Breath Analysis in Real Time

Materials
- SUPER SESI + EXHALION + Your High Resolution MS
- High purity formic acid - water solution 0.1%, (2 cm³)
- Medical grade, antibacterial spirometry filter & mouthpiece

Methods
Follow these simple steps to turn your MS into an advanced breath analysis system:

- Connect Super SESI to your MS
- Connect EXHALION,
- Power up, wait for system to warm up
- Load and start electrospray
- Start acquisition on MS and EXHALION

- Plug disposable antibacterial mouthpiece
- Exhale through mouthpiece (20 seconds)
- Use EXHALION to guide exhalation maneuver
- Wait 1 minute between exhalations to obtain 6 exhalation replicates*

* Breathing naturally and exhaling into SUPER SESI produce different breathing patterns. As a result, the signal intensities display a transient evolution that reach a steady state in 3-4 exhalations. Exhaling 6 times at regular intervals allows for most species to reach the steady state.

Drugs or isotopically labeled metabolites trigger metabolic response

Non-invasive monitoring of endogenous and exogenous metabolites

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Data post-processing
- Synchronize EXHALION and MS data, & differentiate respiratory fractions based on CO₂ profile
- For each fraction, extract peak m/z centroid & intensity list

Number of peaks detected
8000 peaks* for signals integrated during an average exhalation, 2000* in background

* Results obtained with a SUPER SESI coupled with a Q-Exactive Plus; only peaks with signals above 10^3 a.u. were accounted to determine No. of peaks.

High quality data, eliminate confounding factors
- No sample preparation
- No sample handling

Biological relevance
- Low volatility metabolites detected at very low concentrations
- Some molecules identified in breath in the 50-500 Da range.

Breath Biomarker Identification

References
- Standardization procedures for real-time breath analysis by secondary electrospray ionization high-resolution mass spectrometry; Analytical and Bioanalytical Chemistry, 2019