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# SIFT-MS: The Gold Standard for Volatile Biomarker Verification and Validation

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## Introduction

Volatile organic (and inorganic) compounds are universal in chemical communication within and between virtually all living species. They are integral to carbon, nitrogen and sulphur flux through the biosphere and a significant source of atmospheric pollution and greenhouse gas emissions.

Since they are generally present at low to sub-ppm(v) concentrations, their analysis is primarily done by GC-MS with pre-concentration (e.g., onto thermal desorption tubes).

GC-MS is the gold-standard analytical platform for characterising complex mixtures (e.g., volatile biomarker discovery) but, getting reliable measurements is challenging due to the reactivity and stability of the analytes and adsorptive losses in the analytical sample path and the difficulty of analysing high humidity samples by GC-MS.

Current technologies for real-time VOC analysis (ESI, APCI, PTR-MS, IMS, DMS) all have significant shortcomings in several of the following areas: dynamic range, linearity, sensitivity, selectivity and/or specificity. They are susceptible to ion suppression and/or instrument drift and require require routine re-calibration.

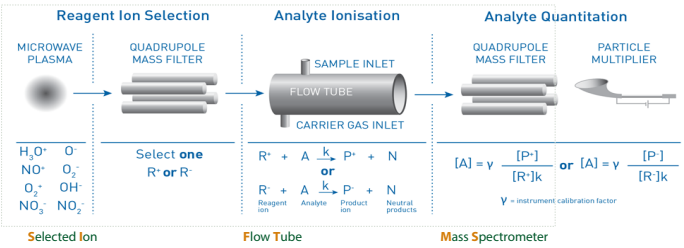
In this poster, we present a new technology, Selected-Ion-Flow-Mass-Spectrometry (SIFT-MS), for volatile biomarker validation and verification.

## How it Works

Reagent ions are generated in a microwave plasma (from humidified air), they are selected in the first quadrupole and transferred into the flow tube.

On entering the flow tube, they interact with the flow gas and are quenched to thermodynamic ground-state. The reagent ions react with the analytes by ultra-soft, ion-molecule (proton transfer, electron transfer, dissociative election transfer, association and hydride abstraction) ionization.

Product ions are analysed in the downstream quadrupole MS analyser and accurate, precise analyte concentrations calculated from product-ion signals.



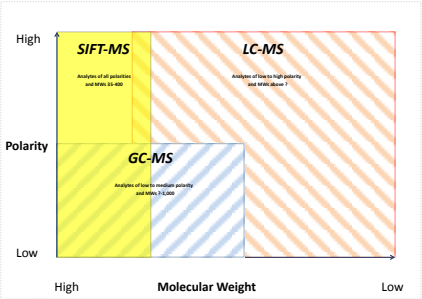

## Benefits

Absolute quantitation, with no need for routine calibration

Single digit ppt(v) sensitivity with large ($10^9$) linear dynamic range

Simultaneous analysis with multiple reagent ions delivers:

- High selectivity and specificity (e.g., speciation of structural isomers)
- Multi-target metabolite analysis without chromatography
- Inert sample path – no adsorptive analyte losses/polarity discrimination
- Minimal services ($N_2$ or He flow gas, DI water and 10A power supply)
- Unaffected by humidity




## Sampling Options

**Direct sampling options**

- High Performance (Hex) Inlet
- Breath Inlet
- Valve Sampling

**Autosampler interface**

- Static headspace (2mL to 1L)
  Vials, exetainers, vacutainers, microbial cultures, bottles, jars, etc.
- Continuous headspace
- Multiple Headspace Extraction (solids, gels, liquids)
- Flow cell - online sampling from gas & liquid streams (e.g., bioreactors)
- Sampling from Tedlar® bags

## Metabolomics Applications

**Breath Research & Human Health**

- Breath Biomarker analysis – non-invasive disease diagnosis
- Therapeutic Disease monitoring (renal dialysis, liver disease)
- Urine/Plasma/tissue volatile biomarker analysis
- Microbial Identification and (microbiome) community analysis

**Ecology, Agriculture and Environment**

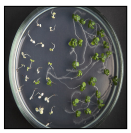
- Biogenic (livestock, plant, soil & microbial) emissions
- Carbon, Nitrogen and Sulphur Flux studies
- Platform scale catchment/remote monitoring
- Biomass and Bioenergy Research (Anaerobic Digestion, Sewage & Biogas. Biomass combustion/pyrolysis)

**Chemical Ecology**

- Chemical attractants, repellents and pheromones
- Responses to pathogenesis/predation
- Non-invasive, real-time measurement of inter- and intra- species interactions in laboratory and field (ecosystem) studies

**Industrial Biotechnology**

- Off-gas analysis, product & reaction process monitoring
- Multi-steam sampling from fermenters, photobioreactors, etc



## Conclusions

SIFT-MS is ideally suited to the analysis of volatile metabolites in metabolomics, synthetic biology, industrial biotechnology and ecological studies.

- Unsurpassed selectivity, sensitivity and selectivity
- Comprehensive inorganic and organic volatile analysis at physiological concentrations (notable exceptions $N_2$, $O_2$, CO, $H_2$, noble gases)
- Calibration free, absolute quantitation with no polarity discrimination
- Real-time analysis delivers high temporal data density (e.g., process monitoring, spatio-temporal and flux studies)
- Long term stability: ideal for longitudinal and large scale volatilomics studies
- Choice of direct or autosampler interfaces and options for laboratory, field and online analysis offer ultimate flexibility and scalable solutions
- No mass discrimination in mass analyser (m/z 10-400) or in-source fragmentation
- Reaches the parts of the metabolome that GC-MS, LC-MS and NMR can't

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