DraMS Thumbnail

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Updated on 2021-10-25:

momadataviewZ.app.zip

Chromatogram Instructions

1. Load a MOMA GCMS run
2. Under "Data Viewers" menu, select "Chromatogram Viewer"
3. From Chromatogram viewer, click "Thumbnail" checkbox (calculation takes time, so there will be a period of unresponsiveness)
4. Create a ZIC or cZIC trace with UI at bottom of window

The 'Z' denotes the thumbnail data, which keeps only the detected peaks that fit within the data volume estimate. If a SIC or cSIC is duplicated with the '+' and the duplicate is changed to a ZIC or cZIC it will stay linked to the original SIC or cSIC when changing m/z. **NOTE:** the linking is only one way ZIC --> SIC, not SIC --> ZIC

Calculation Notes:

- Each summed histogram from the GCMS has a stripped down thumbnail counterpart, which is at most 74 detected peaks
- If a detected peak has a FWHM < 1.5 or > 5.5 bins, it is rejected

Mass Scan Viewer Instructions

1. Under "Data Viewers" menu, select "Mass Scan Viewer"
2. Select a mass scan in the list on the left side of window
3. Click the "Math" popup menu, and select the "Fit All" checkbox
   - This plots the fitted peaks over the raw data
4. To list the details of all the peaks, click "Peaks" popup menu and select the "Show List" checkbox
   - The cutoff can be altered from the default value of 74 peaks with the "Peak Number Cutoff" field
   - The red horizontal line indicates the y-axis value that corresponds to the cutoff

Release History

2021-09-27: Initial release of modified momadataview app for assessing thumbnail product

2021-10-15: [316f106] Feature refinement before wider release (includes dynamic peak cutoff line)

2021-10-25: [bc44147] Update mass scan viewer to reflect thumbnail data

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