

End-to-End Breath Analysis – Purpose-built for SESI-MS Users

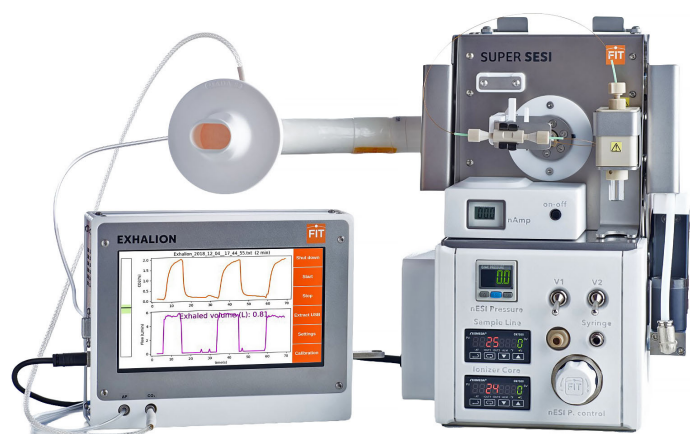
Breath analysis uses **high-resolution mass spectrometry (HRMS)** to detect volatile biomarkers in exhaled breath. In practice, generating high-quality HRMS data is demanding. Without chromatographic separation, all compounds are ionized simultaneously, making fragmentation, low analyte abundance, and physiological variability major obstacles to reliable interpretation.

Secondary electrospray ionization (**SESI**) and the **EXHALION** breath analysis interface by **Fossiliontech** (Salamanca, Spain) enable efficient, soft ionization of trace-level, low-volatility breath compounds and standardizes exhalation, producing reproducible, high-quality data.

The result is rich breath datasets whose value depends on dedicated data handling and interpretation.

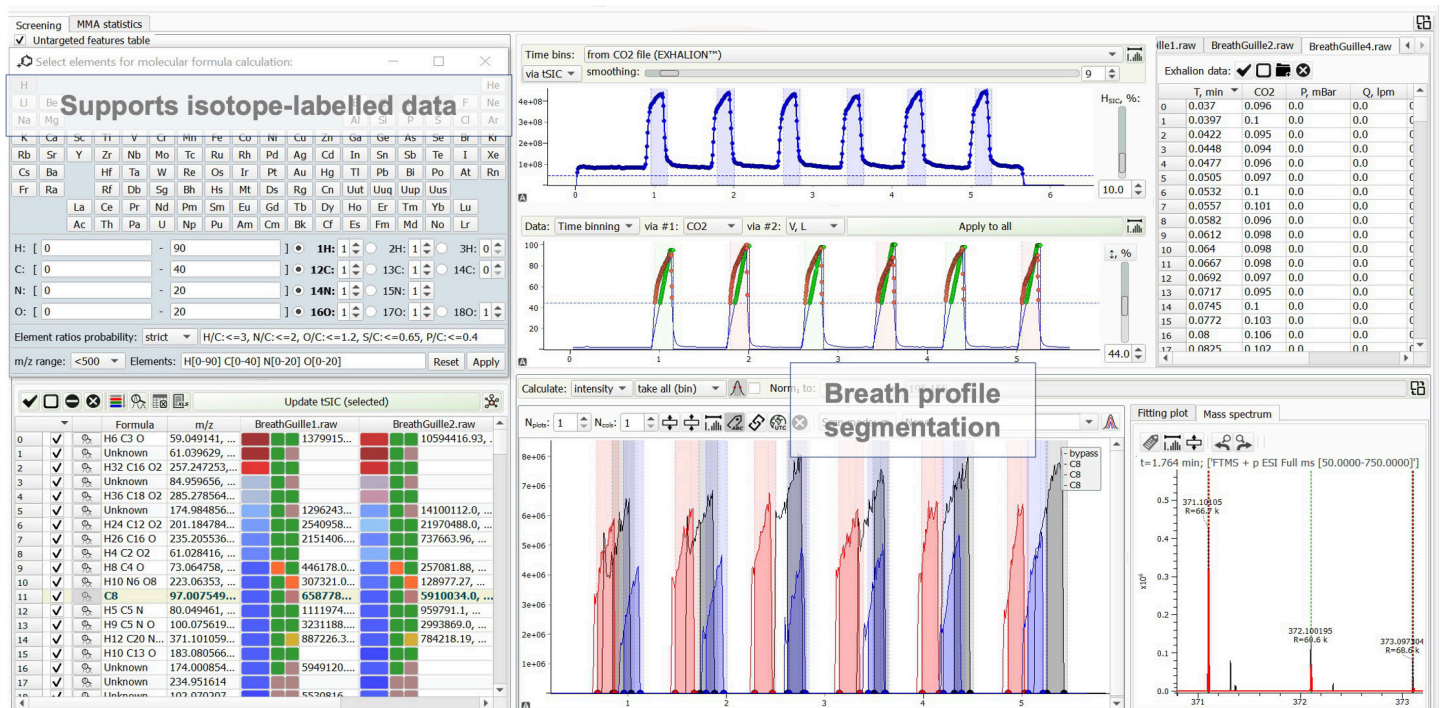


SUPER SESI X



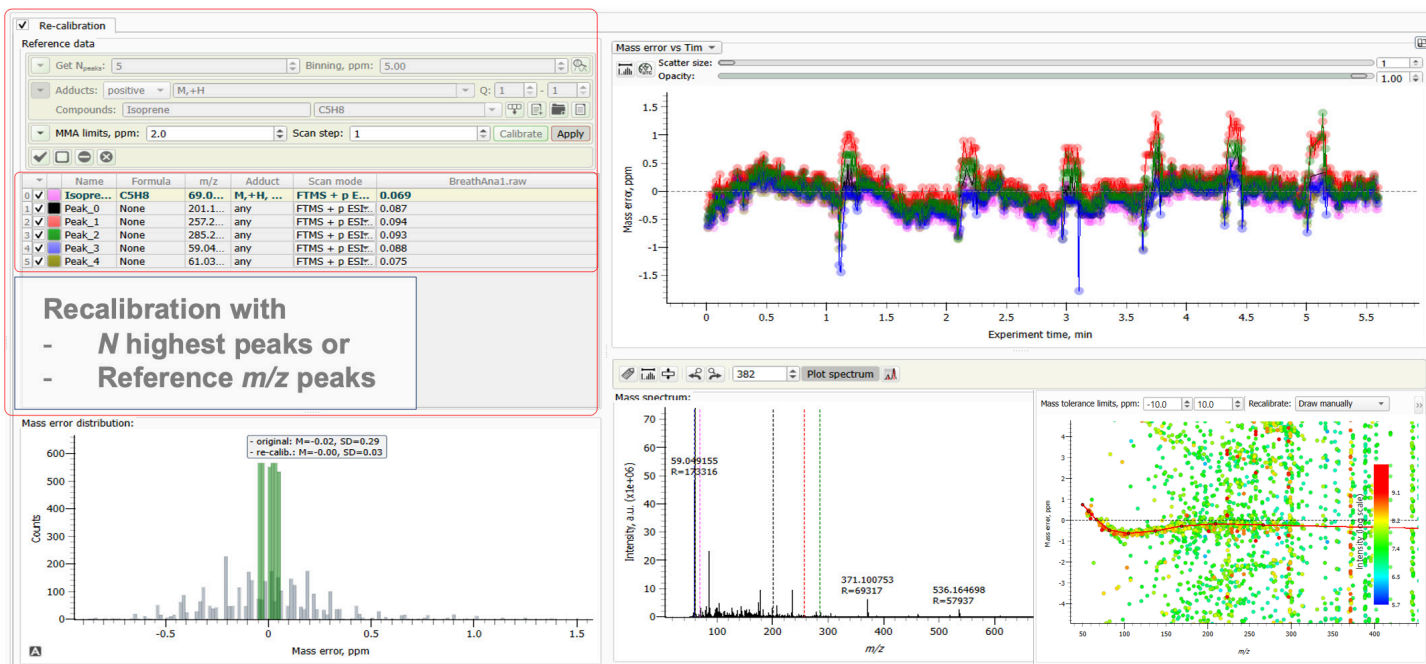
EXHALION

Peak-by-Peak Breath Analysis software from **Spectroswiss** (Lausanne, Switzerland) directly supports breath analysis applications using SESI-MS ion sources coupled to Orbitraps and other types of mass spectrometers. It provides a unified end-to-end workflow for targeted and untargeted molecular analyses, supported by efficient recalibration procedures and scalable data handling for datasets of any size.

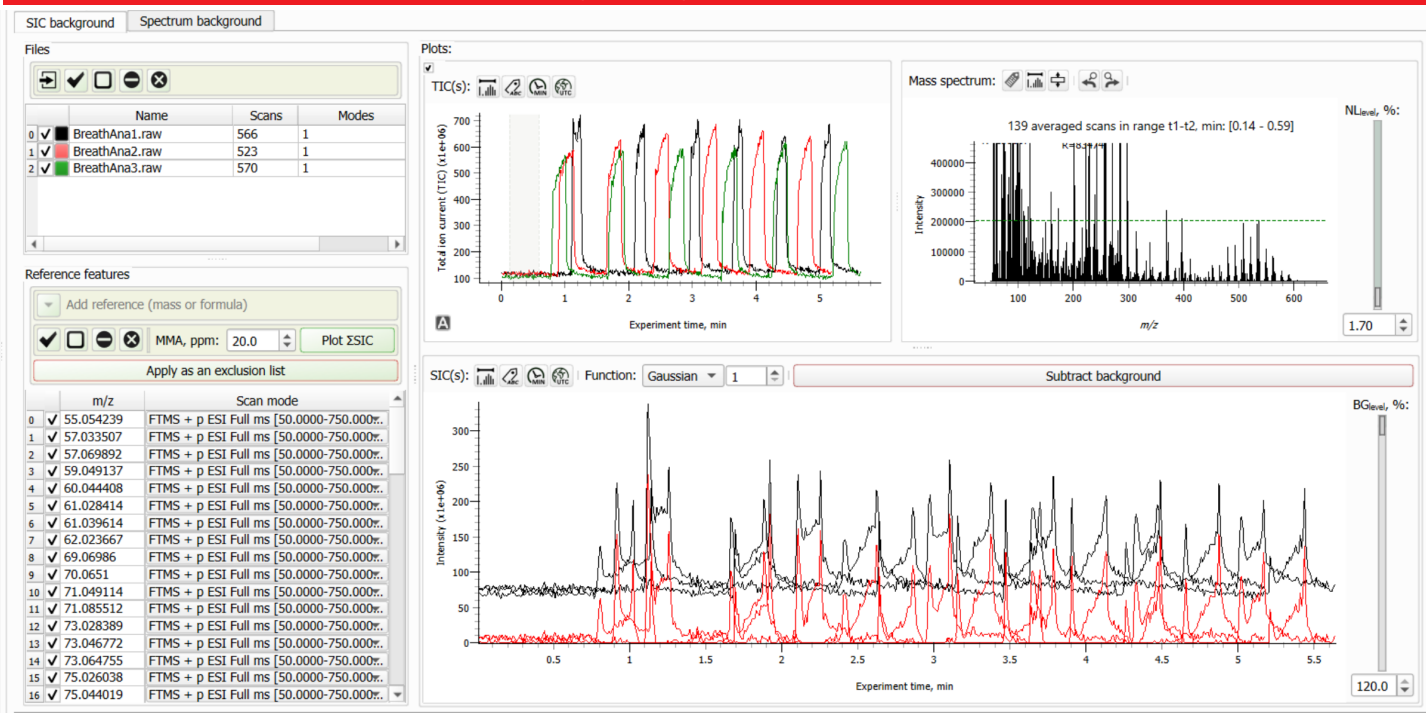


Key Features

- End-to-end processing and analysis for **datasets of any size**, supporting chromatographic and **non-chromatographic** acquisitions
- Secondary electrospray ionization (**SESI**)-ready on any MS platform (e.g., Orbitrap & TOF MS) for **real-time** and **off-line** workflows
- **Time-resolved** breath feature extraction with automatic, manual, or CO₂-guided segmentation (via EXHALION)
- **Multi-experiment** project support, including batch handling and interactive visualization of extracted traces across many features
- Configurable data processing and filtering, including **background subtraction**, exclusion lists, and custom rule-based filters
- Mass accuracy monitoring, **adaptive spectral recalibration**, and integrated QC/validation checks
- **Untargeted feature detection** and clustering, including **multivariate analysis** (e.g., PCA/LDA) and support for stable-isotope labeling
- Untargeted discovery utilities, including database-free **molecular formula assignment** and semi-automated event detection/annotation
- **High-throughput** performance, enabled by a Python-based compute engine, HDF-backed storage, and multi-threaded processing
- Flexible **export** to CSV/TXT/XLSX with configurable output formats, ready for your downstream statistics, ML, and QA/QC pipelines



Advanced Data Processing: Background Subtraction, Exclusion List, etc.



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