What's new in Tofware V2.1?

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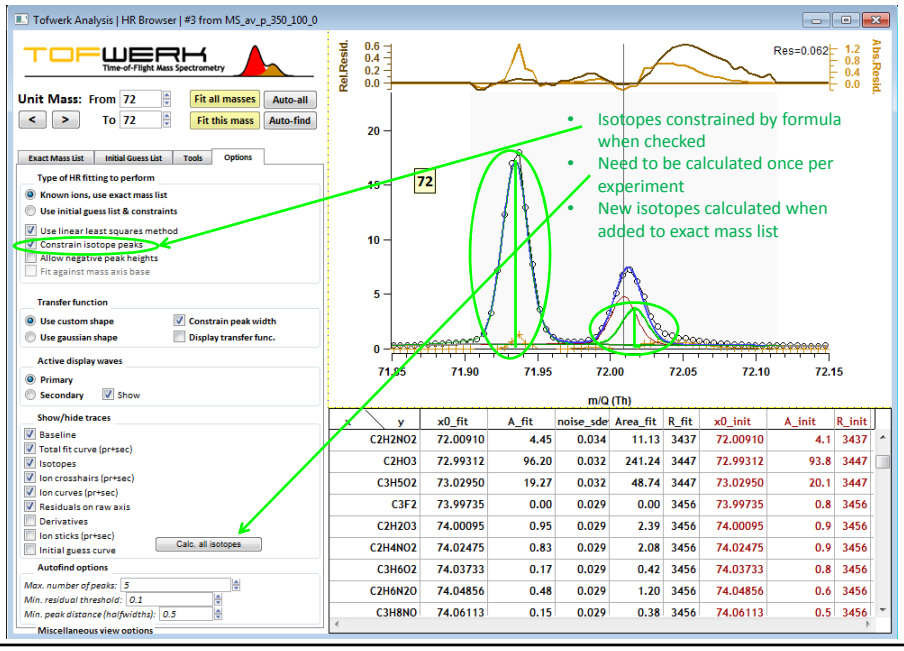
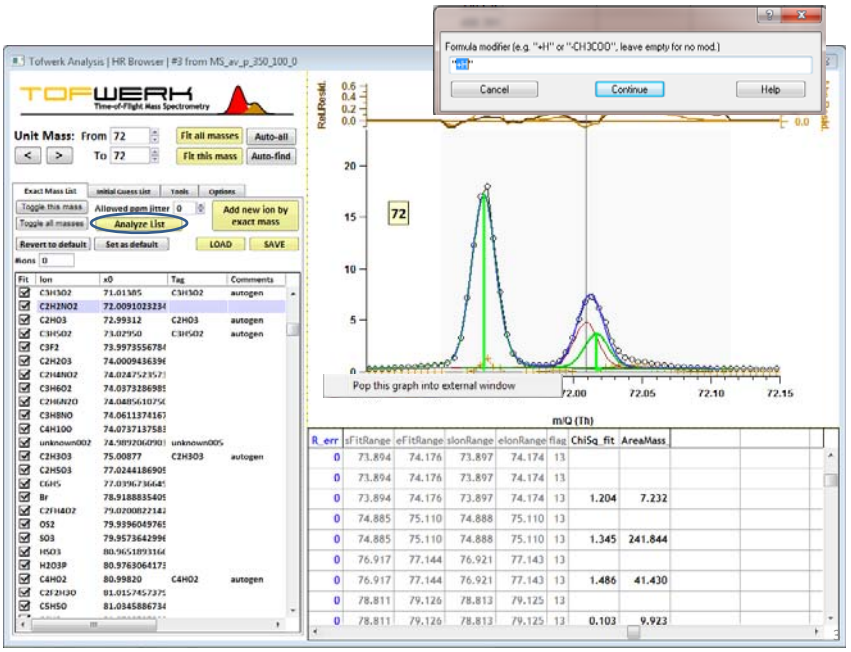
TOFWERK Time-of-Flight Mass Spectrometry

Isotopes



More Analysis tools



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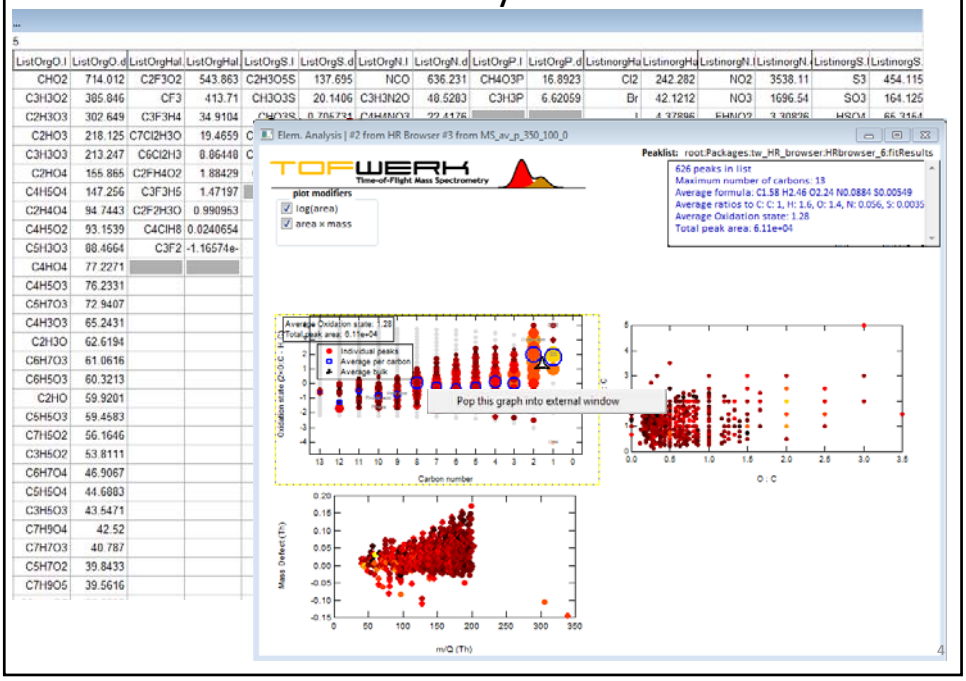

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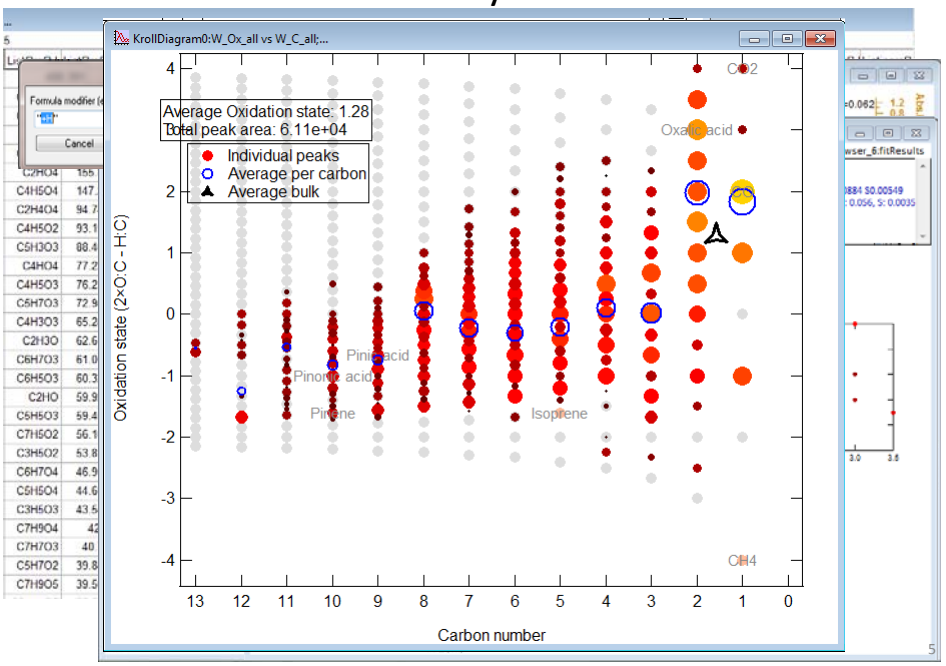
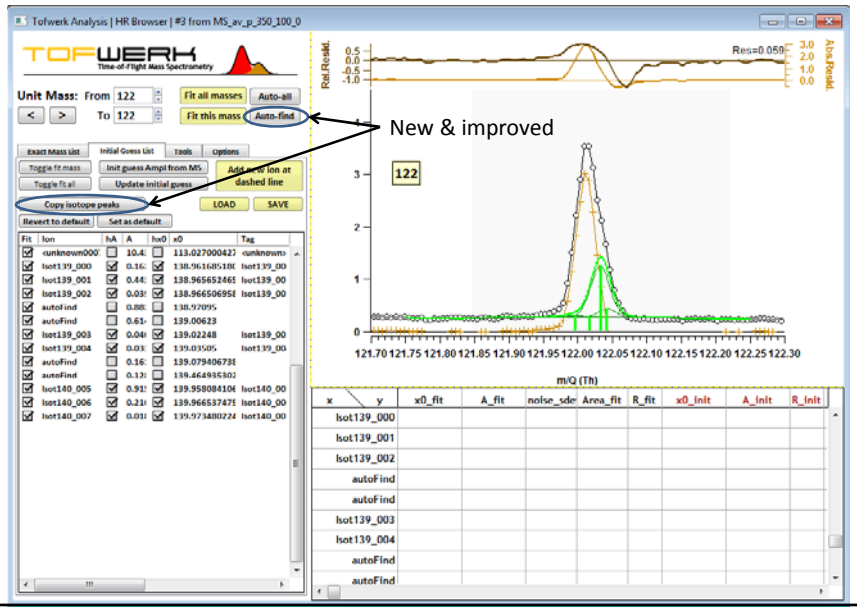


Easier peak finding and identification



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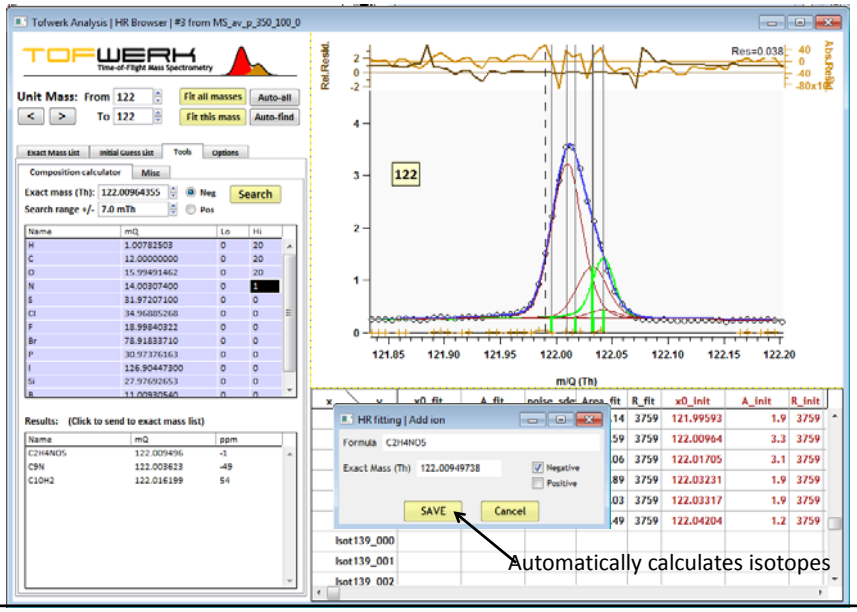
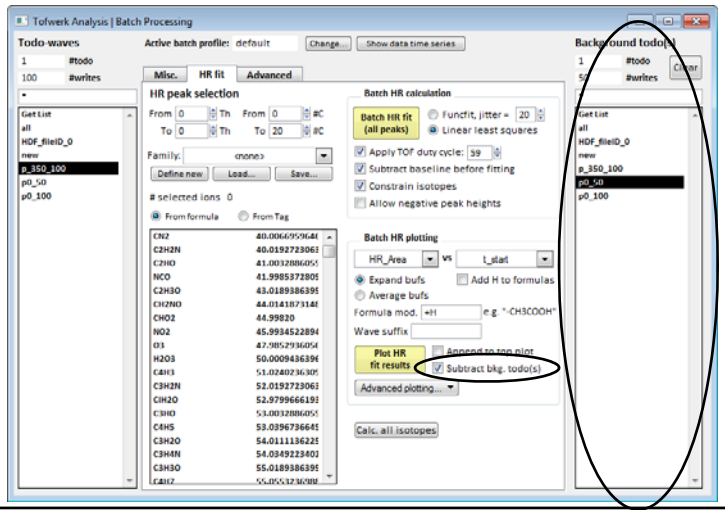


New items in HR batch fitting panel

Background subtraction:

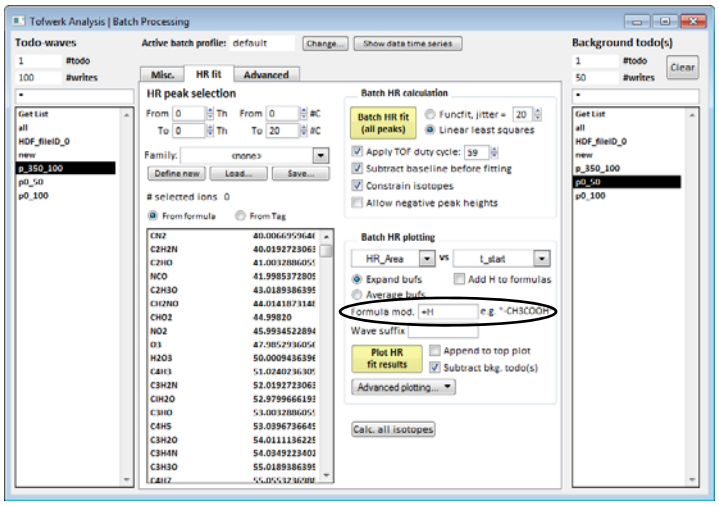
- Select either 1 background todo or as many as signal todo waves
- Will subtract average of background todo (currently no normalization)



New items in HR batch fitting panel

Formula modifier:

- Allows adjustment for ion chemistry
- More accurate calculation of elemental properties (e.g. OsC)



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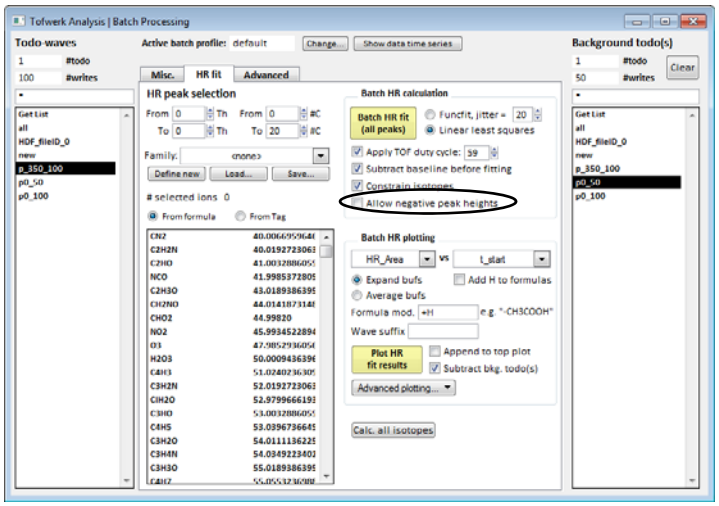
New items in HR batch fitting panel

Negative peak heights:

- Handle with extreme care!



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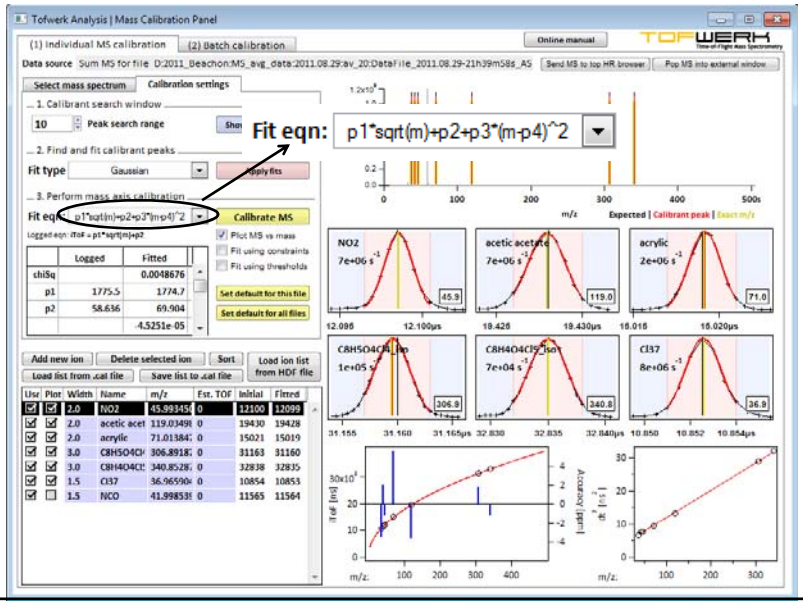
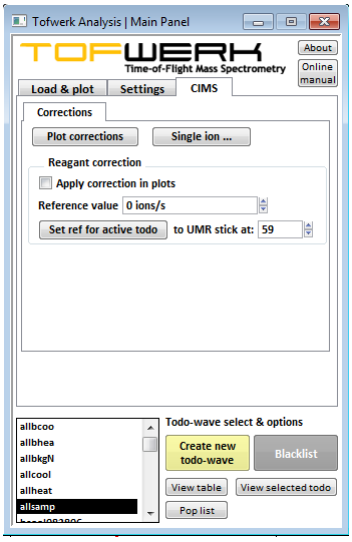
New m/Q calibration function



CIMS-specific tab in main panel



- Addition of CIMS-specific functionality to Tofware:
  - normalization of UMR data to reagent ion
  - display single ion signal
- Other instrument-specific tabs exist (ACSM, pToF, …)
- Currently: only one can be loaded at the same time

Internal changes

- Bug fixes
- Toftools XOP speeds up many tasks
  - Composition calculator
  - Isotope calculation
  - iTof ↔ m/Q

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Perspective: future implementations

- Adapt to new EyeON data output
- More MOVI-specific functions (thermograms, etc.)
- Frag tables (user input needed: what do we know about fragmentation in the CIMS?)
- Spectra arithmetics
- More analysis tools
- Switch to numeric-only hdf files (will speed up HR batch fitting)
- More frequent updates (monthly, biweekly?)
- …?
- Bugs and comments: https://sites.google.com/site/citofms/analysis-software/bug-reports

Thanks to all beta testers!

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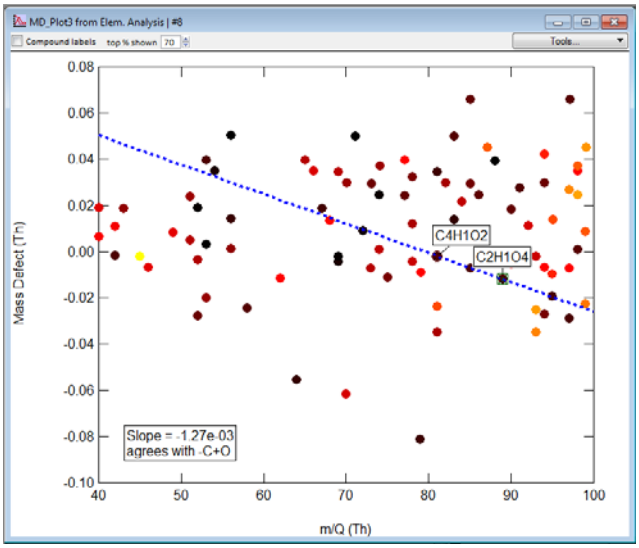
More analysis tools for mass defect plots

Auto-updating plot

- compound labels
- select percentile shown

Will be included in next beta release!



Cursors draw line and try to assign transition

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Extra slides

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Bad use of negative peak heights

Don't use to get a better fit!

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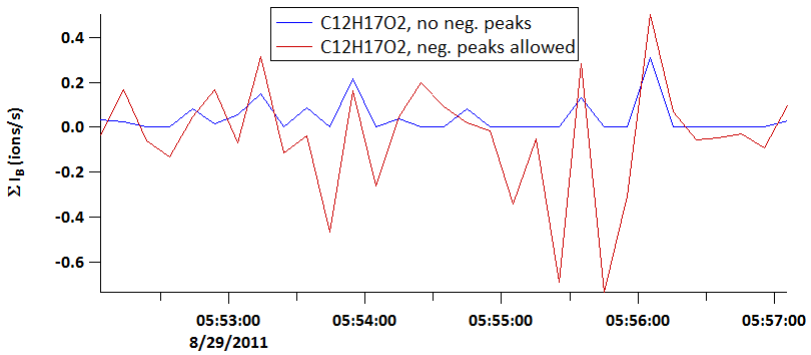
Good use of negative peak heights?

- Can avoid positive bias in HR time series
- Problem: noise typically higher due to more degrees of freedom
- Better: use standard deviation (not always possible, e.g. heating cycles)



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