What’s new in Tofware V2.1?

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Isotopes

- Isotopes constrained by formula when checked
- Need to be calculated once per experiment
- New isotopes calculated when added to exact mass list
More Analysis tools

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Easier peak finding and identification

New & improved
Easier peak finding and identification

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)

New items in HR batch fitting panel

Negative peak heights:
• Handle with extreme care!
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 \leftrightarrow m/Q

Perspective: future implementations

• Adapt to new EyeON data output
• More MOVIR-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!
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

Extra slides
Bad use of negative peak heights

Don’t use to get a better fit!

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)