# SUPER SESI

### (Application note)



### An introduction: Breath Analysis in Real Time

Biologically relevant molecules Reduced confounding factors



#### Materials

- SUPER SESI + EXHALION + Your High Resolution MS
- High purity formic acid water solution 0.1%, (2 cm<sup>3</sup>)
- Medical grade, antibacterial spirometry filter & mouthpiece

### Methods

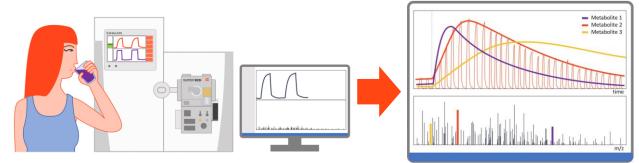
Follow these simple steps to turn your MS into an advanced breath analysis system:



- 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

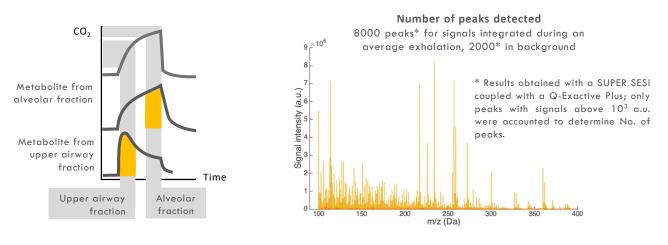


## SUPER SESI

### Data post-processing

- Synchronize EXHALION and MS data, & differentiate respiratory fractions based on  $\mathrm{CO}_2$  profile

- For each fraction, extract peak  $\ensuremath{\text{m/z}}$  centroid & intensity list

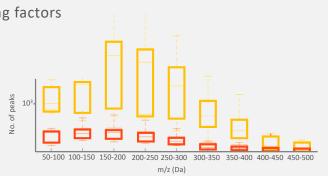


### High quality data, eliminate confounding factors

- 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
- Real-Time Breath Analysis Reveals Specific Metabolic Signatures of COPD Exacerbations; CHEST Journal (Official publication of the American colleague of chest physicians), 2019.
- Real-Time Monitoring of Tricarboxylic Acid Metabolites in Exhaled Breath; Analytical Chemistry, 2018.
- Translating Secondary Electrospray Ionization–High-Resolution Mass Spectrometry to the Clinical Environment; Journal of Breath Research, 2018.
- Real-time Mass spectrometric identification of metabolites characteristic of chronic obstructive pulmonary disease in exhaled breath; Clinical Mass Spectrometry, 2018.
- Metabolic effects of inhaled salbutamol determined by exhaled breath analysis; Journal of Breath Research, 2017.