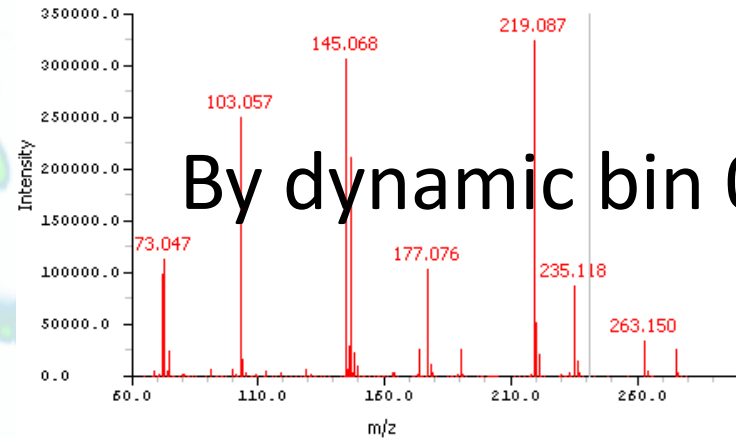
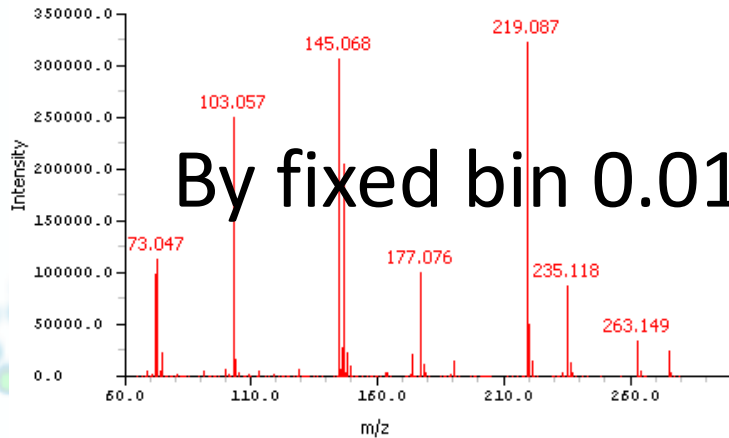
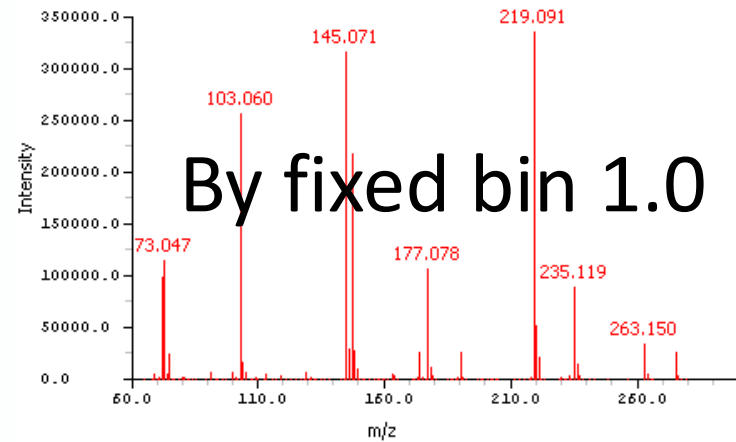
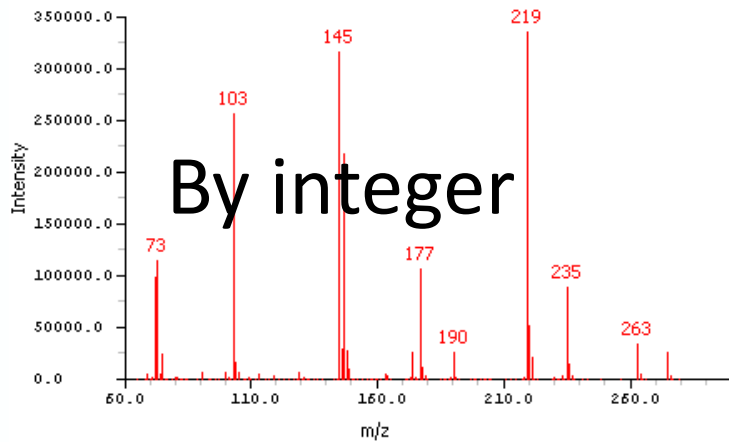
- Issue: Blob/area integrated spectra require adding multiple spectra in which the same ion may have slightly different  $m/z$ .
- In previous versions, spectra were summed within integer intervals.
- GC Image R2.5 also can generate HRMS integrated spectra by two new ways:
  - Within decimal intervals (1, 0.1, 0.01, 0.001, ...)
  - Within dynamic bins using user-specified tolerance

## HRMS - Blob/Area Integrated Spectra



User-controlled configuration. Integration within dynamic bins uses large intensity ions as a tent-pole around which smaller intensities within the tolerance are integrated.

## HRMS - Blob/Area Integrated Spectra

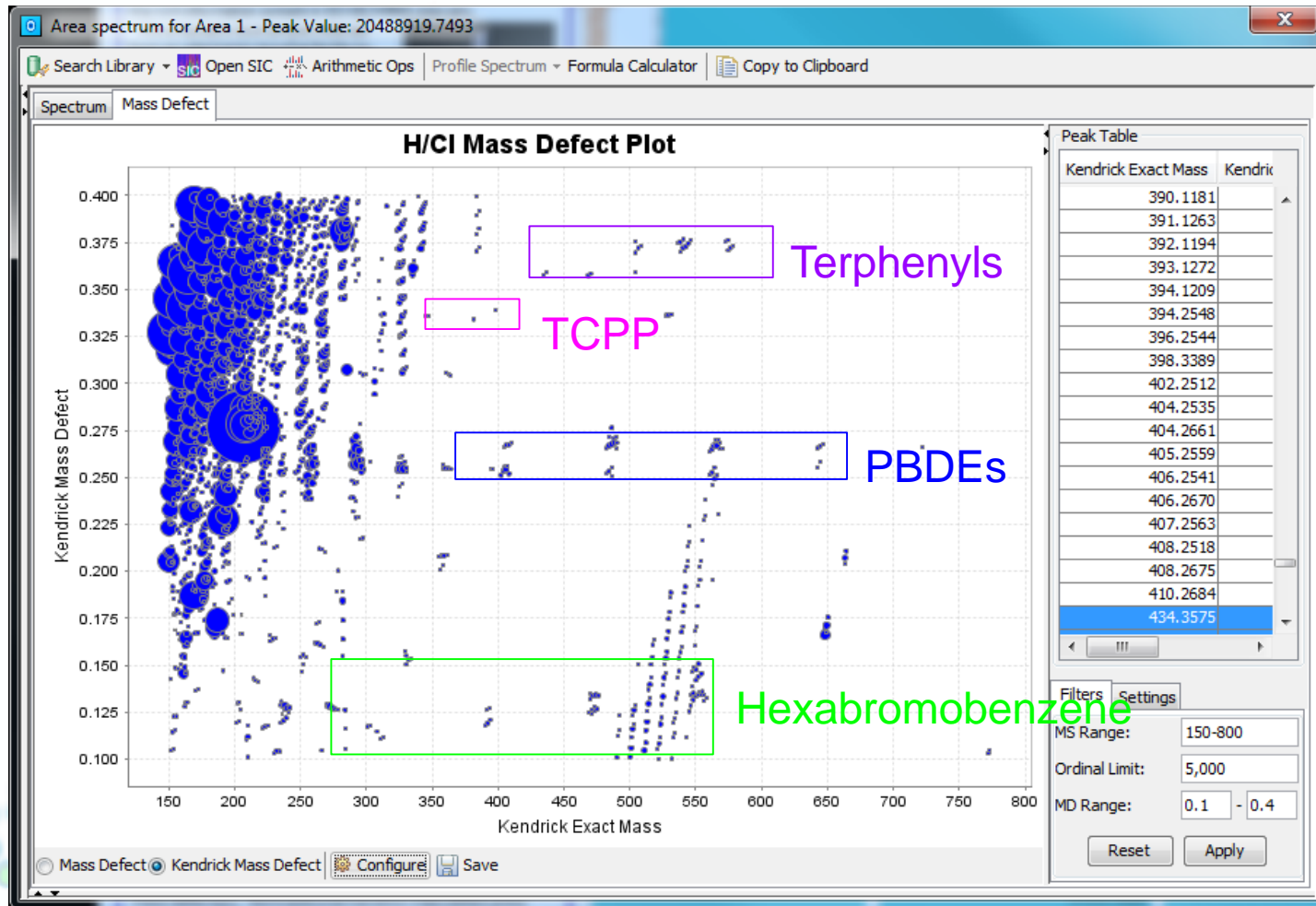


## HRMS - Mass Defects

- Mass Defect and Kendrick Mass Defect analyses in MS Viewer
- For given mass spectrum, each ion shown:
  - In table, with mass, mass defect, & intensity
  - In graph, with mass x mass defect
- Ions selectable in table or graph for SIC



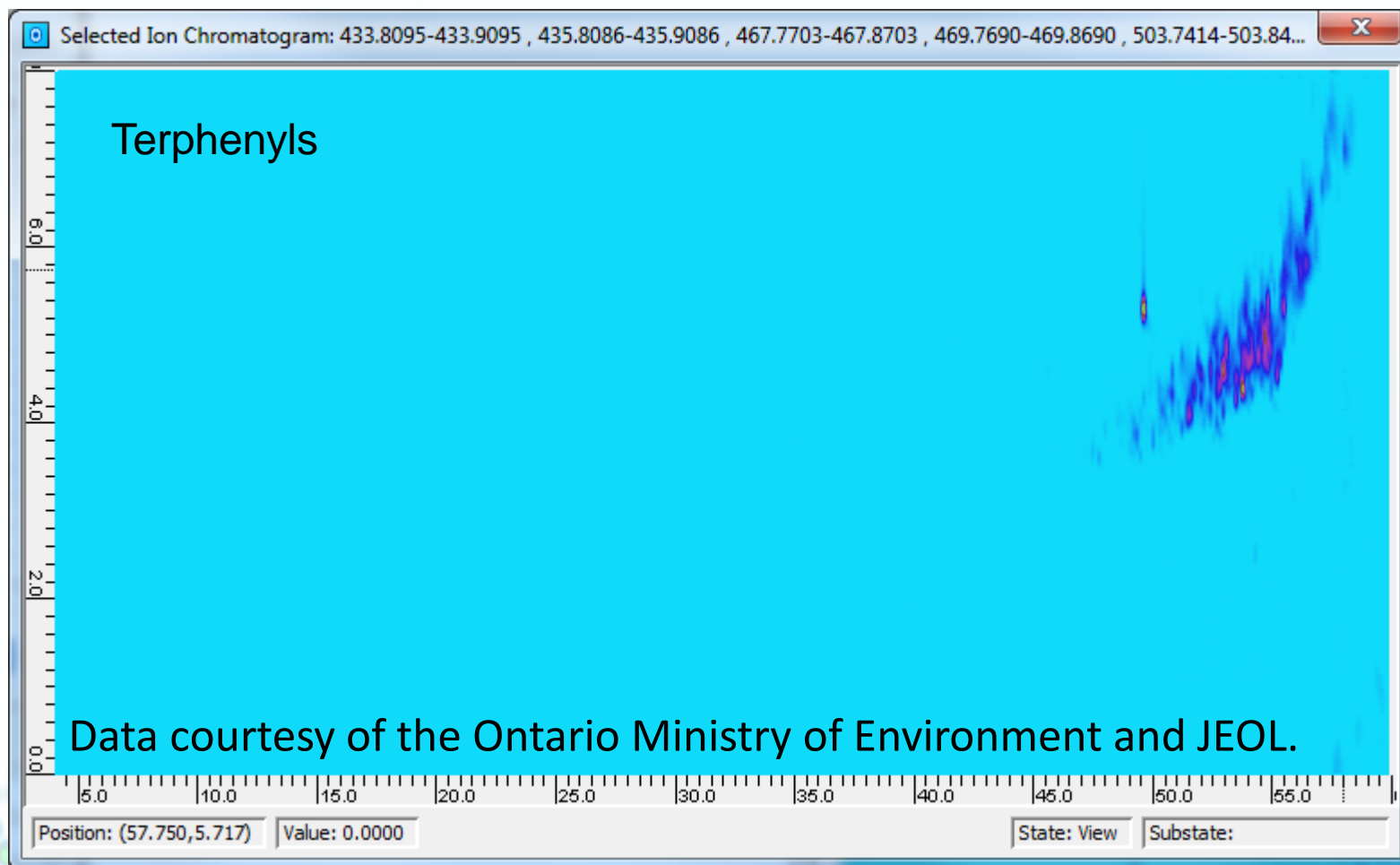
## HRMS - Mass Defects - Example



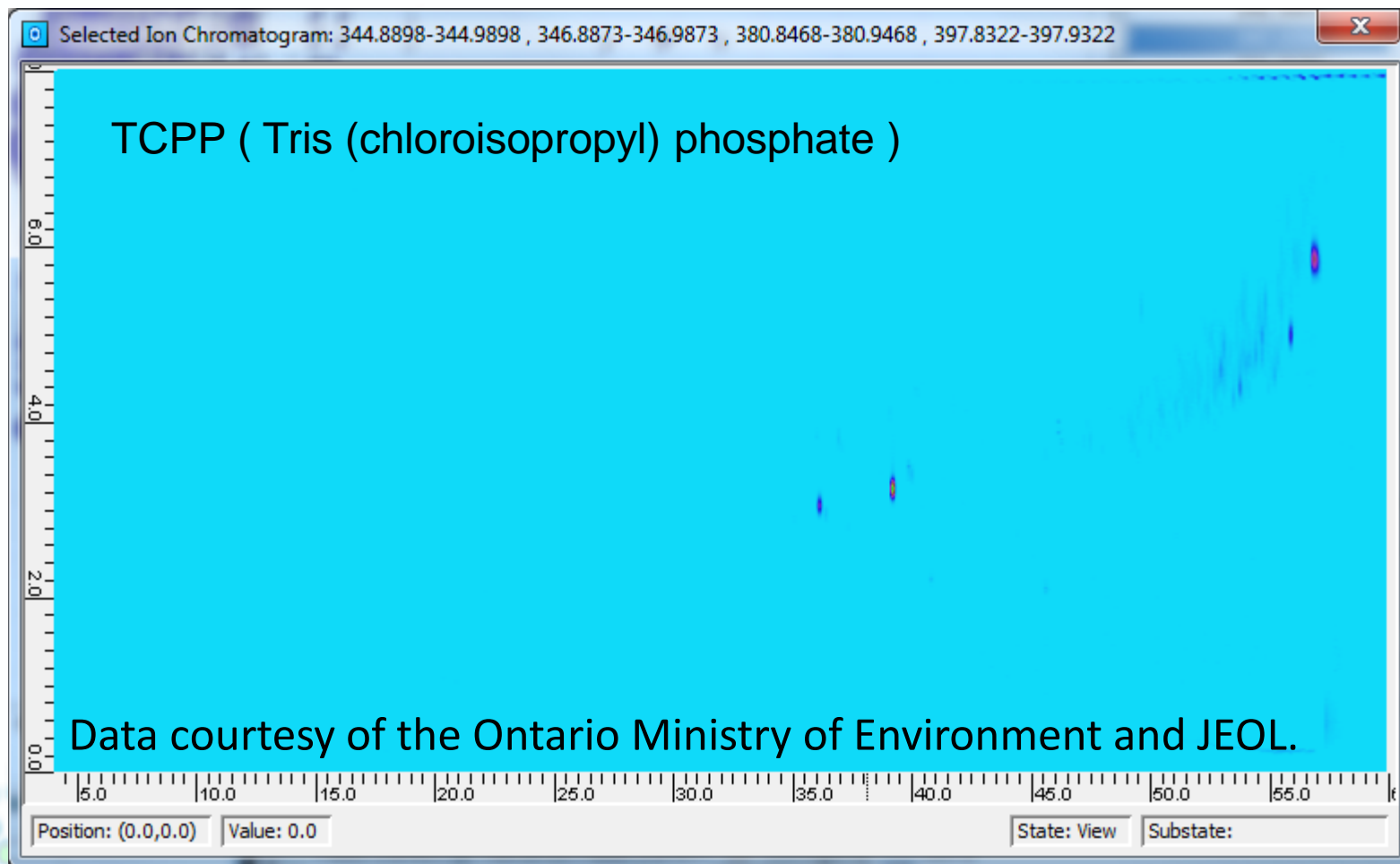
Area object spectrum from entire chromatogram for analysis.

Example data courtesy of the Ontario Ministry of Environment and JEOL.

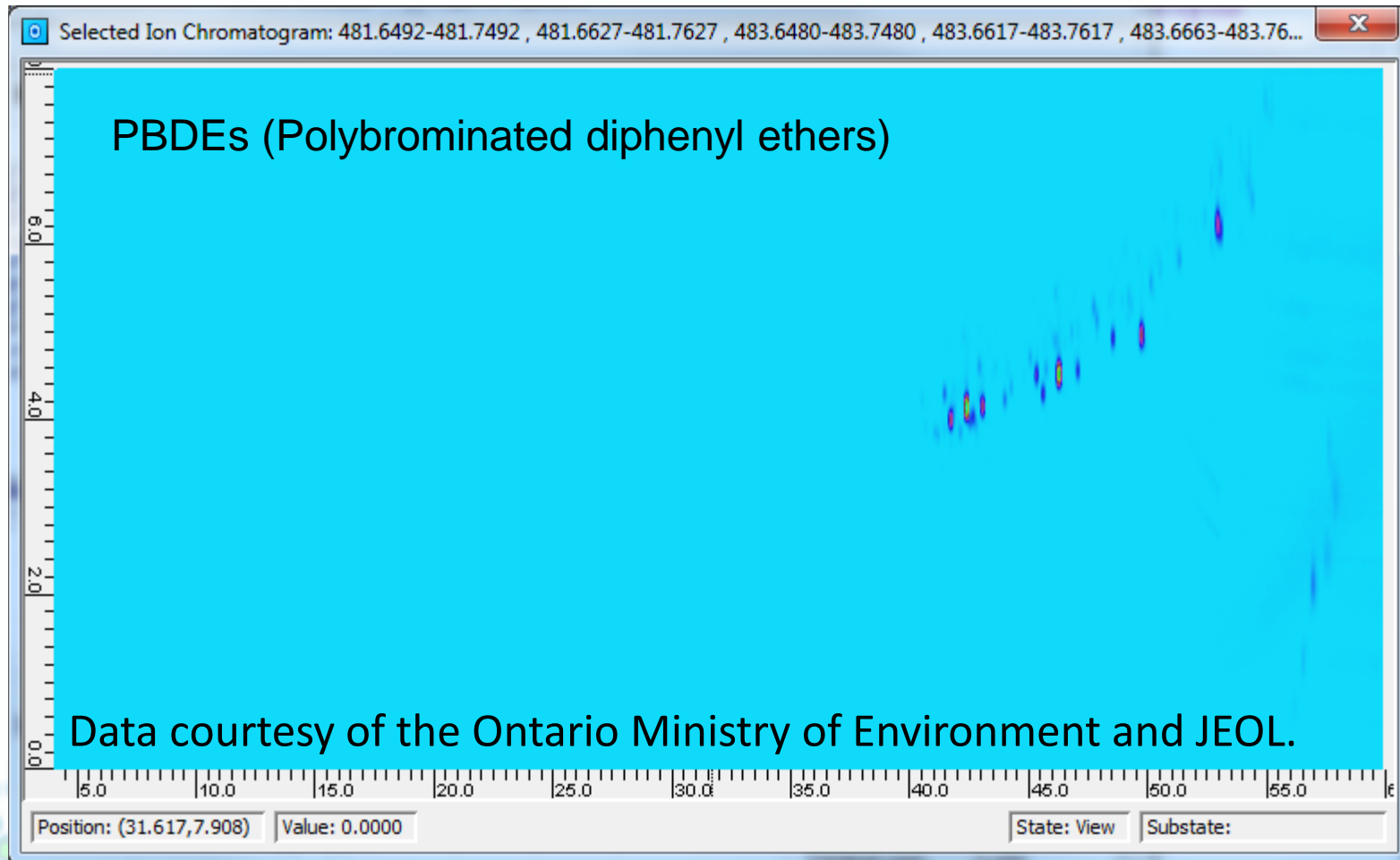
## HRMS - Mass Defects - Example



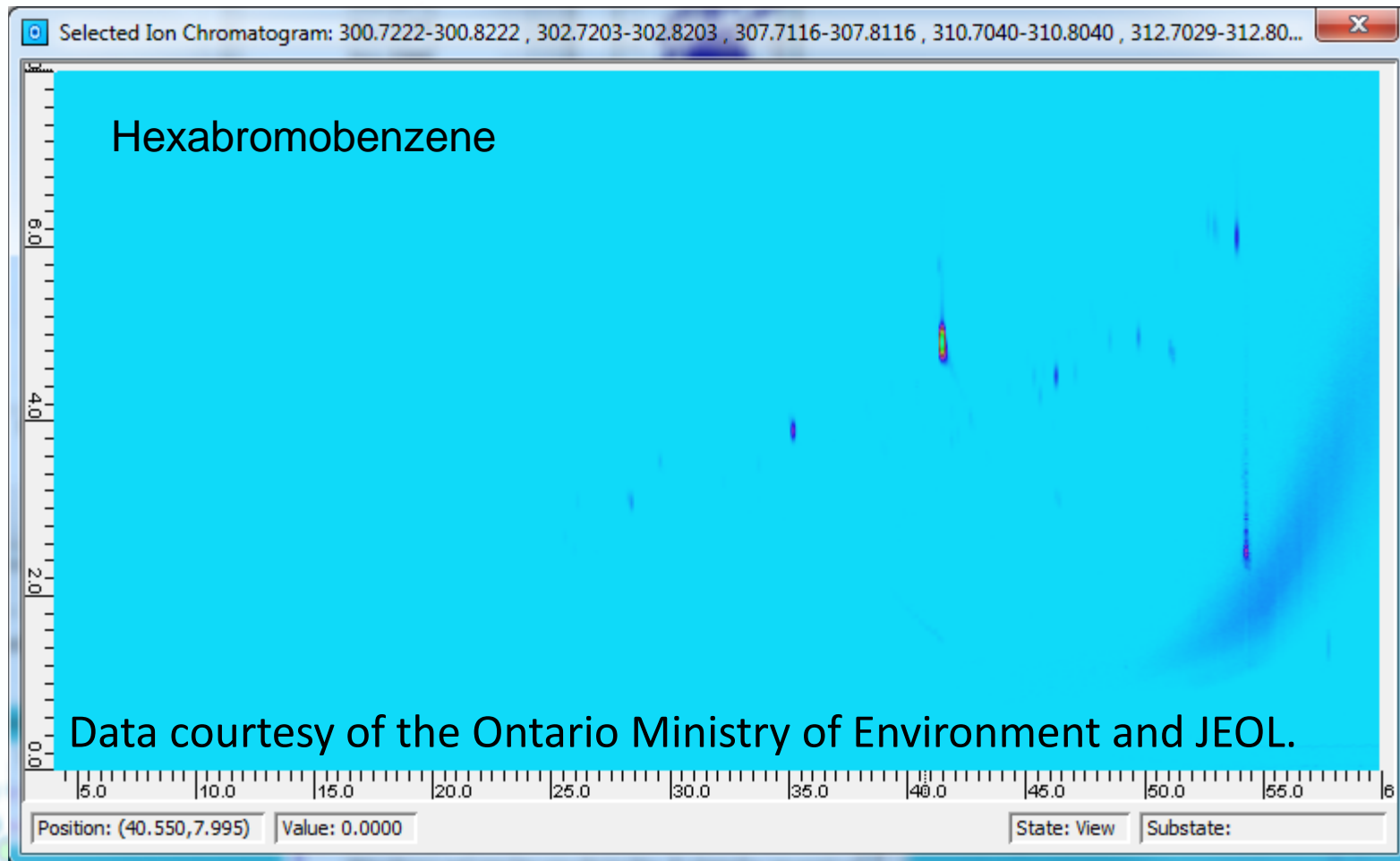
## HRMS - Mass Defects - Example



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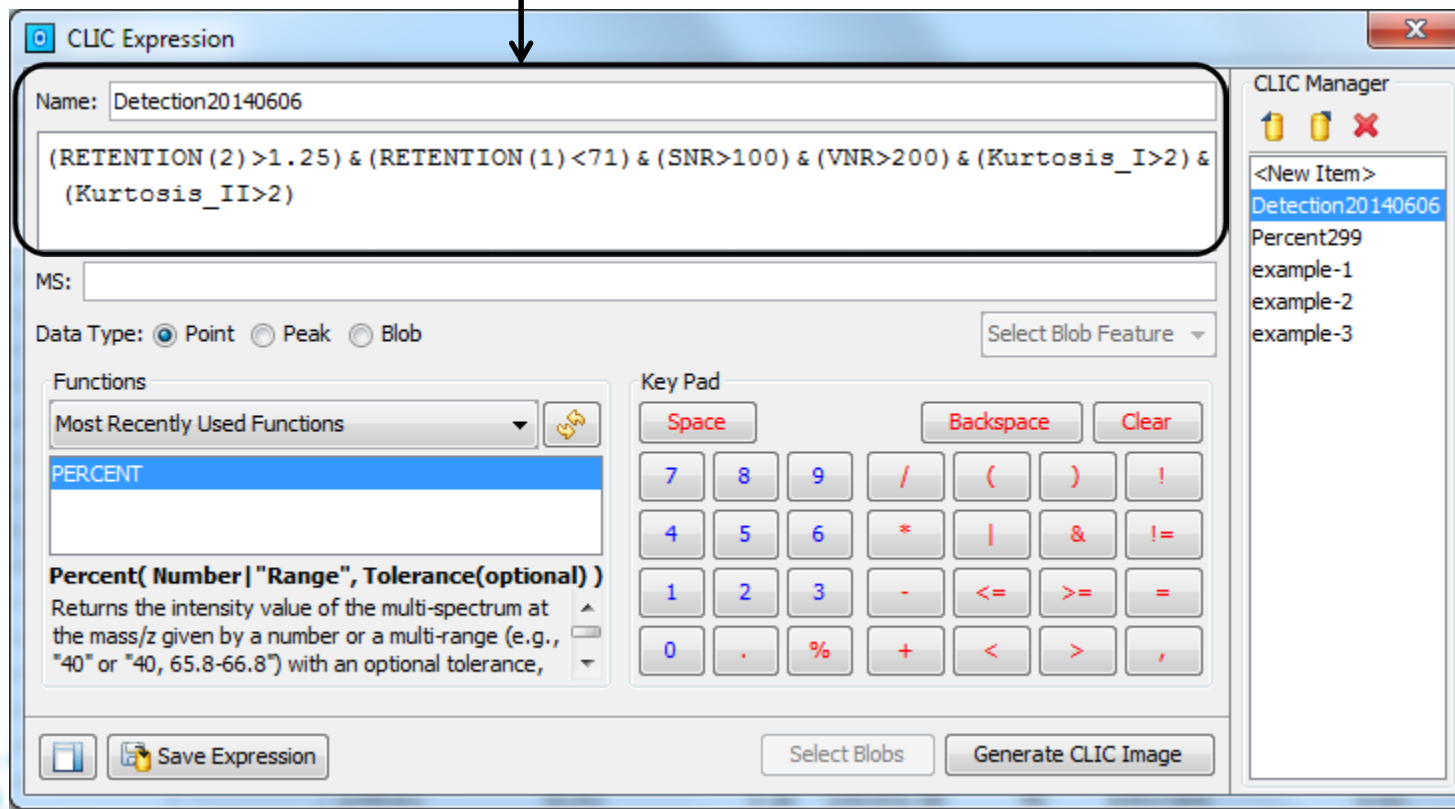


## HRMS – Other New Features

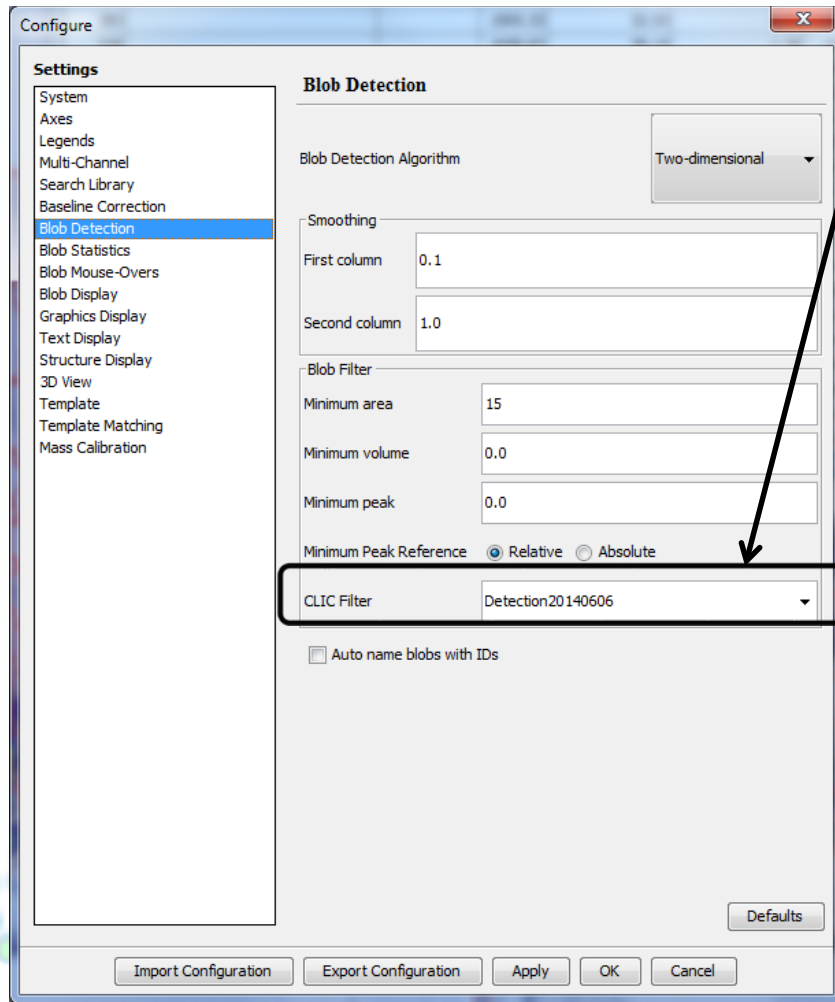
- HRMS quantifier & qualifier ions
- HRMS in CLIC expressions
- Export HRMS spectra for blobs and areas with Export Image plug-in
- Sortable measures of isotopic similarities in the Formula Calculator [pending]
- HRMS SICs in MS Cube [pending]
- Calibration for HRMS centroid data [pending]

# Blob Detection - CLIC Filter

1. Create named CLIC expression (optional).



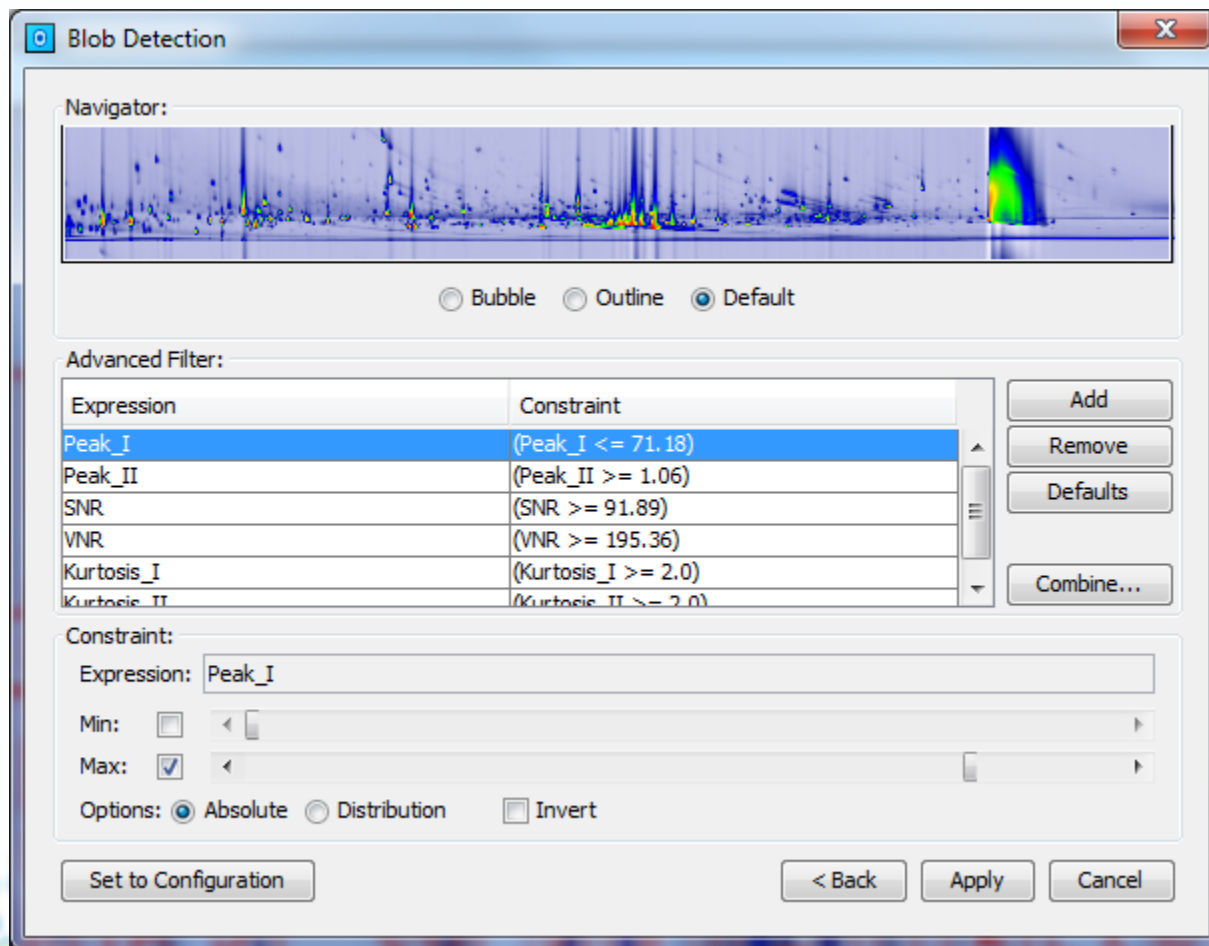
## Blob Detection - CLIC Filter



2. Specify CLIC expression to filter blobs. Can be named expression or an unnamed expression typed into configuration.
3. Detect blobs.



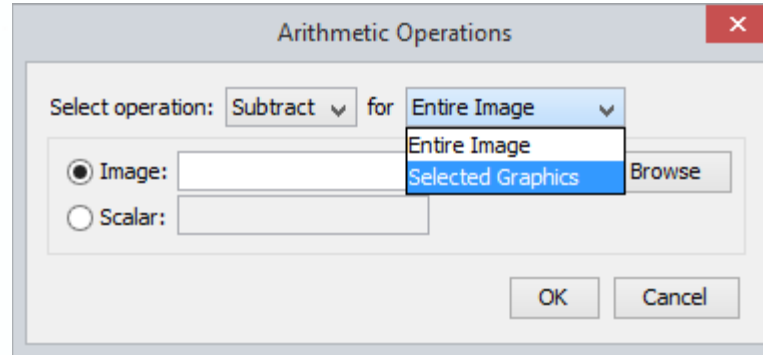
## Blob Detection - Interactive Filter



Filters are applied in combination. As a filter is changed, e.g., with slider, blobs are added or removed.

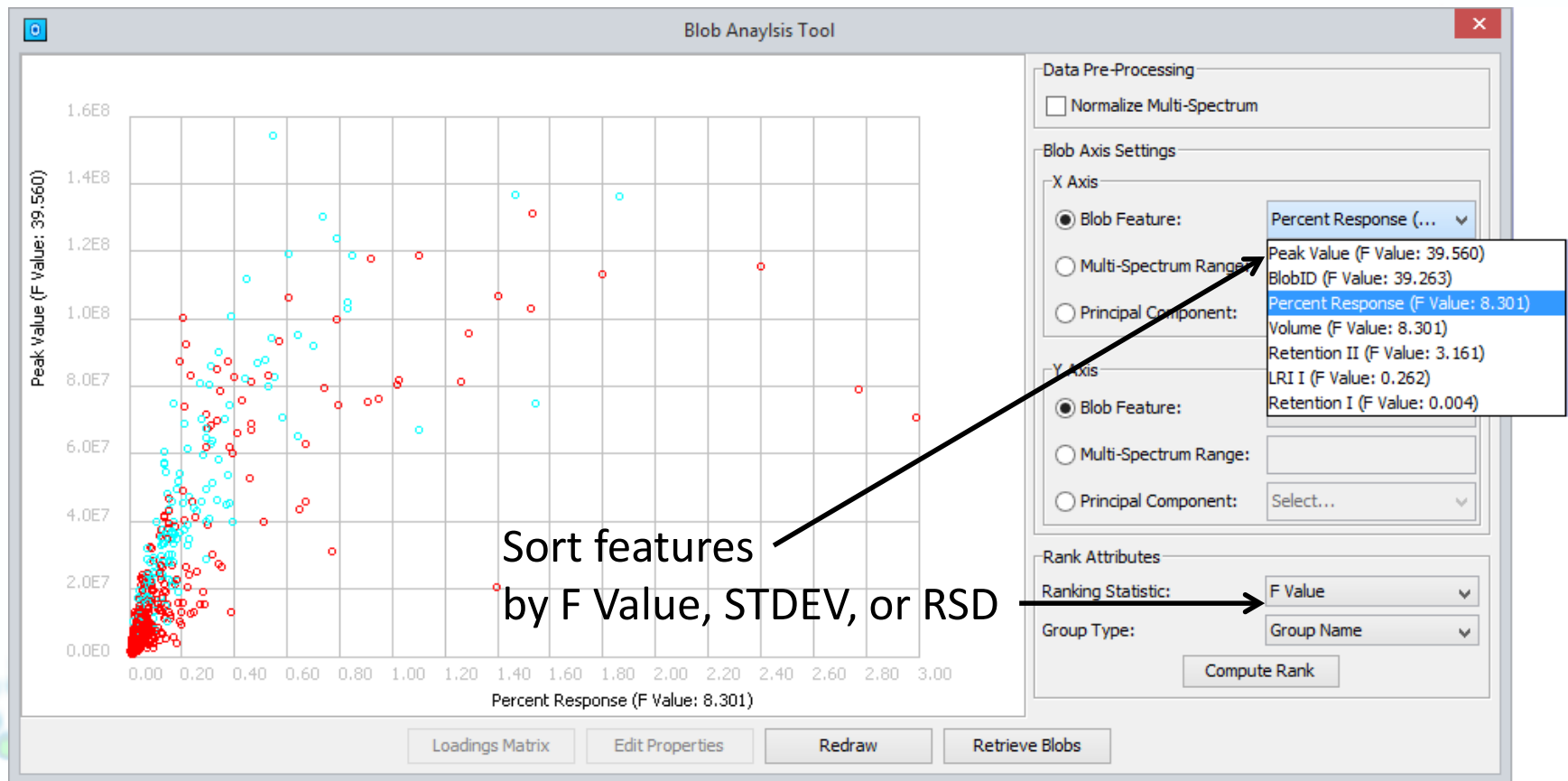
## Data Processing - Regional Arithmetic

- Arithmetic operations for selected region(s)



## Data Processing - Analyze Blobs

- Sort by group statistics in Analyze Blobs



# Data Processing - Other Operations

- Generate peak-region Area objects from selected blobs (as is done in Image Investigator Auto-Feature Analysis)
- Configure geometry for including data points in Areas or blobs in Graphics, as either leading time (used in earlier versions) or center time
- Additional options for gradient baseline correction [pending].

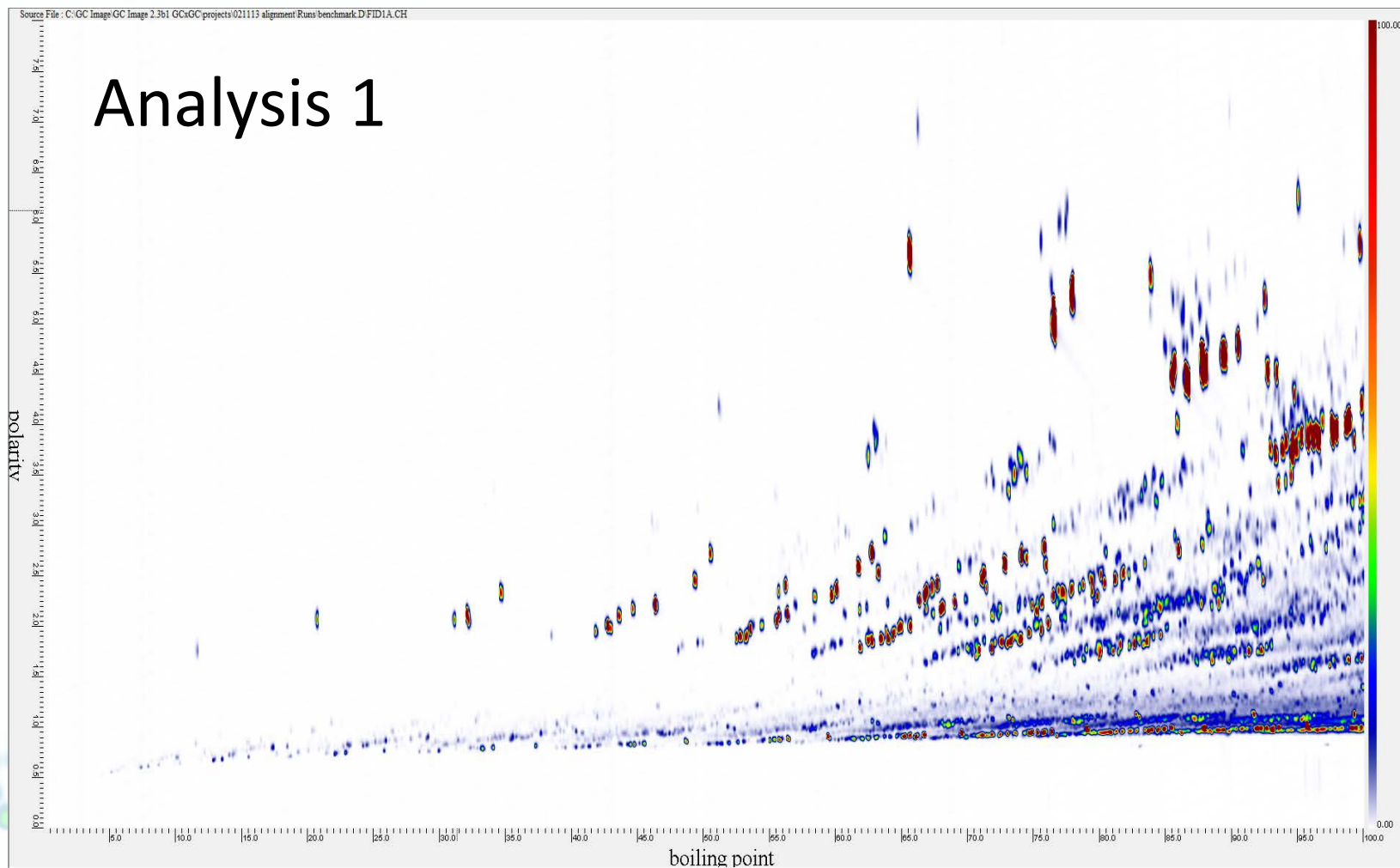
# Template Transformations

- Many causes of retention-time differences between chromatograms
  - Different detectors (e.g., FID & MS) & detector differences
  - Different columns & column differences (e.g., decomposition)
  - Operational variations (e.g., injection volume, flow rate, temperature)
  - Matrix effects

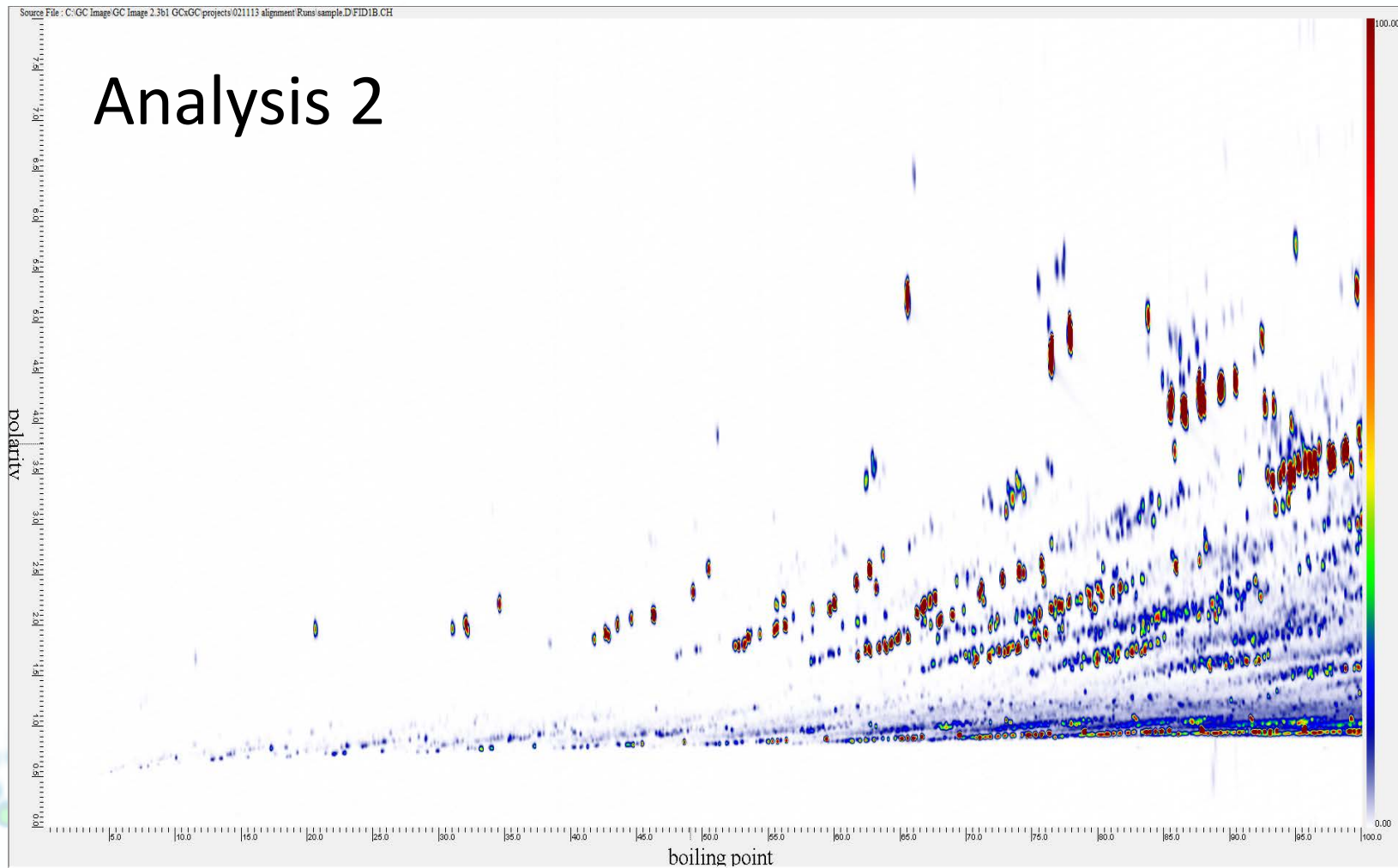
# Template Transformations

- New tools for aligning templates with chromatograms
  - Transformation based on marker peaks
  - Local transformations that limit region of transformation
  - Transformation mapping to adjust degree of transformation along either axis or both

## Template Transformations

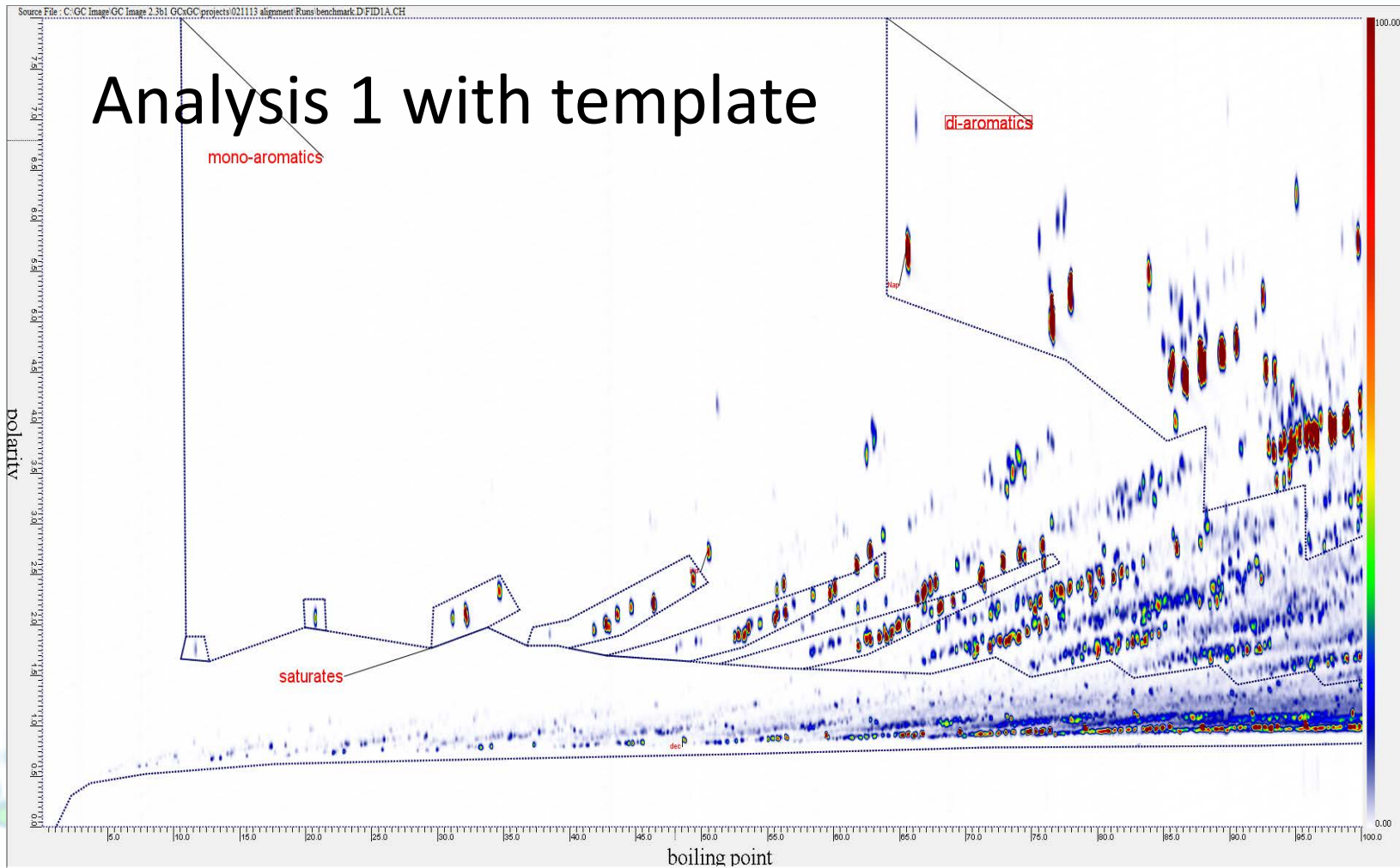


## Template Transformations

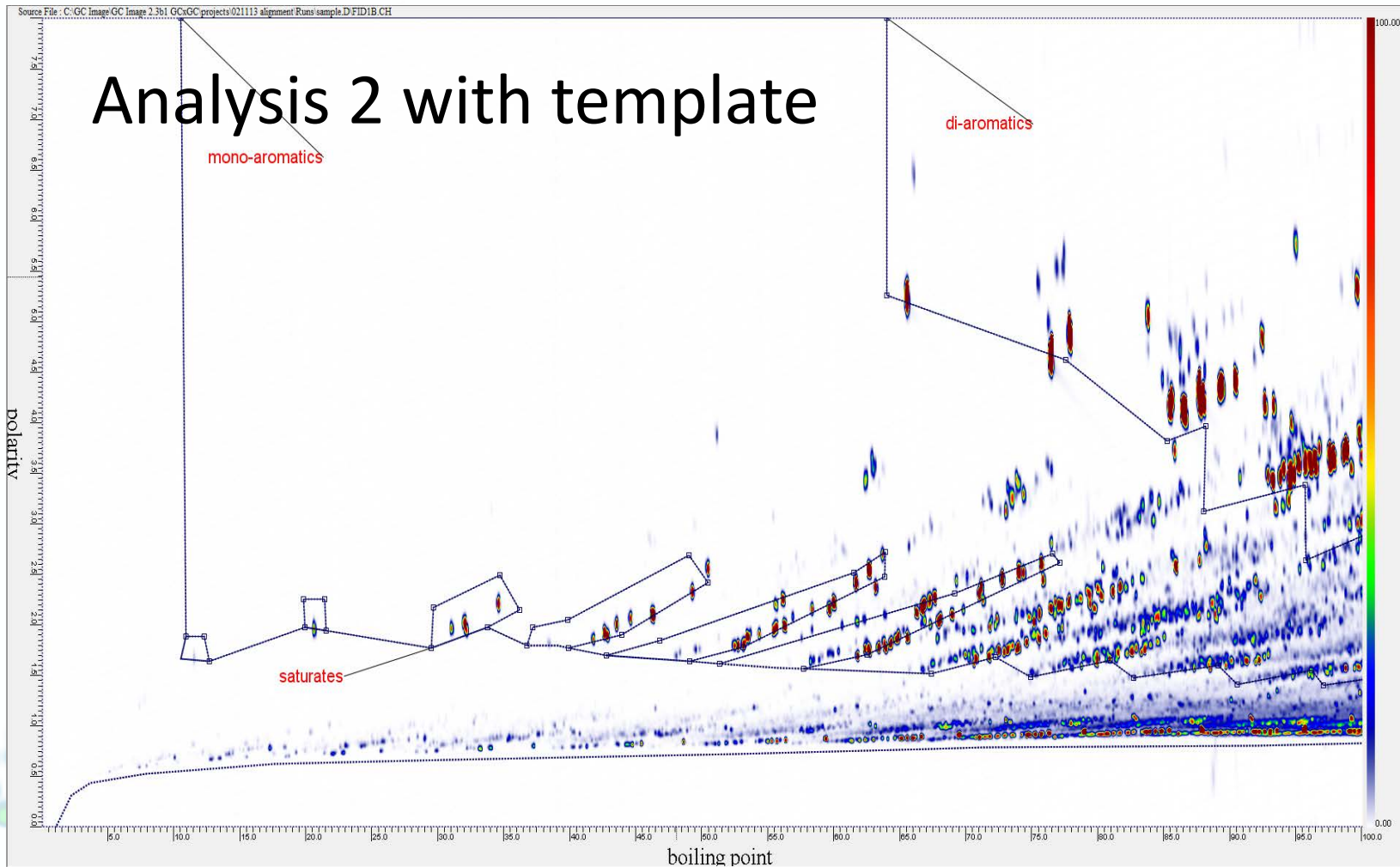




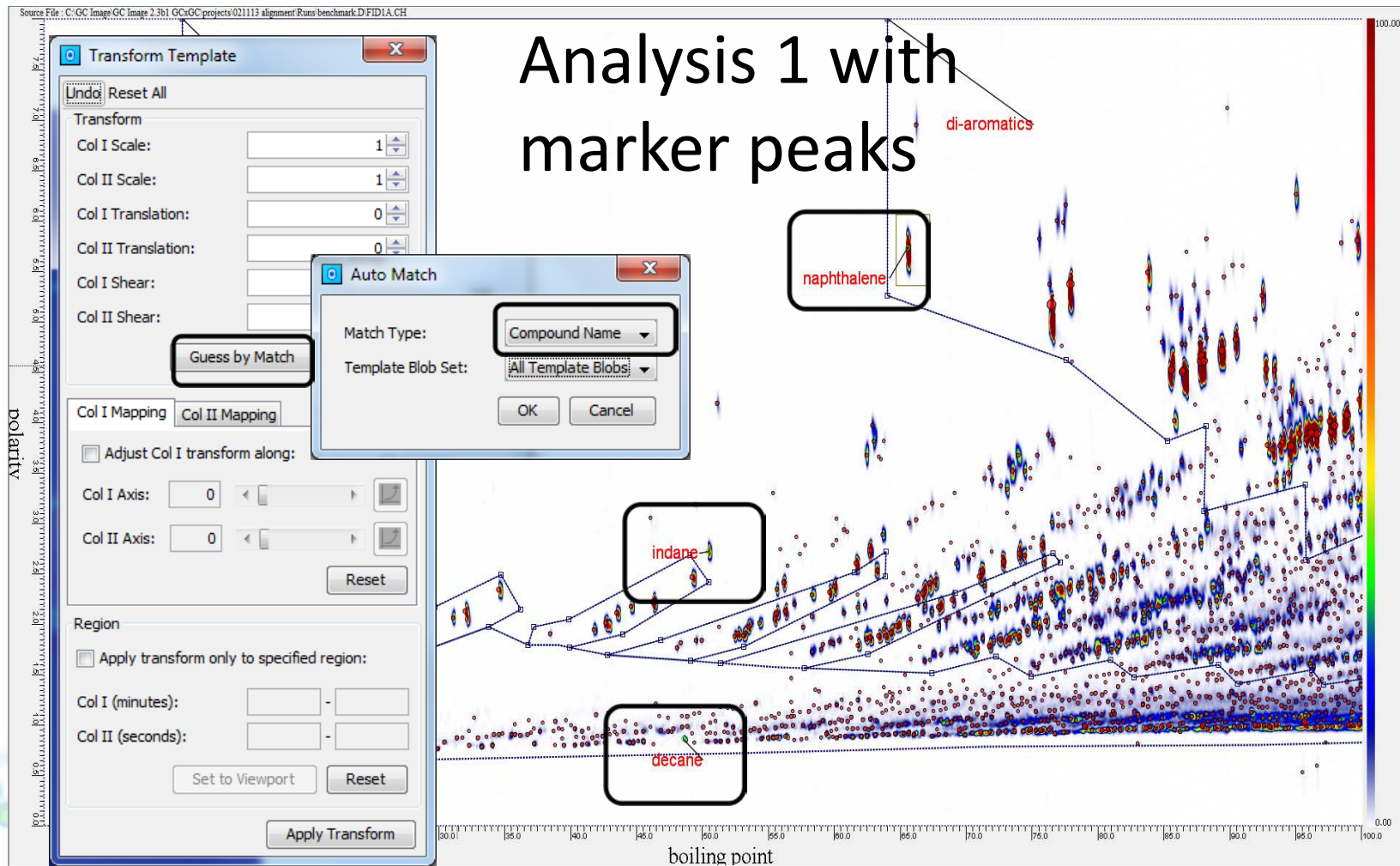
## Template Transformations



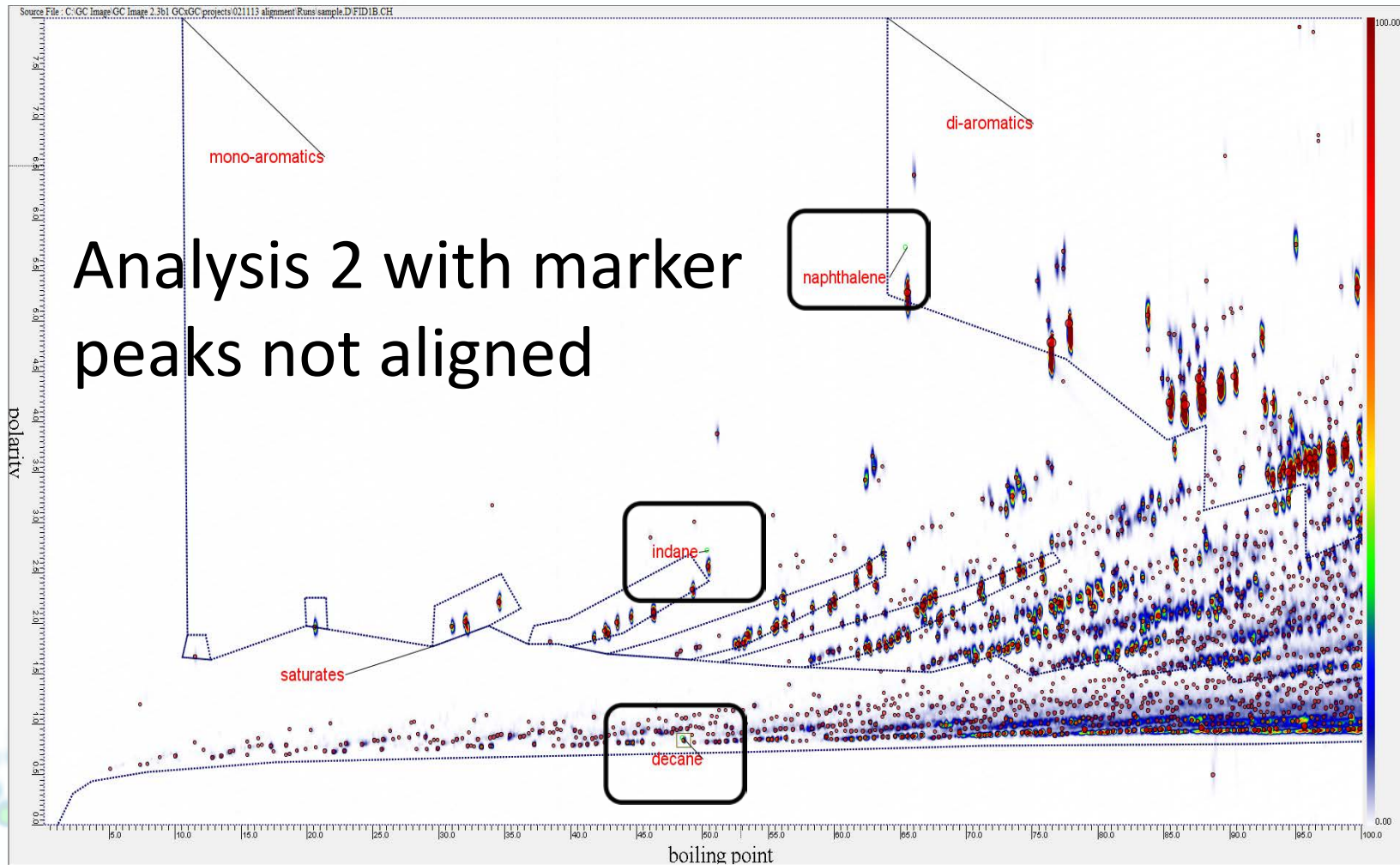
## Template Transformations



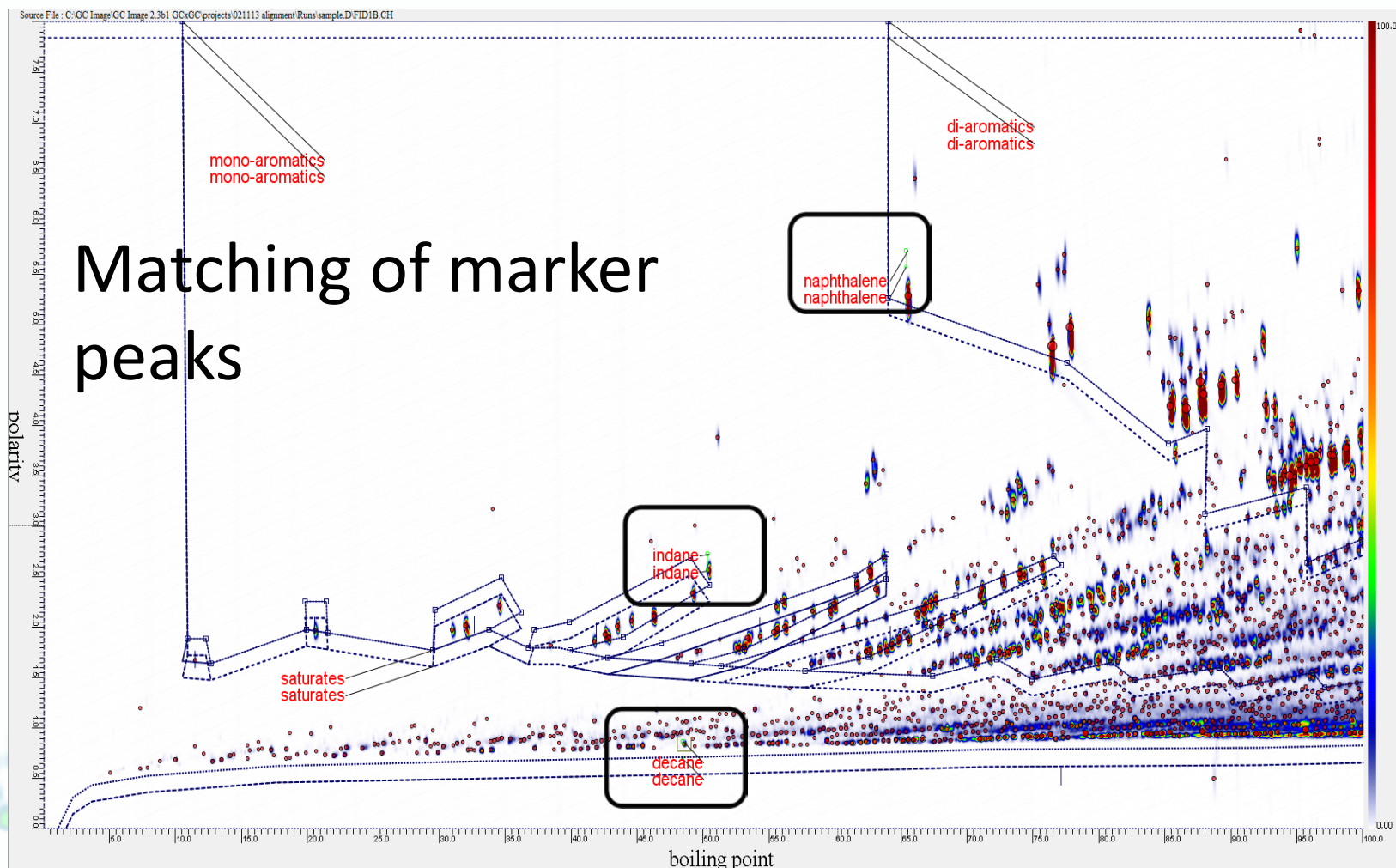
## Template Transformations



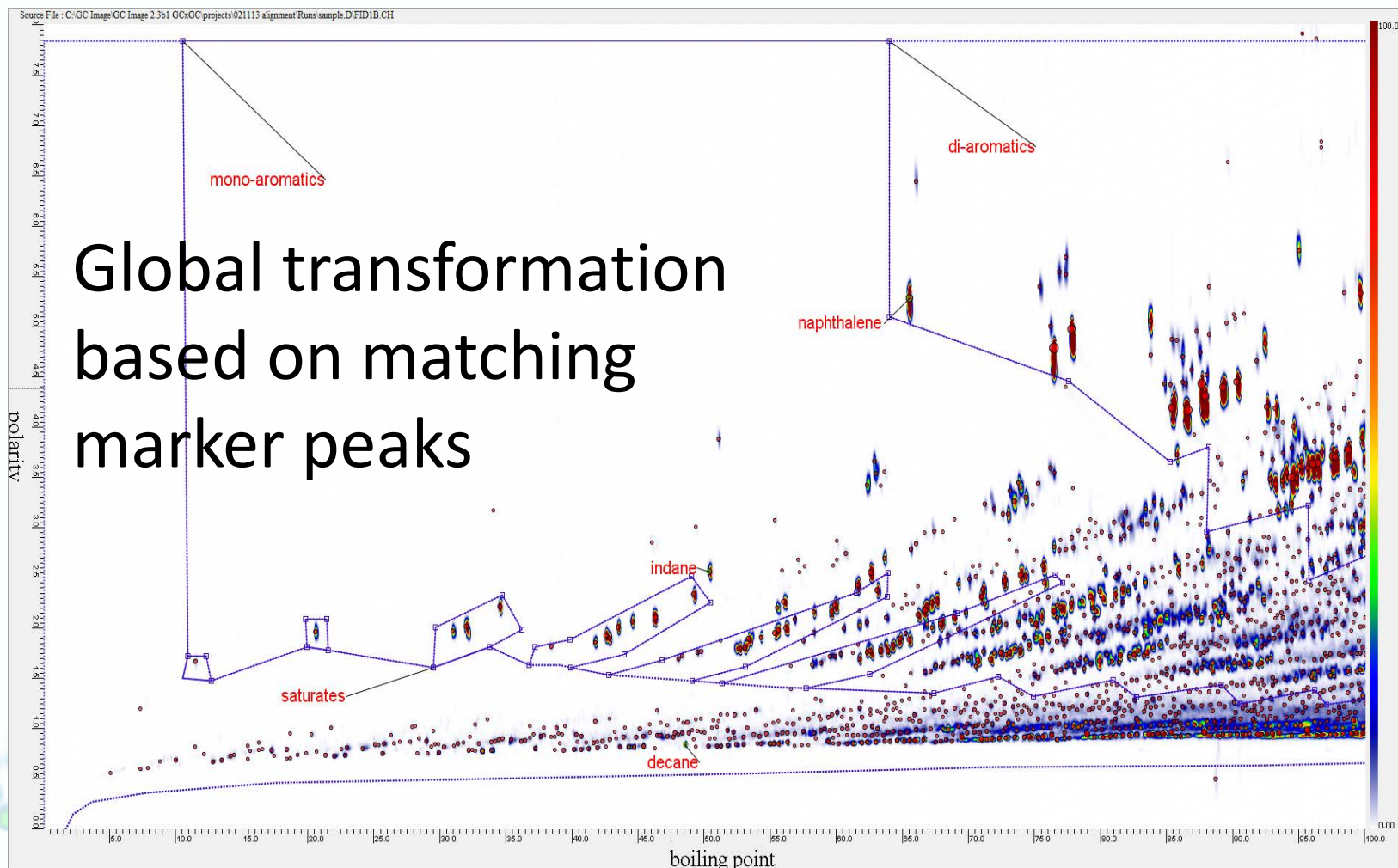
## Template Transformations



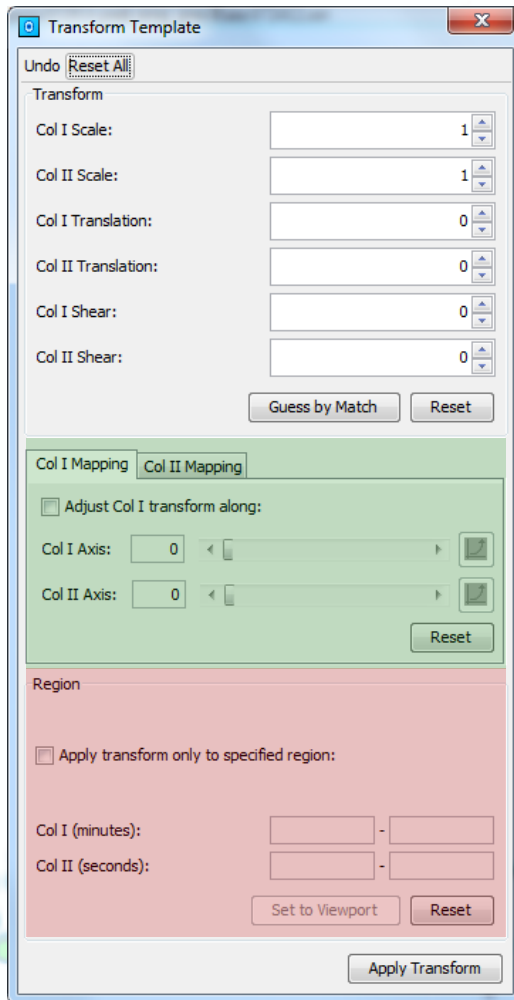
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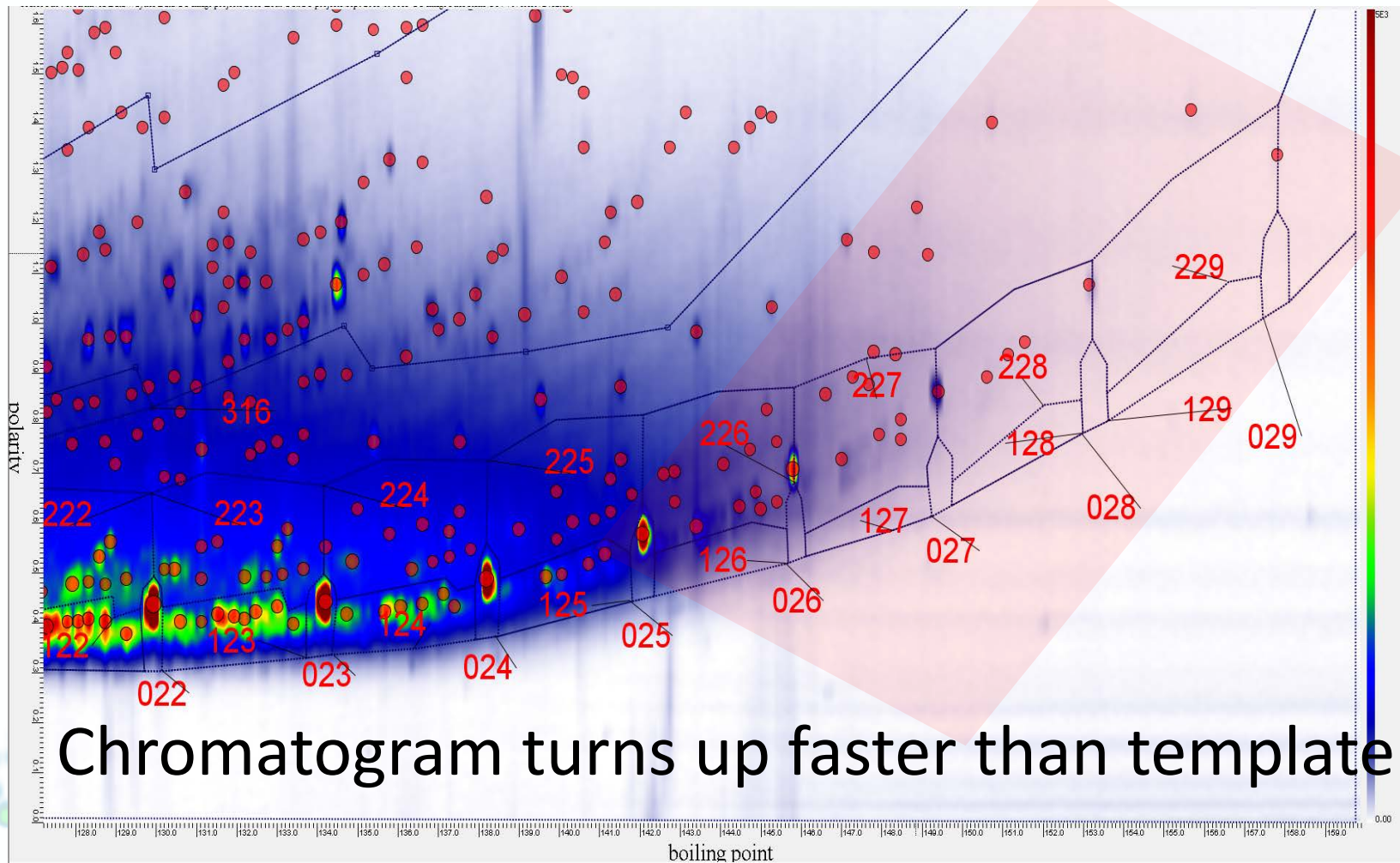


## Template Transformations



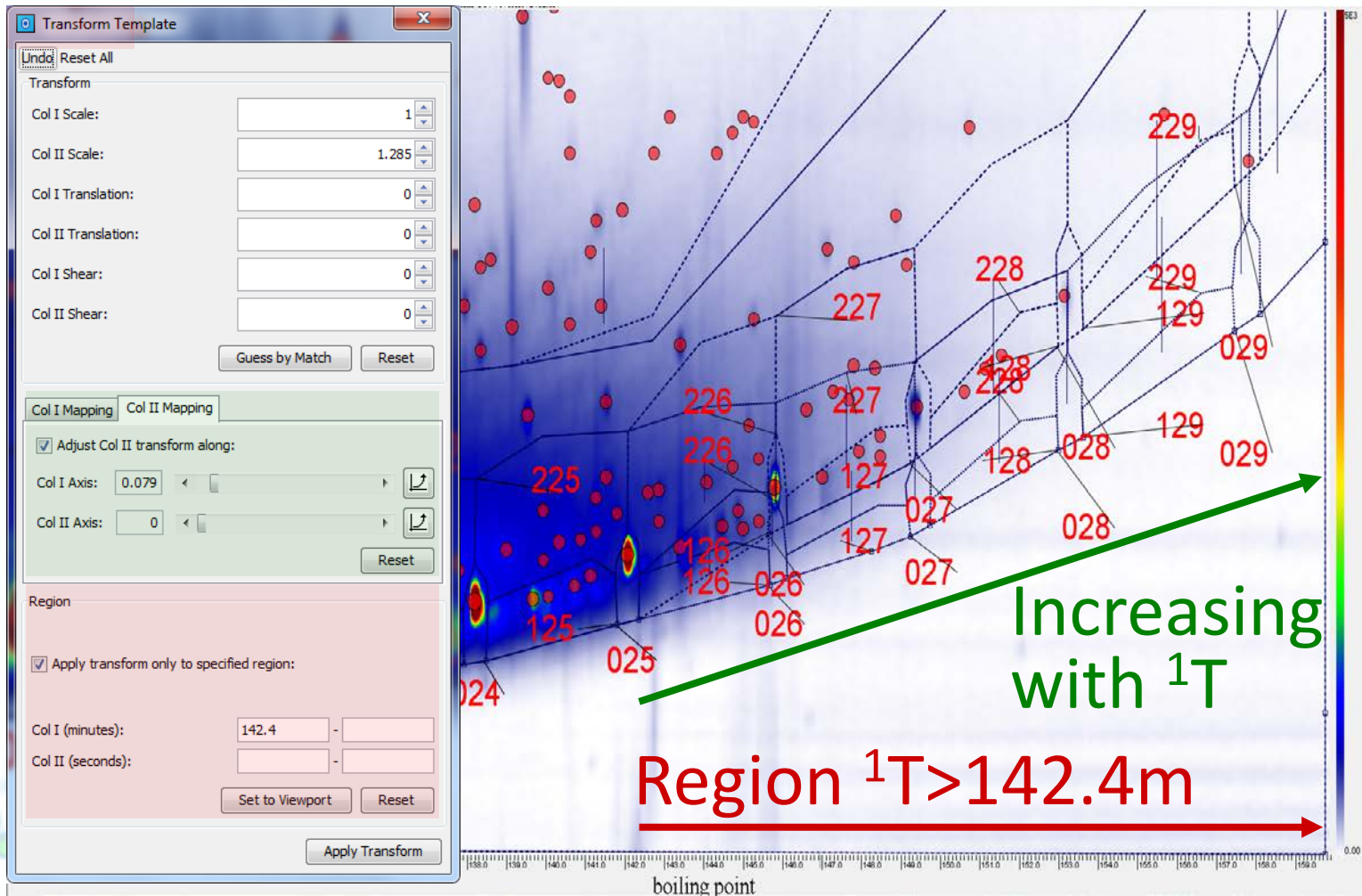
- Upper pane configures transformation (as in R2.4)
- Middle pane (green) allows variable degree of transformation along axes
- Bottom pane (red) allows transformation limited to specified region

## Template Transformations

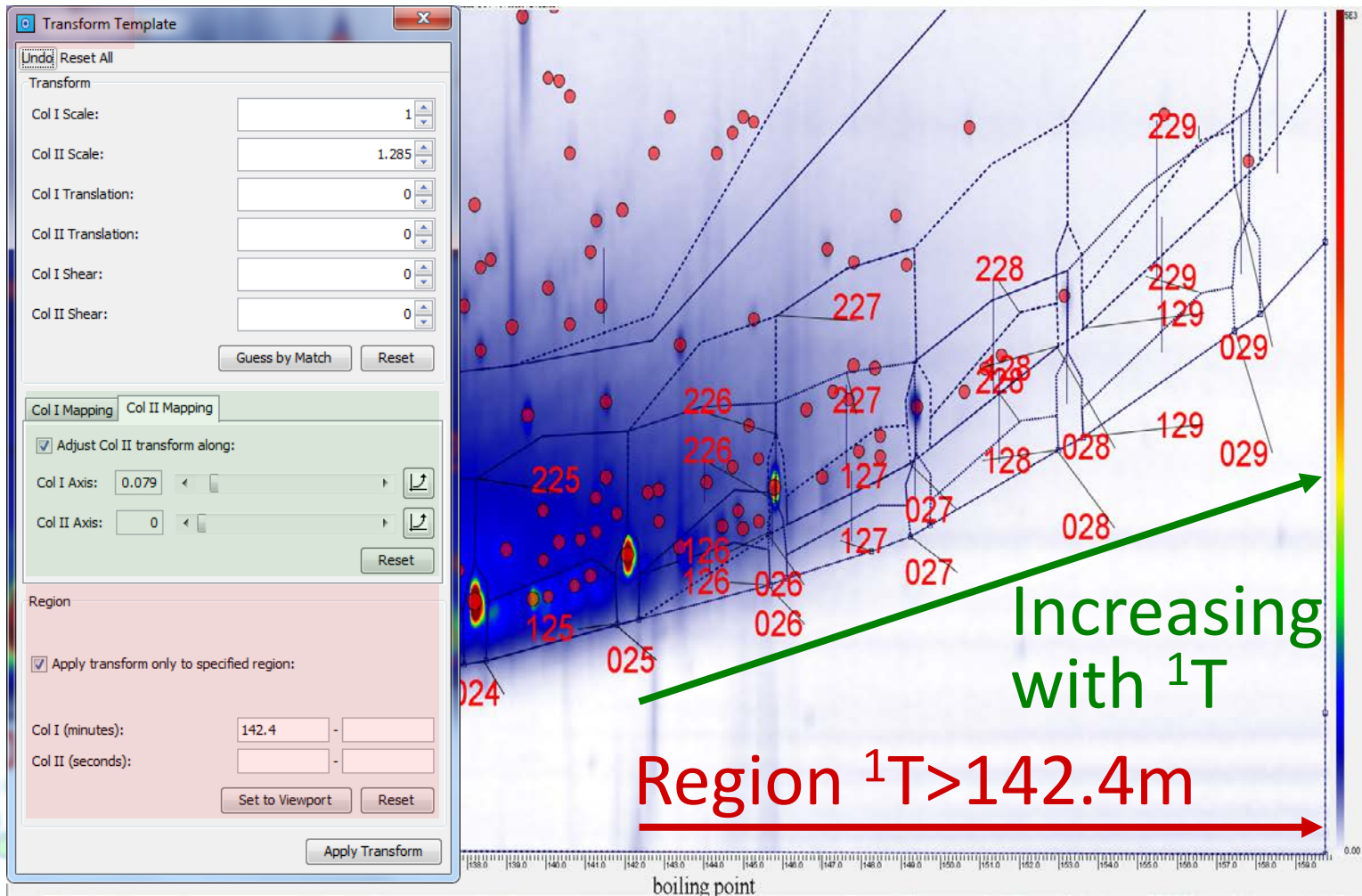




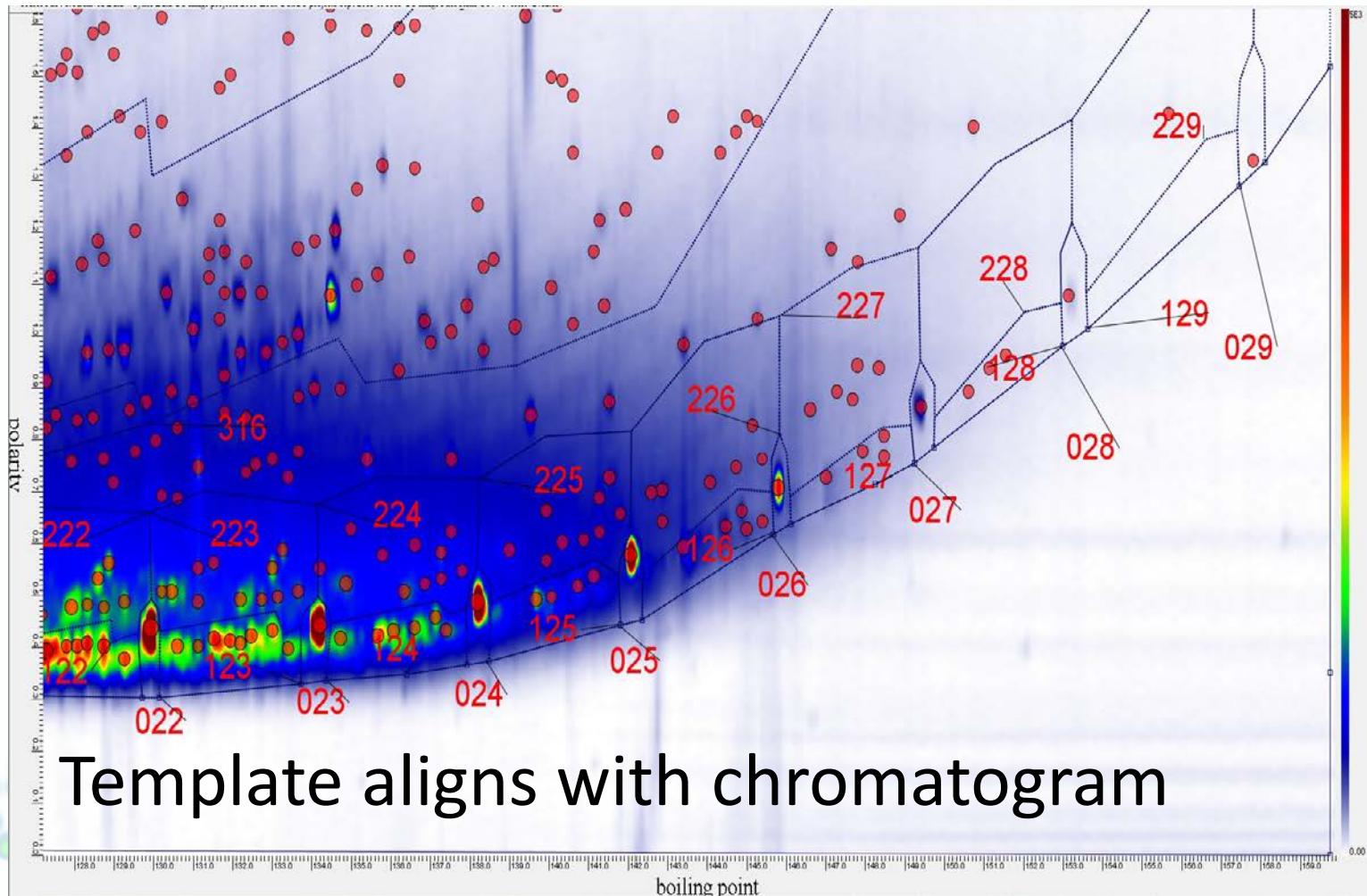
## Template Transformations



## Template Transformations



## Template Transformations



Template aligns with chromatogram

# Image Investigator

- For feature template with Auto Features, generate qCLICs from composite
- Keep compound identifications for feature template with Auto Features
- Remove chromatograms from analysis set without reloading
- Assign class labels of chromatograms without reloading

## 3D Modeling & Visualizations

- In MS Cube, adjustable value mapping for individual SICs
- In 3D View, export surface as 3D model to [Visualization Toolkit \(VTK\)](#) format file
  - VTK is open-source, multiplatform software for visualization
  - VTK format is used by many software packages
  - Easy to create 3D fly-around videos with [ParaView](#), open-source software

## Slice Reports (ASTM D2887)

- User-specified slices with fixed degree intervals
- Custom cut-points (either BP or %-off) in CSV string
- Temperature unit configuration
- Latest D2287 oil batches, repeatability, & reproducibility standards

# Molecular Weight Distributions

- From R2.5, GC Image will have growing support for polymer analysis
- New blob & area table columns
  - $M_p$  Molecular weight at peak apex
  - $M_n$  Number average molecular weight
  - $M_w$  Weight average molecular weight
  - $M_z$  Z-Weight average molecular weight
- Configurable linear calibration

## Tables & Reports

- Sorting on text field recognizes numbers in tables & Comparison Report
- Optional field for graphics group name(s) in Blob Table
- Optional description field in Comparison Reports
- Option to show or not show residual group in Blob Sets Tables & Areas Tables



## I/O Features

- Export selected regions from Export Image in text formats
- Save SIC and CLIC images from chromatograms with variable modulation periods
- Mass Hunter speed improvements [pending]
- Improved options for sampling rate interpolation without padding [pending]

## Miscellaneous

- Populate LRI Table has Append option
- User-specified locations for Text label relative to object
- View journal from GC Project
- Sticky modes for Cursor Palette buttons for creating new objects
- Toolbar reorganization

## In Progress

- NIST14 interoperation, especially enhancements for RIs [pending]
- Align chromatogram to template and resample [pending]