

# SIFT-MS

SELECTED ION FLOW TUBE MASS SPECTROMETRY

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TECHNOLOGY OVERVIEW \ SYFT TECHNOLOGIES





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## SELECTED ION FLOW TUBE MASS SPECTROMETRY TECHNOLOGY OVERVIEW

Selected ion flow tube mass spectrometry (SIFT-MS) is a form of direct mass spectrometry that analyses volatile organic compounds (VOCs) in air with typical detection limits at parts-per-trillion level (by volume; pptv). Real-time, quantitative analysis is achieved by applying precisely controlled soft chemical ionization and eliminating sample preparation, pre-concentration and chromatography.

### BENEFITS OF SIFT-MS INCLUDE:

- Instantaneous, quantitative analysis of air and headspace with very high sensitivity and selectivity
- Simultaneous analysis of chemically diverse VOCs (e.g. aldehydes, amines and organosulfurs)
- Direct analysis of high humidity samples
- Simplicity of operation
- Simple integration with existing infrastructure
- Low maintenance and long-term stability.

SIFT-MS is, therefore, an ideal tool for high-throughput and real-time gas analysis applications. Syft's SIFT-MS instrumentation is industry proven, providing non-technical operators with laboratory-grade chemical analysis presented in a format that they can understand and act on.

This document equips technical readers with an understanding of the fundamentals of SIFT-MS and outlines the key benefits of Syft's SIFT-MS solutions.

# 1. AN OVERVIEW OF SIFT-MS



SIFT-MS is a form of direct mass spectrometry. It applies precisely controlled chemical ionization reactions to detect and quantify trace amounts of volatile organic compounds (VOCs) and inorganic gases.

## THERE ARE THREE ELEMENTS OF THE SIFT-MS TECHNIQUE (FIGURE 1):

In SIFT-MS, highly controlled soft ionization enables real-time absolute quantitation of analytes

### 1. Reagent ion generation and selection

The eight SIFT-MS reagent ions –  $H_3O^+$ ,  $NO^+$ ,  $O_2^+$ ,  $O^-$ ,  $O_2^-$ ,  $OH^-$ ,  $NO_2^-$ , and  $NO_3^-$  – are all formed by microwave discharge through moist or dry air. The reagent ion of choice is then selected using a quadrupole mass filter.

### 2. Analyte ionization

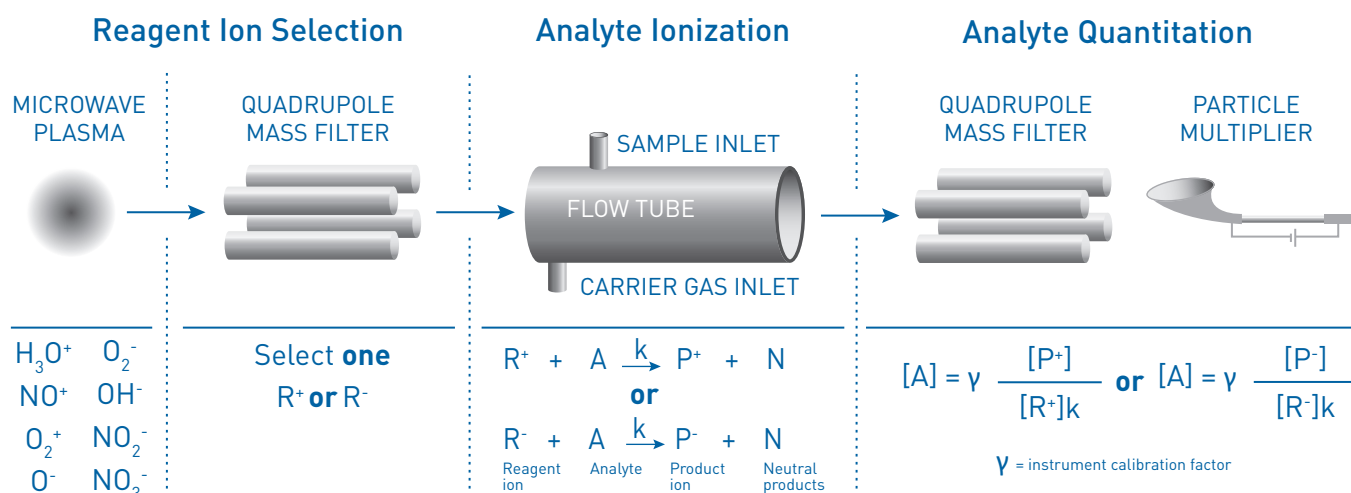
The selected reagent ion is injected into the flow tube and excess energy is removed through collisions with the carrier gas. The sample is then introduced at a known flow rate and the reactive compounds it contains are ionized by the reagent ion to form well-characterized product ions.

### 3. Analyte quantitation

Product ions and unreacted reagent ions are sampled into a second quadrupole mass spectrometer. Utilizing Syft's compound library, the software instantaneously calculates each analyte's absolute concentration.

The next section provides more information on the unique application of chemical ionization in SIFT-MS.

Figure 1. Schematic representation of the SIFT-MS technique.



## 2. PRINCIPLES OF SIFT-MS



Soft chemical ionization is applied very precisely in SIFT-MS, allowing it to provide unparalleled selectivity among direct mass spectrometry techniques.

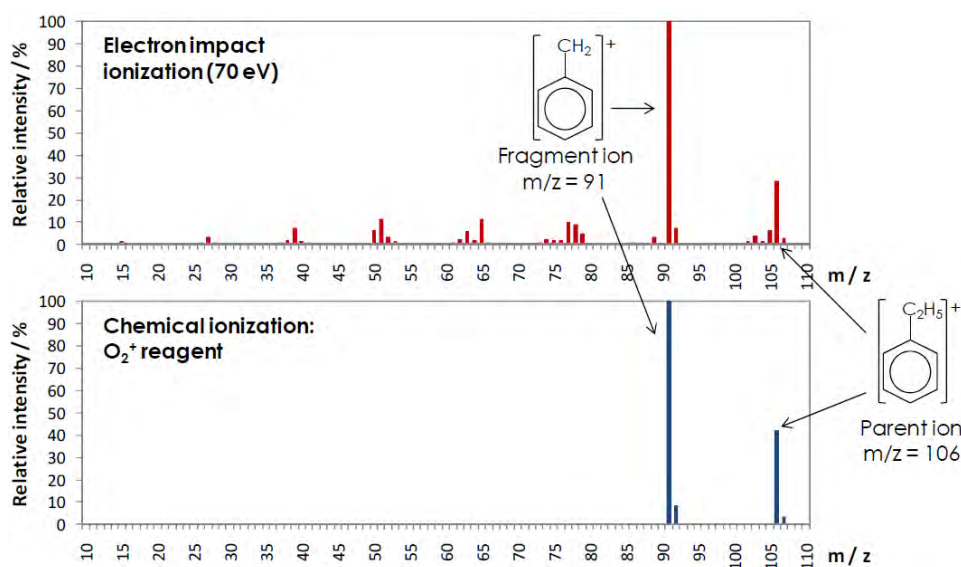
SIFT-MS is unique: it provides reproducible, real-time quantitative analysis

### a. Why chemical ionization?

Chemical ionization (CI) uses a molecular ion to transfer charge onto the target compound (analyte). CI is "softer" than many other types of ionization, so it transfers less energy to the analyte, resulting in reduced fragmentation. SIFT-MS is a unique CI-MS technique because it precisely controls reagent ion energies to allow repeatable, real-time quantitative analysis. A further benefit is long-term calibration stability.

Figure 2 compares ionization of ethylbenzene using 70-eV EI (as used in GC/MS) and  $O_2^+$  CI (as used in SIFT-MS). Reduced fragmentation means chromatography is unnecessary, which allows SIFT-MS to be applied as a real-time technique.

Figure 2. Electron impact and chemical ionization of ethylbenzene illustrates the much simpler fragmentation observed for SIFT-MS than standard GC/MS.



## 2. PRINCIPLES OF SIFT-MS

SIFT-MS, provides unparalleled real-time selectivity by utilizing rapid reagent ion switching

### b. Why multiple reagent ions?

Eight reagent ions ( $\text{H}_3\text{O}^+$ ,  $\text{NO}^+$ ,  $\text{O}_2^+$ ,  $\text{O}^-$ ,  $\text{O}_2^-$ ,  $\text{OH}^-$ ,  $\text{NO}_2^-$ , and  $\text{NO}_3^-$ ) can be used in SIFT-MS because they enhance specificity and allow a wide range of compounds to be detected. These reagent ions exhibit a variety of reaction mechanisms, which means that they often react differently with each compound. The dominant mechanisms are:

- $\text{H}_3\text{O}^+$ : proton transfer (PT)
- $\text{NO}^+$ : electron transfer (ET), association, hydride ( $\text{H}^-$ ) abstraction
- $\text{O}_2^+$ : ET, dissociative ET
- $\text{O}^-$ : ET, proton abstraction (PAb), association, displacement
- $\text{O}_2^-$ : dissociative ET, PAb, association
- $\text{OH}^-$ : ET, PAb, displacement, elimination
- $\text{NO}_2^-$ : ET, dissociative ET, PAb, association
- $\text{NO}_3^-$ : PAb, association

Different reaction mechanisms yield different "fingerprints" for the analytes in the sample – often with a different "fingerprint" for each reagent ion.

This provides greater opportunity to detect and selectively quantify the compound. A simple example is provided in Table 1 for two isomers of  $\text{C}_3\text{H}_6\text{O}$ : acetone and propanal. The  $\text{NO}^+$  reagent ion provides the most effective differentiation because it reacts via a different mechanism for the two compounds and yields a single product ion for each.

A significant benefit of SIFT-MS is that all reagent ions are produced from moist air. Furthermore, reagent ion switching occurs within 10 milliseconds for ions of the same polarity produced under the same ion source conditions (e.g. the positive reagent ions), because it simply involves changing the reagent ion mass in the quadrupole mass filter. This enables complex samples to be analyzed in real time (e.g. in breath-by-breath analysis or monitoring dynamic processes). This characteristic is unique to SIFT-MS.

Table 1. Product ions formed from reaction of the SIFT-MS  $\text{H}_3\text{O}^+$ ,  $\text{NO}^+$  and  $\text{O}_2^+$  reagent ions with isomeric compounds acetone and propanal.

Reagent ion	Acetone product ion (m/z)	Propanal product ion (m/z)
$\text{H}_3\text{O}^+$	$(\text{CH}_3)_2\text{CO.H}^+$ (59)	$\text{CH}_3\text{CH}_2\text{CHO.H}^+$ (59)
$\text{NO}^+$	$(\text{CH}_3)_2\text{CO.NO}^+$ (88)	$\text{CH}_3\text{CH}_2\text{CO}^+$ (57)
$\text{O}_2^+$	$(\text{CH}_3)_2\text{CO}^+$ (58); $\text{CH}_3\text{CO}^+$ (43)	$\text{CH}_3\text{CH}_2\text{CHO}^+$ (58); $\text{CH}_3\text{CH}_2\text{CO}^+$ (57)

SIFT-MS provides unsurpassed on-line absolute quantitation through tightly controlled ionization

### c. How does SIFT-MS achieve high measurement precision?

Consistency of reagent ion energy is one of the most critical factors in controlling analyte ionization, which in turn provides reproducible product ion formation and reliable, stable absolute quantitation.

In SIFT-MS the use of a carrier gas enables the CI process to be controlled very effectively compared to EI ionization and other forms of CI mass spectrometry (such as PTR-MS, APCI-MS and DART). The carrier gas used in SIFT-MS plays two very important roles in controlling ionization:

- It thermalizes the reagent ions prior to introduction of sample. This ensures that reagent ion energies are low and uniform, providing predictable, precise, and ultra-soft CI.

- It transports the product ions and unreacted reagent ions along the flow tube to the detection region without addition of excess energy. For example, no electric field gradient is used to accelerate ions toward the detection region. This low energy transport minimizes fragmentation and maximizes spectral simplicity, selectivity, and the ability to uniquely identify and quantify compounds.

## 2. PRINCIPLES OF SIFT-MS

### d. How does a SIFT-MS instrument provide absolute quantitation in real time?

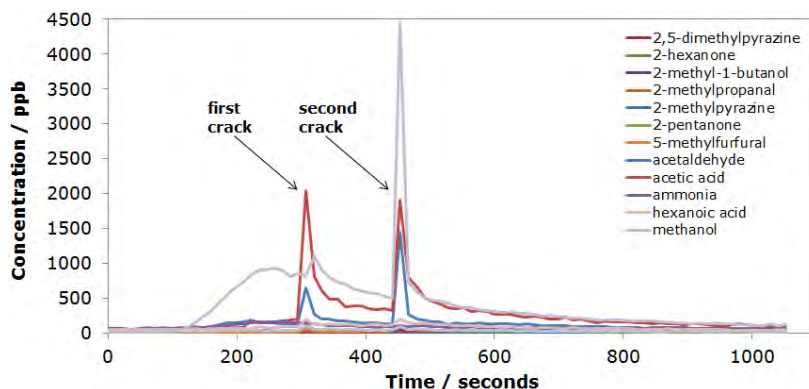
SIFT-MS selected ion mode (SIM) scans are analogous to GC/MS SIM scans and involve targeting known compounds. In this mode, specific reagent and product ions are selected and their count rates measured repeatedly. Combining this experimental information with the known rate coefficient ( $k$ ) from the Syft library for reaction of the reagent ion and analyte, and the known dilution of the sample gas into the carrier gas, the absolute concentration of an analyte is calculated and displayed in real time (see Figure 3).

Simply put, a higher concentration of a compound in the sample will result in a greater proportion of the reagent ion

reacting and hence more of the product ions for that compound will be observed. The number of product ions is an absolute measure of the concentration of compound in the sample. This gives a linear range from low-pptv to about 50 ppmv – over six orders of magnitude. Higher concentration samples are analyzed either by attenuating the sample flow or by diluting the sample.

SIFT-MS also has a wide dynamic range: compounds at pptv levels can be detected in the presence of compounds at mid- to high-ppm concentrations.

Figure 3. Real-time quantitation of VOCs produced during coffee bean roasting. Beans 'crack' during roasting, releasing additional VOCs.



### e. Calibration of SIFT-MS instruments

SIFT-MS enables absolute quantitation of target compounds at high precision based on the compound data contained in the Syft library (namely, the reaction rate coefficient and the product masses together with their branching ratios). A formal calibration can also be performed in the normal way to provide even higher accuracy. Once calibrated for a particular compound, the SIFT-MS calibration remains valid by applying the Syft automated daily validation standard.

Certified gas standards are used for calibration of SIFT-MS instruments. The two main commercial options for suitable standards are compressed gases and permeation tubes.

### 3. OPERATIONAL ADVANTAGES OF SIFT-MS



The inherent technical characteristics of SIFT-MS (including the precise ionization control and elimination of the chromatographic column) has allowed Syft Technologies to develop commercial instruments with significant usability and integration advantages compared to chromatographic and other direct mass spectrometric techniques.

Syft Technologies' instruments are the most user-friendly mass spectrometers available

#### a. Ease of use

Syft has developed software that enables the powerful SIFT-MS technology to deliver laboratory-grade analytical results even for minimally trained users. Features designed for such users include:

- Simplified workflows for very easy operation
- Intuitive touchscreen, menu-driven analysis
- Completely customizable target compound lists
- Instantaneous reporting of quantitative results when the analysis is finished

- Alarms raised when a specific compound is above a user-defined threshold or if a pattern or trend indicates that a process is outside specification.

Figure 4 illustrates how a laboratory-grade analysis has been configured for simple operation for non-technical users.

For technical users, Syft also offers the LabSyft suite of analysis tools, which allows advanced users to view data during and after scans, manipulate and export data, search and expand the compound library, create and edit analytical methods, execute batch schedules and interface the instrument with other devices.

Figure 4. The Voice-Series software is readily configured for use and interpretation by non-technical operators. These screenshots from the Voice200 instrument's touchscreen show two results screens from a worker safety application. RT is a reporting threshold that the employer has chosen, below which the results are hidden from the operator to avoid causing unnecessary alarm. One screen shows a pass result with acceptable levels of target compounds, while the other shows unacceptable formaldehyde levels.

Scan Results	
voice200	
Fumigant Analysis	✓
ID 12573	11-11 16:56
chloropicrin	<RT
ethylene dibromide	<RT
ethylene oxide	<RT
formaldehyde	<RT
hydrogen cyanide	<RT
methyl bromide	<RT
phosphine	<RT
vikane	<RT

Scan Results	
voice200	
Fumigant Analysis	⚠
ID 12572	11-11 16:33
formaldehyde	2.4 ppm ⚠
chloropicrin	<RT
ethylene dibromide	<RT
ethylene oxide	<RT
hydrogen cyanide	<RT
methyl bromide	<RT
phosphine	<RT
vikane	<RT

### 3. OPERATIONAL ADVANTAGES OF SYFT SIFT-MS

Syft Technologies' instruments have full internet connectivity, supporting simple remote operation

#### b. Remote operation

Syft Voice-series SIFT-MS instruments are fully networkable, meaning instrument operation, data handling, and troubleshooting can be performed remotely, from anywhere in the world, even using smartphones or tablets.

This allows scanning to be fully automated and top-level support and fault diagnostics can be quickly delivered to any location and time zone.

#### c. Low maintenance

The absence of chromatographic columns, a very clean microwave ion source and detection system, and gas-only analysis mean that routine maintenance tasks are minimized for SIFT-MS.

A key benefit of eliminating chromatography and using clean, stable chemical ionization is

that SIFT-MS has long-term calibration stability, confirmed daily by use of the automated instrument validation routine. Automated validation includes analysis of a multiple component certified gas standard (the so-called Syft Calibrant Standard), which confirms that the instrument's response is stable through the entire mass range.

#### d. Technical support

Syft and its distributors offer extensive maintenance and support services for Voice-series instruments, accessories and their applications. In particular, the remote access feature of the Voice-series instruments

allows instruments to be monitored and supported anywhere that internet access is available. Remote diagnosis, combined with modular design, means that a faulty component can be identified and replaced rapidly, minimizing instrument down-time.

## 4. SUMMARY

SIFT-MS offers high sensitivity, real-time and non-discriminatory analysis of VOCs and inorganic gases in whole air in a very easy-to-use package. The absence of chromatography columns and very clean, precise chemical ionization reduce maintenance requirements and increase stability, compared to other mass spectrometry techniques. These benefits make SIFT-MS an extremely powerful analytical tool for industry and the laboratory.

