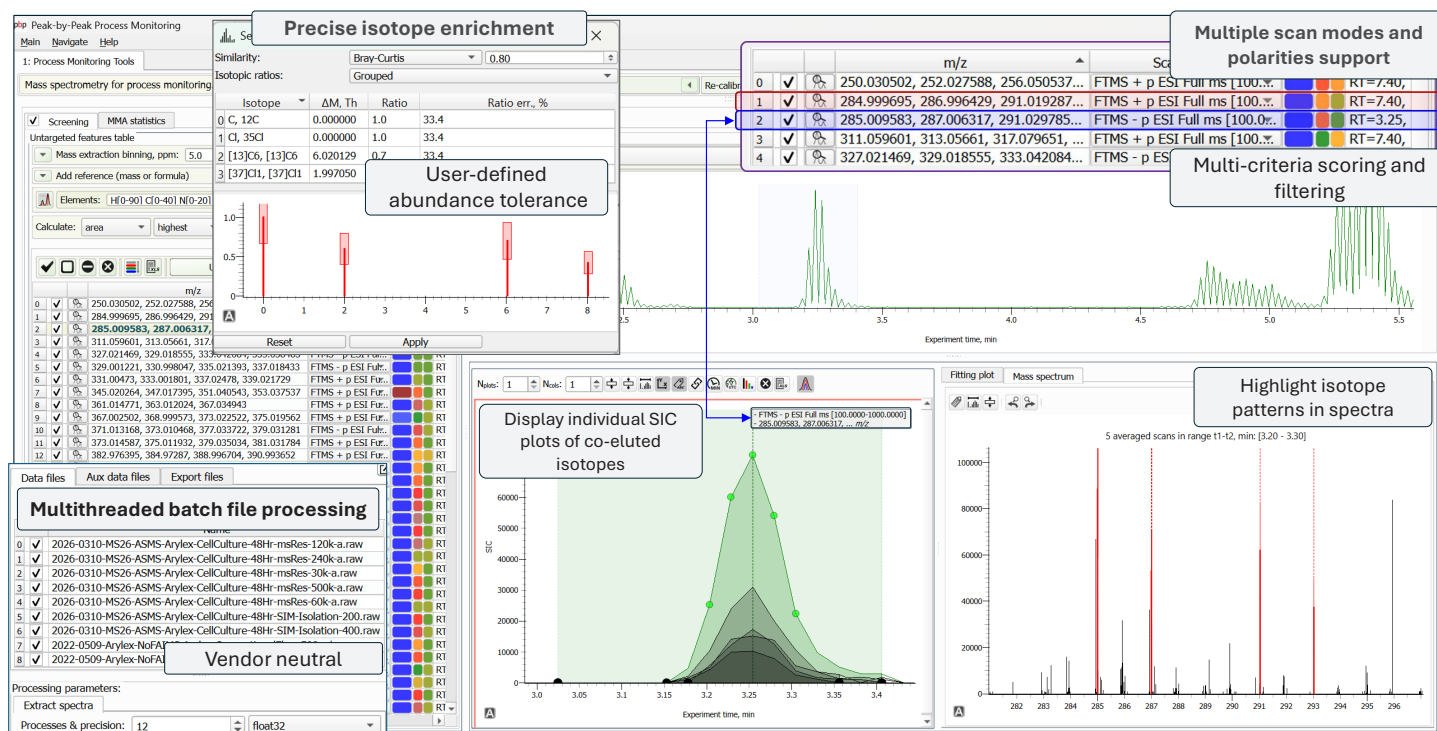


IsoChains: untargeted extraction of stable isotope labelled patterns

IsoChains is a module of Peak-by-Peak Isotope Analysis software that groups co-eluting isotope signals, scores pattern similarity, and highlights candidates for rapid validation. Best for: untargeted tracing, xenobiotic metabolite ID, labelled-feature screening. Discover labelled metabolites and isotope-enriched features without a fixed target list.

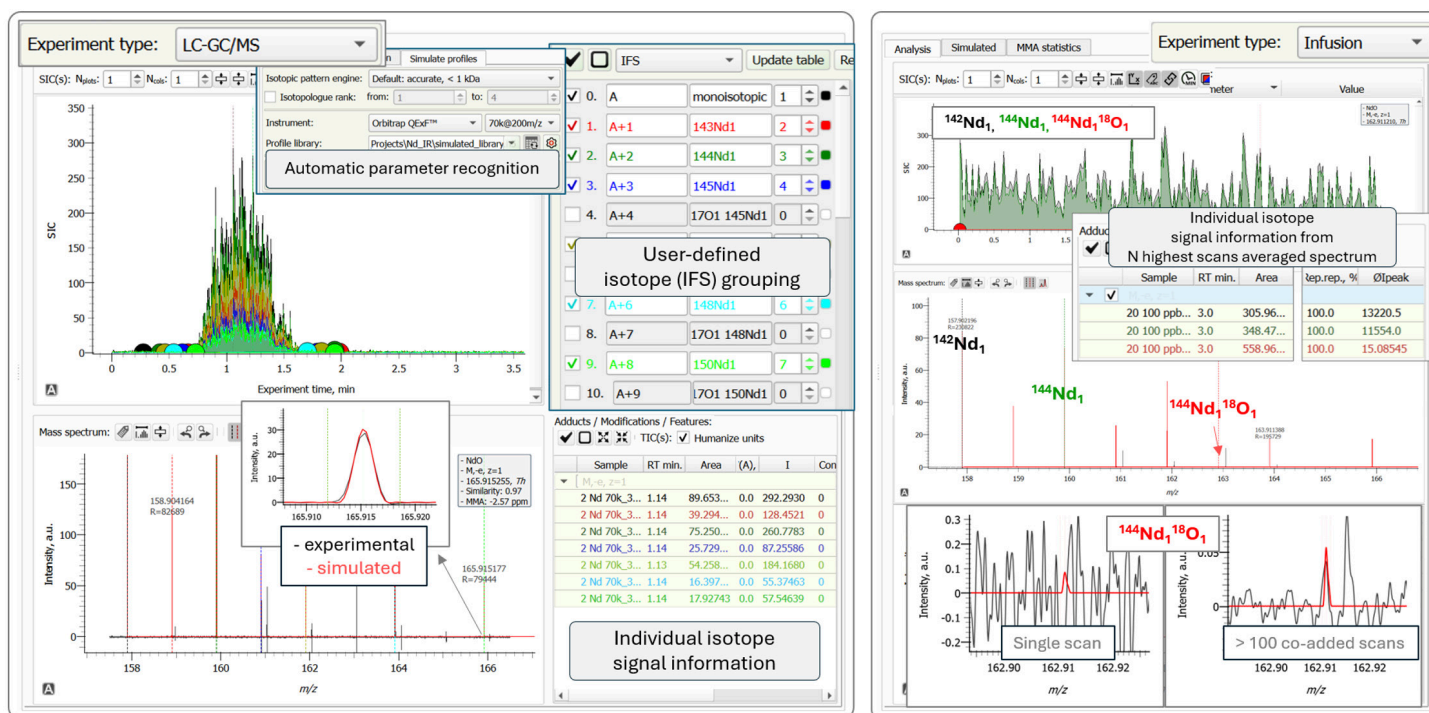


Key Features

- Complete processing workflow for datasets of any size
- Rapid batch file processing for high-throughput: 100 files in under 30 minutes
- Multi-vendor & instrument-agnostic tool with a direct data loading in a vendor format
- Precise isotope enrichment and customizable isotope abundances
- Feature extraction based on isotope pattern in a targeted or untargeted approach
- Multiple scan modes support including common modes (MS, SIM, MSn) and polarities
- Multi-criteria data filtering: abundance, co-elution, and isotopic pattern similarity scores
- Highlighting isotope patterns in mass spectra and co-eluting SIC profiles for validation
- Mass accuracy evaluation, adaptive re-calibration and molecular formula assignment
- Fast calculations: python, HDF file structure, & multi-threading data processing
- Flexible CSV/XLSX export for reporting and downstream analysis

IsoRatios: targeted extraction of isotope ratios

IsoRatios is a module of Peak-by-Peak Isotope Analysis software that quantifies user-defined isotopic groups by calculating theoretical isotopic distributions from molecular formulas, accurately simulating isotopic peak profiles for exact instrument settings, and extracting **isotope ratios (IR)** from mass spectrometry data.



Key Features

- Supports LC/GC MS or direct infusion experiment types
- Capable of processing time-domain ion signals (transients) from **FTMS Booster** systems
- Full profile data support for improved sensitivity, including absorption mode FT (aFT)
- Feature extraction for user-defined isotopic groups, including isotopic fine structure
- Direct infusion mode allows to conditionally co-add scans for improved sensitivity
- Precise isotope enrichment and customizable isotope abundances
- Mass accuracy evaluation, adaptive re-calibration and molecular formula assignment
- High speed of calculations: python, HDF file structure, & multi-threading data processing
- Flexible and customized dynamic data export, including in CSV and XLSX file formats
- Selected customer publications:
 - **Utilization of the LS-APGD microplasma/Orbitrap-FTMS Booster system for detection and isotopic analysis of neodymium nanoparticles**, Ken Marcus et al., *Spectrochimica Acta Part B: Atomic Spectroscopy* (2026) 236, 107398
 - **Improved uranium isotope ratio analysis in LS-APGD/Orbitrap FTMS coupling through the use of an external data acquisition system**, Ken Marcus et al., *J. Am. Soc. Mass Spectrom.* 2021, 32, 5, 1224–1236

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