Spectroswiss

peakbypeak PROCESS ANALYSIS

Empower Your Real-Time Mass Spectrometry Research

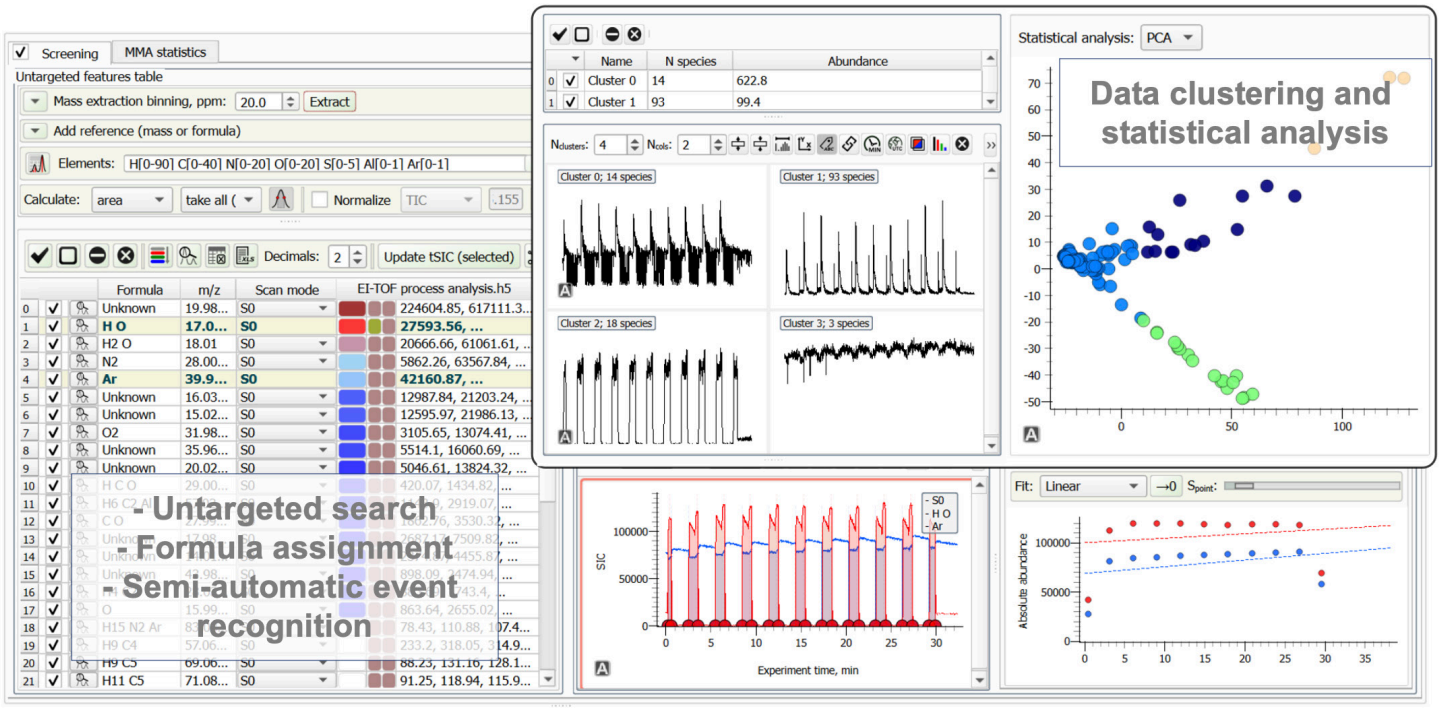
Process, Analyze, and Visualize Real-Time MS Data – No Matter the File Size

Industrial processes and environmental monitoring increasingly rely on high-performance mass spectrometry (MS) to deliver real-time insights and support both targeted and untargeted molecular analyses.

Real-time MS, however, presents significant challenges, including extended acquisition times, rapidly changing signals, harsh operating environments, wide concentration ranges, and limited access to calibration standards.

TOFWERK (Thun, Switzerland) addresses these challenges with its Process Analysis, Air Quality Monitoring, and Cleanroom Monitoring MS instruments, enabling robust real-time MS over extended acquisition periods.

Peak-by-Peak Process Analysis software from **Spectroswiss** (Lausanne, Switzerland) is purpose-built for processing data generated by TOFWERK instruments. The software supports both targeted and untargeted analyses (illustrated in the example screenshot below) and provides efficient recalibration workflows together with scalable data handling, suitable for applications ranging from short measurement campaigns to long-term monitoring studies.



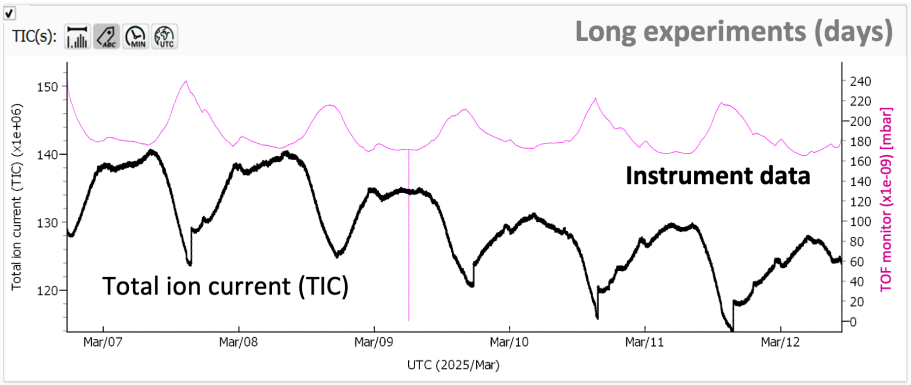
Key Features

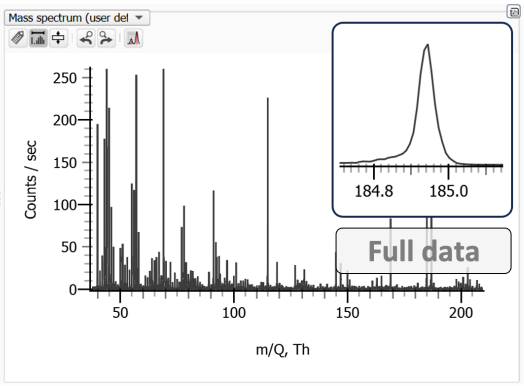
- A full cycle of **real-time MS** data processing & analysis, also for data of any size
- Directly compatible with **TOFWERK** mass spectrometers data, including **profile** mass spectral data
- Alignment of mass spectra and **instrument data** (pressure, temperature, voltage, digital inputs, *etc.*)
- Adjustable time axis with conversion between seconds, minutes, & **UTC** (coordinated universal time)
- No *m/z* scale binning & advanced peak data management: avoiding artifacts & increasing processing speed
- Mass accuracy evaluation & mass spectra **adaptive recalibration** and data validation
- Multiple experiments support & **multiple features high-resolution** SIC extraction & visualization
- Untargeted search, **molecular formula assignment**, semi-automatic recognition of events
- Data clustering and statistical analysis
- **High speed** of calculations: python, HDF file structure, & multi-threading data processing
- Flexible and customized dynamic **data export**, including in CSV, TXT, XLSX file formats

High-speed adaptive re-calibration of mass spectra for process monitoring, Nagornov et al., MOC pm 15:10, 73rd ASMS, Baltimore, MD, 2 June 2025

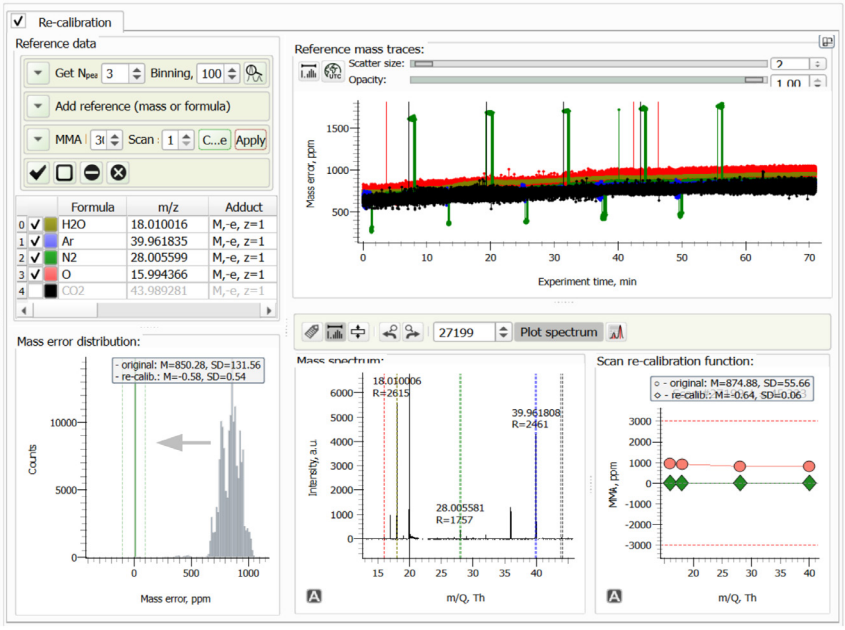
The following examples illustrate step-by-step data processing and analysis using the **Peak-by-Peak Process Analysis** software. Through real screenshots, they demonstrate full-data loading and visualization for long-duration experiments, comprehensive pre-processing workflows, and advanced analysis capabilities, highlighting key features such as flexible time-axis handling, multi-experiment support, and advanced signal extraction and visualization.

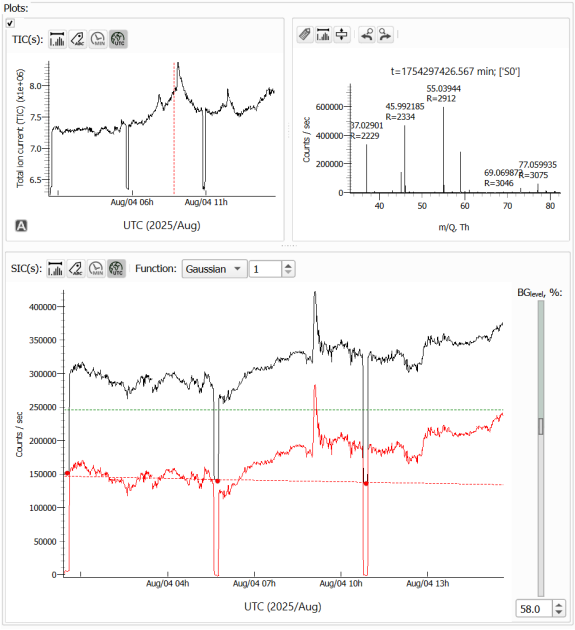
Step 1: Data Loading, Project Initiation, Alignment with Instrument Data, ...



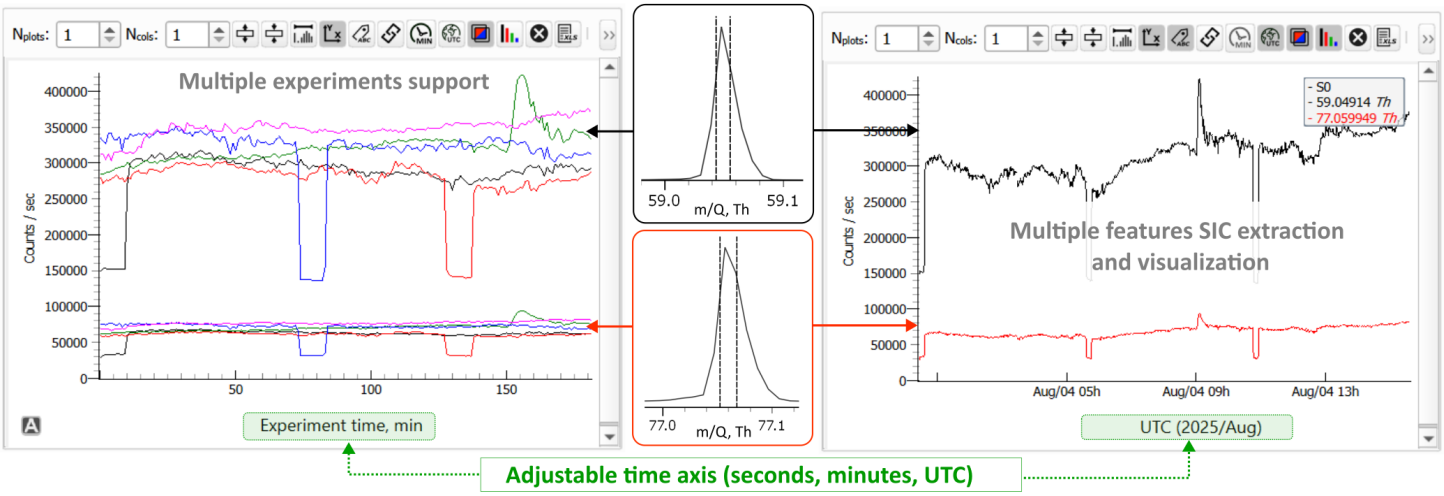


Step 2: Data Pre-Processing: Overview, Recalibration, Background subtraction, ...





Step 3: Advanced Data Processing



To learn more about our software tools or to get your free evaluation license, you are most welcome to visit https://spectroswiss.ch/software/ and to contact us at info@spectroswiss.ch

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