SIFT-MS: An All-In-One Air Analysis Technique

Barry Prince
Syft Technologies Ltd

Summary

Introduction to SIFT-MS

Key characteristics of SIFT-MS for all-in-one air analysis

Air analysis applications using SIFT-MS

Who uses Syft's products?

Customer	Application	Solution
Baker Hughes Norway	**Mud Logging** 	Testing head space of mud to look for larger hydrocarbons. Solution required nitrogen carrier gas, dilution rig and to talk to BH software. All this was completed in 3 weeks.
SMIC China	**Semiconductors** 	Controlling airborne molecular contaminants (AMCs) is a critical aspect of semiconductor manufacture. SIFT detection allows for monitoring of more compounds with enhanced temporal resolution.
Samsung Korea	**Odor Monitoring** 	Samsung wanted to test for a wide variety of odor compounds at their fabrication plants. Syft developed a solution that allows 24/7 monitoring.

Real-time analysers are increasing in popularity

TheScientist
EXPLORING LIFE, INSPIRING INNOVATION

News Magazine Multimedia Subjects Surveys Careers

The Scientist » The Nutshell

GC-MS Distorts Data?

A study suggests that gas chromatography-mass spectrometry modifies or destroys sample compounds, but some are skeptical.

By Jef Akst | October 22, 2015

FLICKR, NOAA

For more than 50 years, researchers have used gas chromatography-mass spectrometry (GC-MS) to identify unknown compounds within biological samples. But according to new work from Gary Siuzdak of the Scripps Research Institute in La Jolla, California, and his colleagues, the method's heating stage, used to volatilize and separate sample components, changes or destroys many of the compounds analyzed. Siuzdak's team published its results this month (October 4) in *Analytical Chemistry*, questioning whether GC-MS is picking up the desired compounds of a sample or simply thermal degradation products.

the Analytical Scientist Content Filter App Notes Product Profiles

RIP GC?

When disruptive technology comes along, it can be hard to defend the technique under attack for some applications – even if we have embraced it for decades.

By Ray Perkins, Managing Director, Anatune, Cambridge, UK. June 2016.

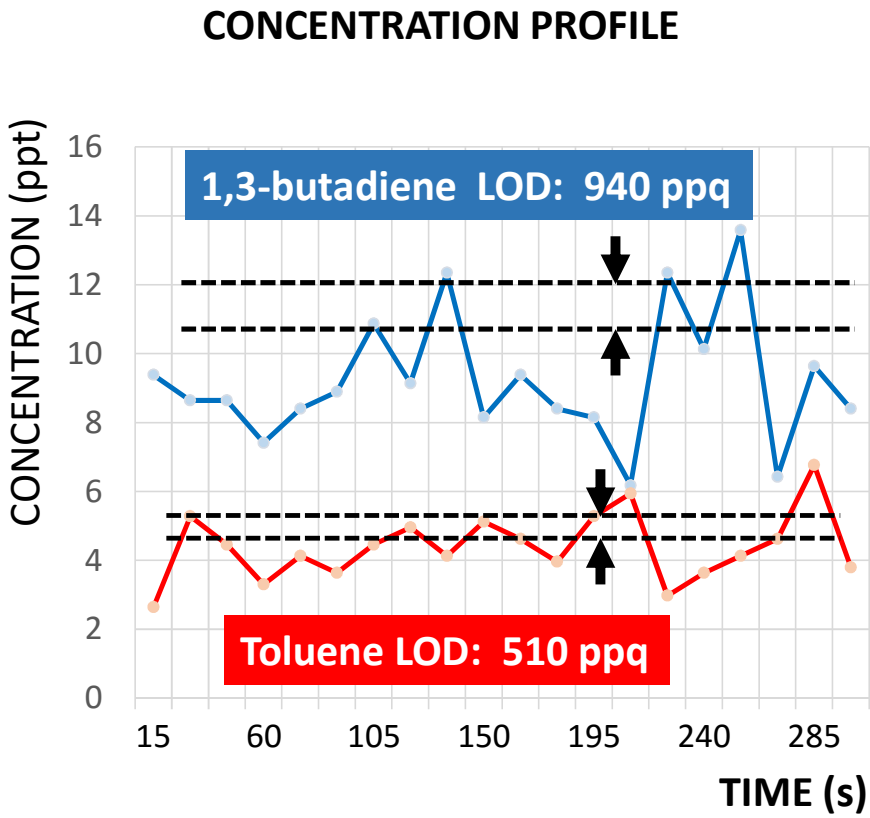
For the first time, I find myself viewing gas chromatography as quaintly passé. It's the same sensation I experienced when, as a Nokia mobile phone user, I picked up an iPhone for the first time. It's the feeling you get when you find yourself staring the future in the face; it has crept upon me as I have become acquainted with selected ion flow tube mass spectrometry (SIFT-MS).

GC has served us well for more than half a century, separating mixtures of non-polar volatile organics and presenting the components to a detector as a time series for identification and measurement. Hyphenated with MS, GC does a good job, but long familiarity kept me blind to

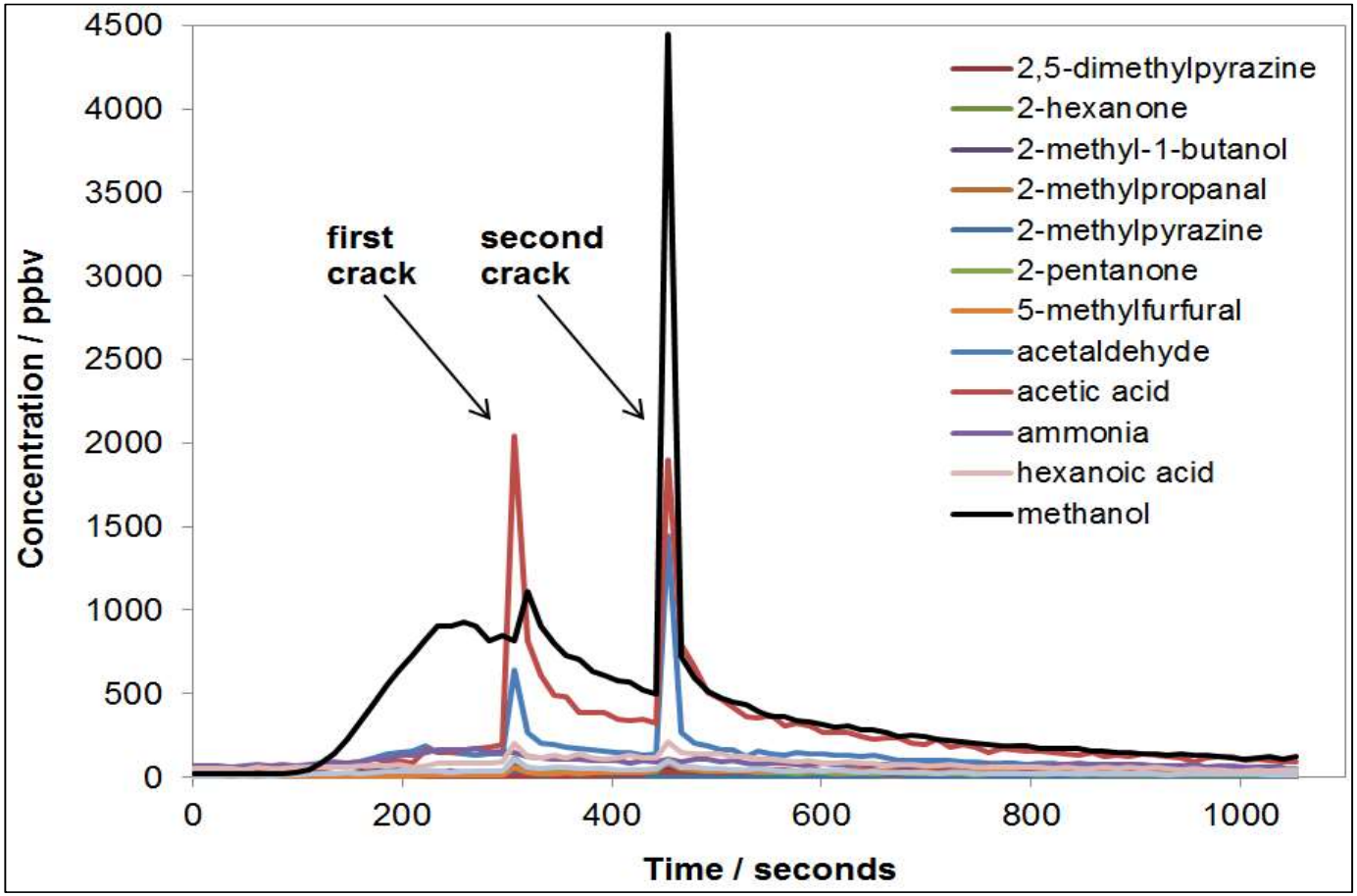
Key Benefit 1: SIFT-MS can measure most VOCs and inorganic compounds

hydrocarbons	alkanes, alkenes, aromatics, monoterpenes
oxygenates	alcohols, aldehydes, ketones, esters, ethers, carboxylic acids, formaldehyde
nitrogen compounds	amines, amides, nitriles, nitrated organics
sulfur compounds	mercaptans, thioethers, carbonyl sulfide
halogenated compounds	aliphatic and aromatic fluorides, chlorides, bromides and iodides
inorganics	ammonia, hydrogen cyanide, hydrogen sulfide, nitrogen dioxide, phosphine, hydrogen chloride, hydrogen fluoride, carbon dioxide, sulfur dioxide, ozone

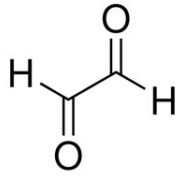
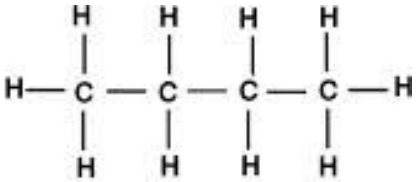
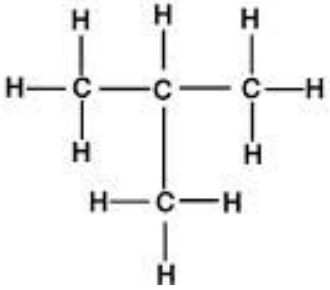
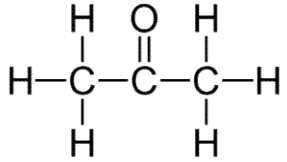
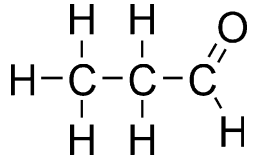
Key Benefit 2: The Voice200*Ultra* for ultra sensitive measurements



Key Benefit 3: Concentrations can be monitored in real time

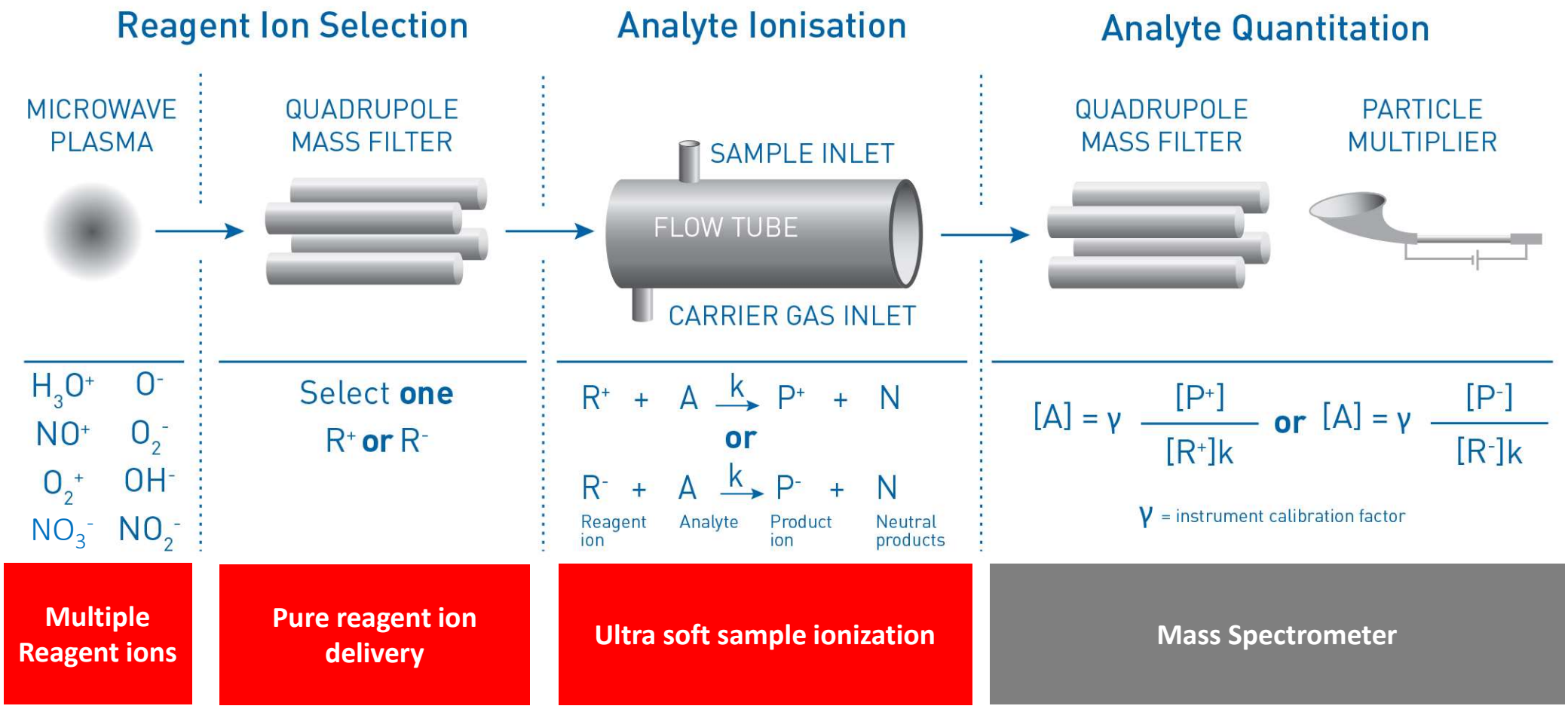


The challenge for real-time MS techniques is selectivity

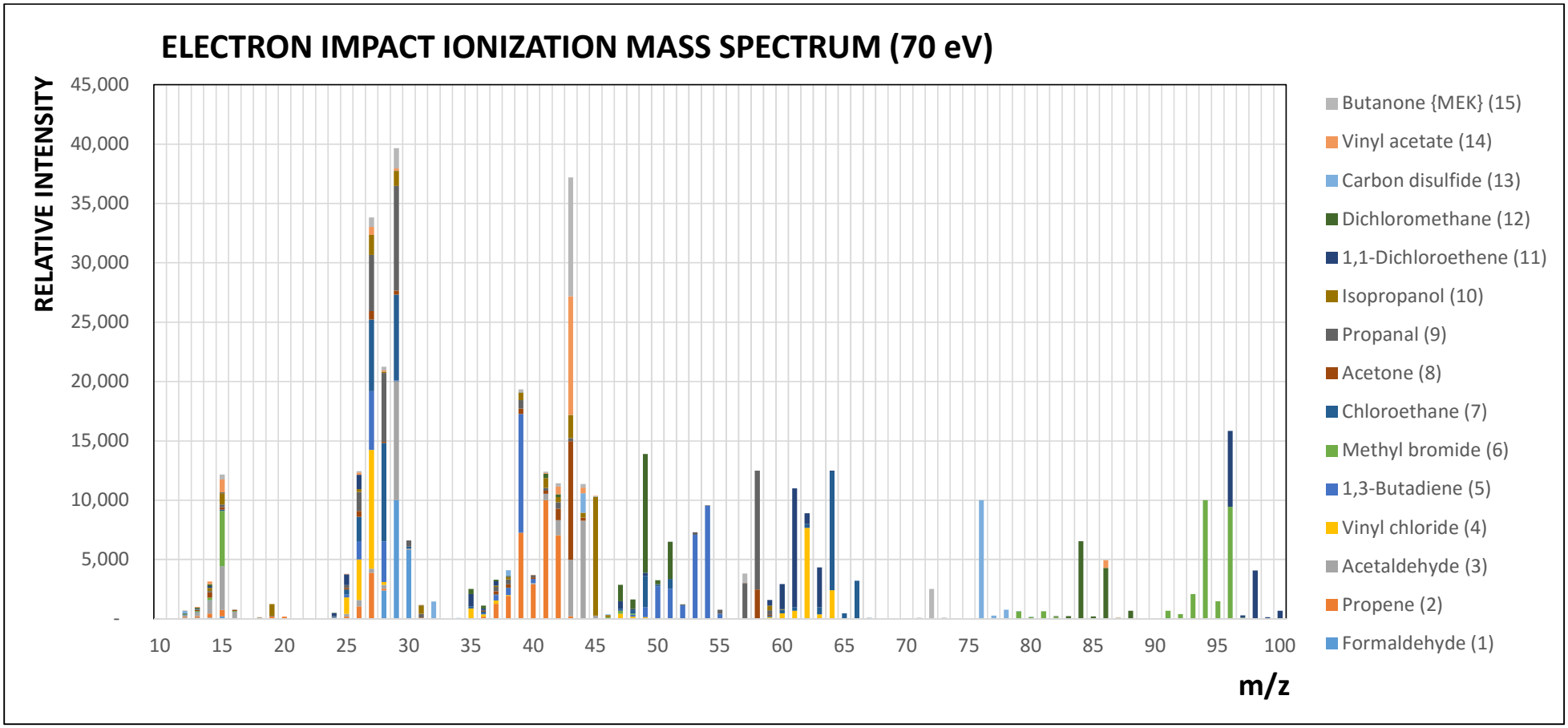
$C_2H_2O_2$	Glyoxal 		
C_4H_{10}	butane  *iso*-butane 	C_3H_6O	Acetone  Propanal 

"The more power a technique has for differentiation of isomers and isobars the more useful it will be for the analysis of real world samples."

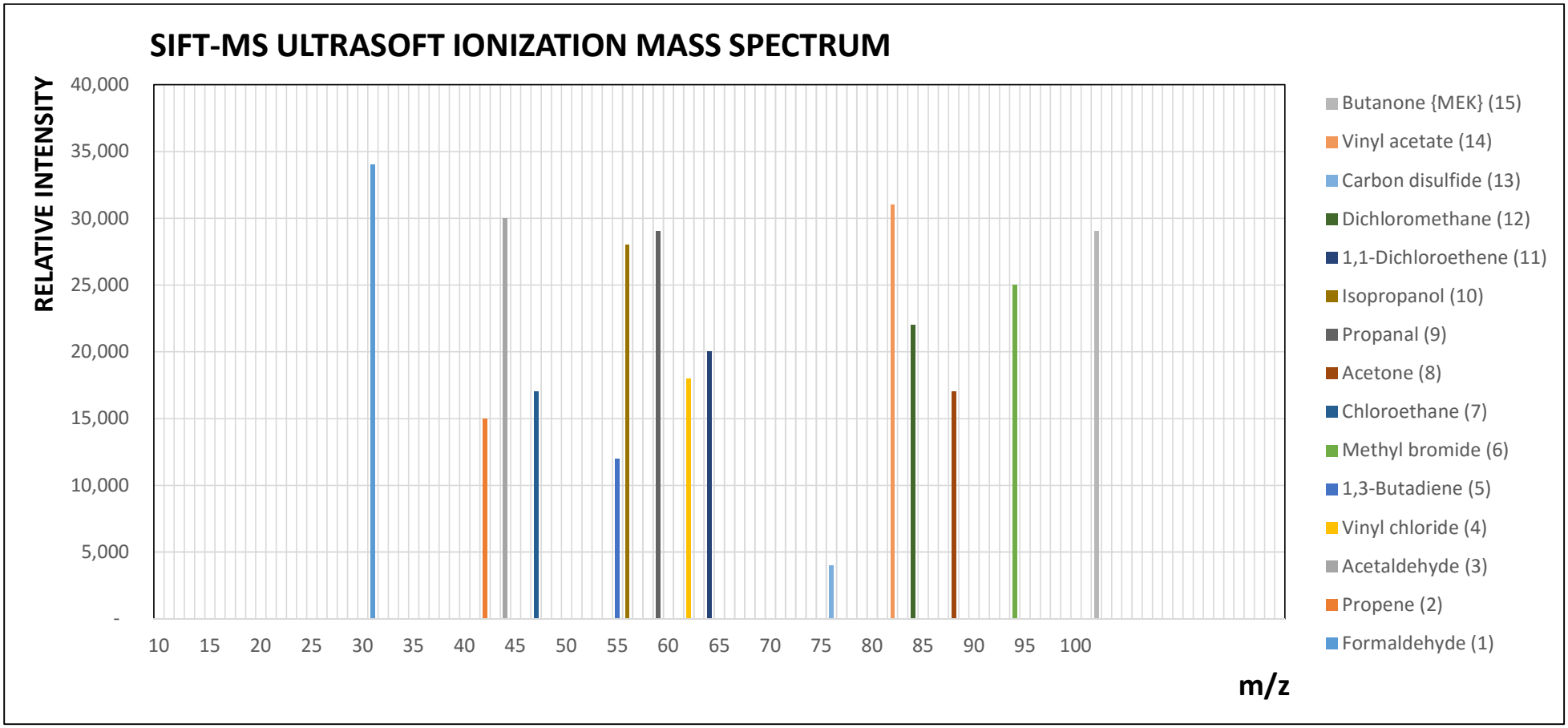
SIFT-MS – how this soft chemical ionization technique works



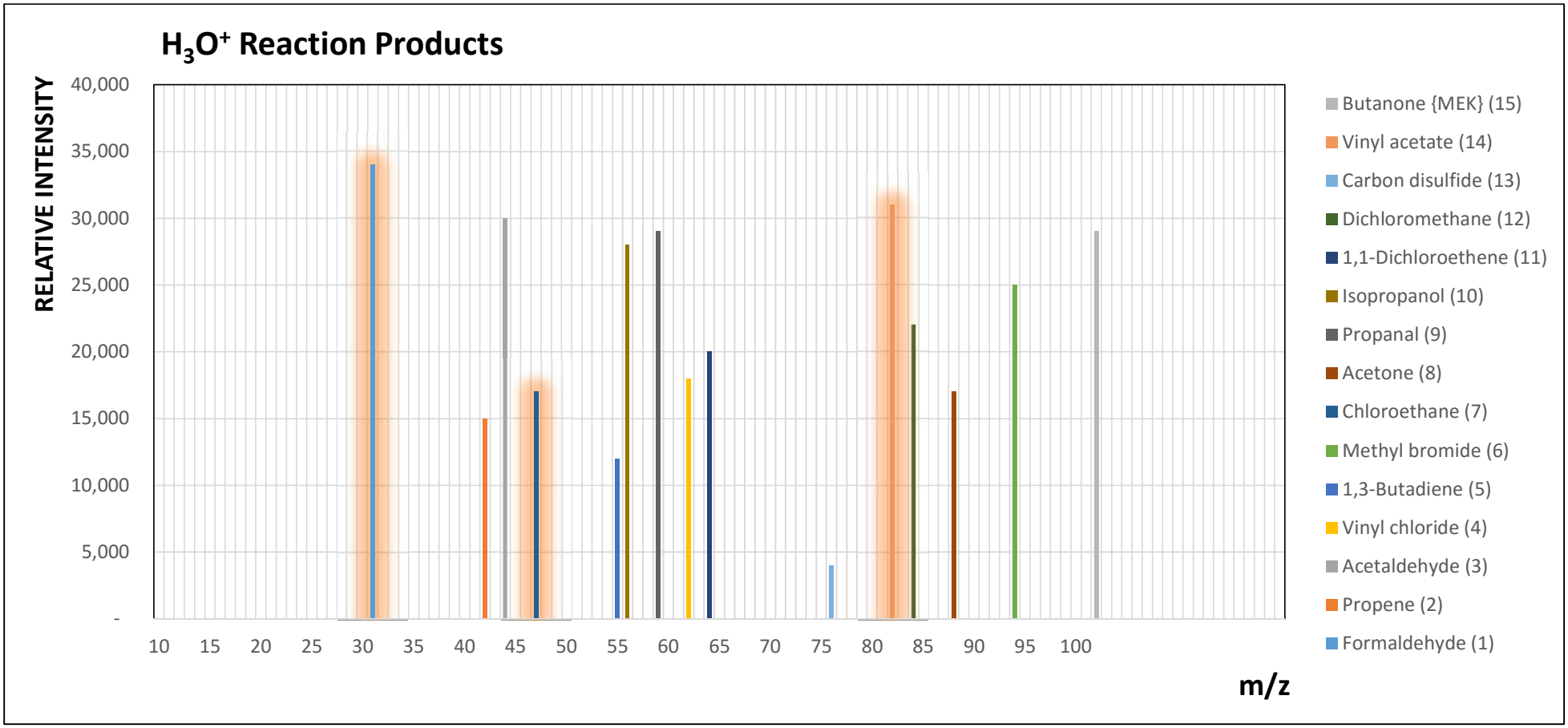
Key Fact 1 - SIFT uses the softest possible ionization



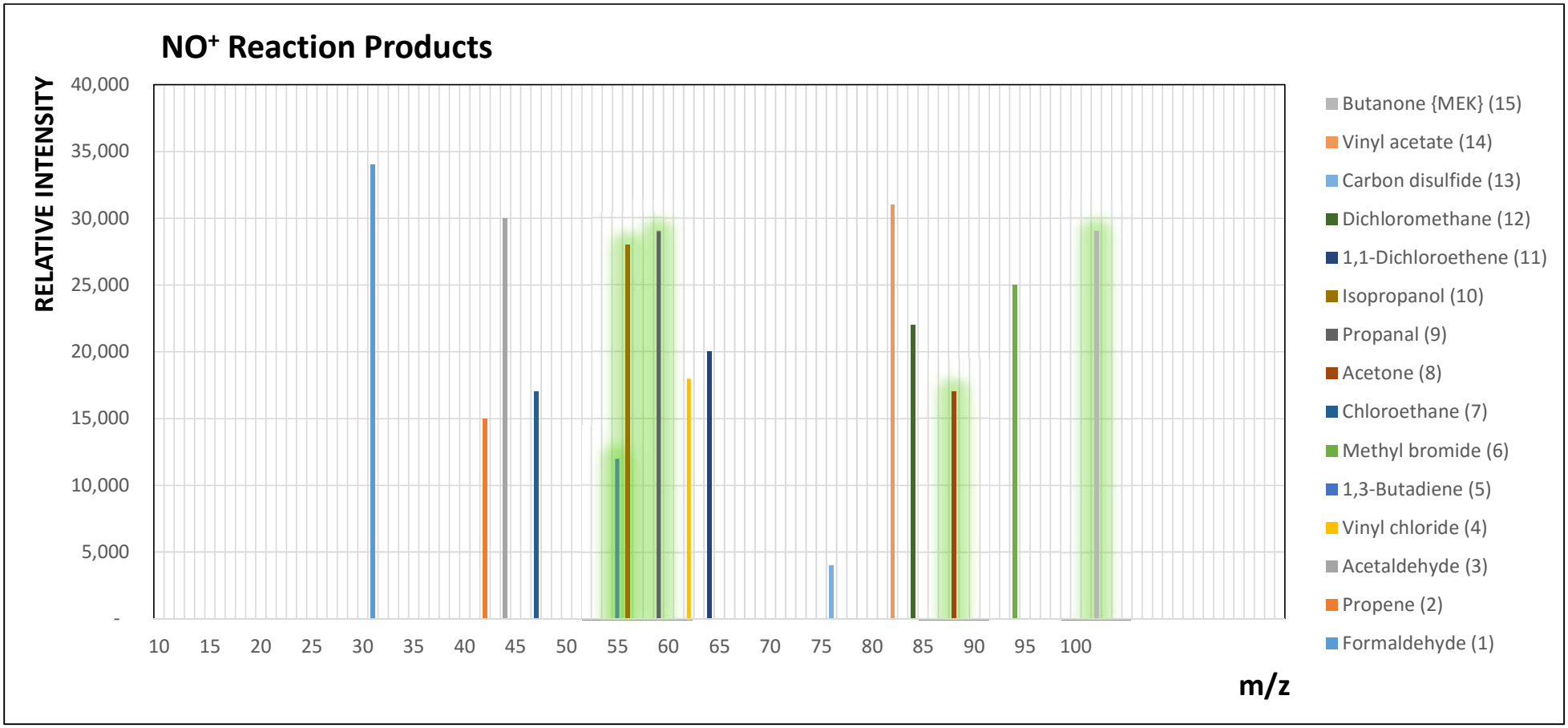
Key Fact 1 - SIFT uses the softest possible ionization



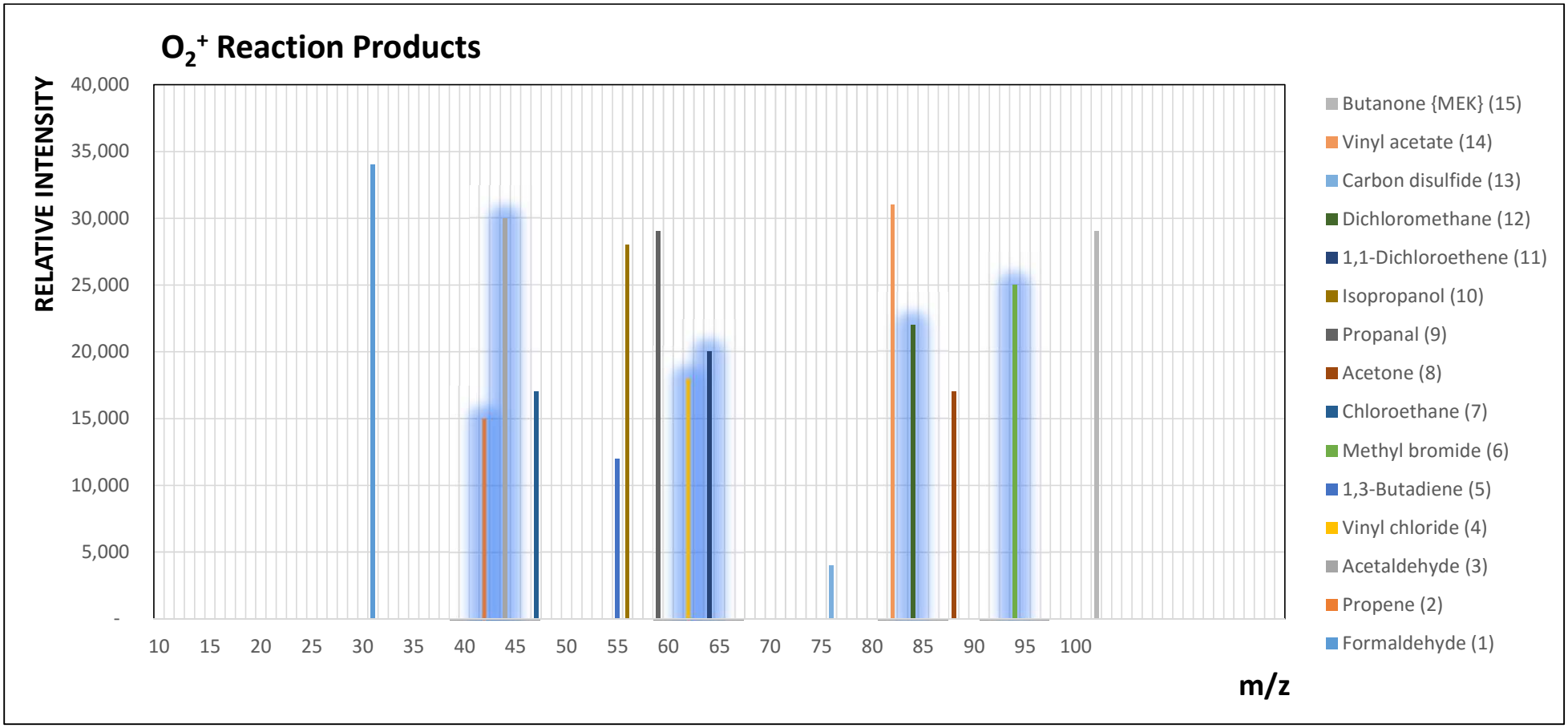
Key Fact 1 - SIFT uses the softest possible ionization



Key Fact 1 - SIFT uses the softest possible ionization



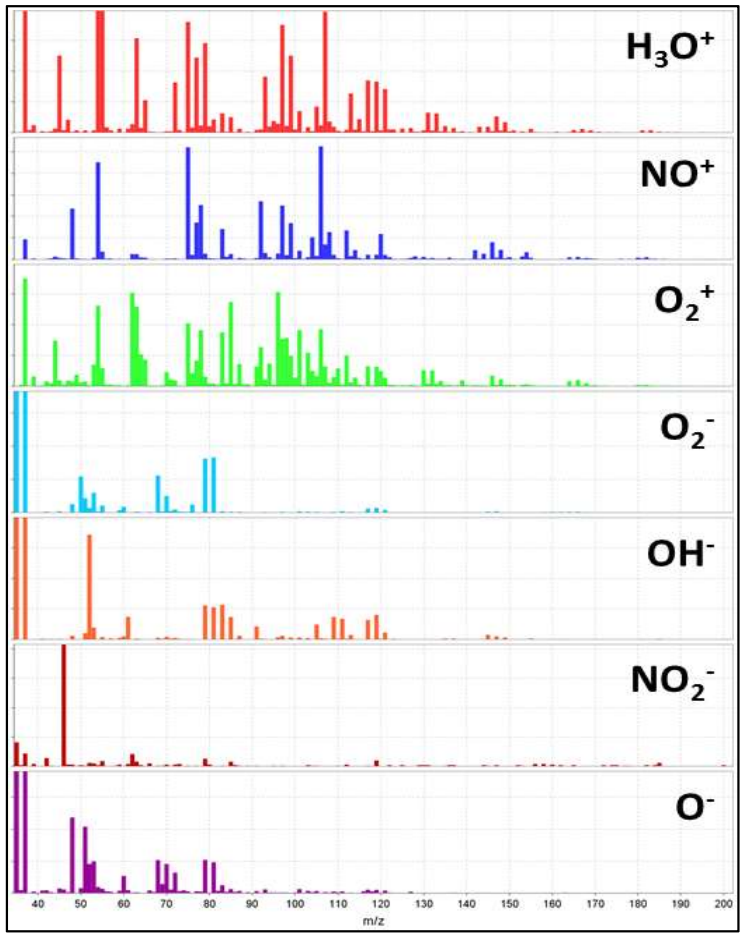
Key Fact 1 - SIFT uses the softest possible ionization



SIFT-MS separates isomers and isobars through chemistry

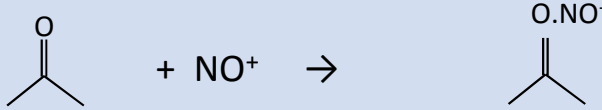
Mechanism	H_3O^+	NO^+	O_2^+	OH^-	O^-	O_2^-	NO_2^-	NO_3^-
Proton transfer (PT)	✓	×	×					
Electron transfer (ET)	×	✓	✓					
Dissociative ET	×	✓	✓					
Hydride abstraction	×	✓	×					
Association	✓	✓	×	✓	✓	✓	×	×
Proton Abstraction				✓	✓	✓	✓	✓
Electron attachment				×	×	✓	×	×
Associative Detachment				✓	✓	✓	×	×
Displacement/Elimination				✓	✓	×	×	×

Separation through ion chemistry



propanol vs acetone (m/z = 58)

m/z = 57



m/z = 88

phosphine vs hydrogen sulfide (m/z = 34)

$H_2S + O_2^- \rightarrow O_2 + HS^-$ *m/z = 33*

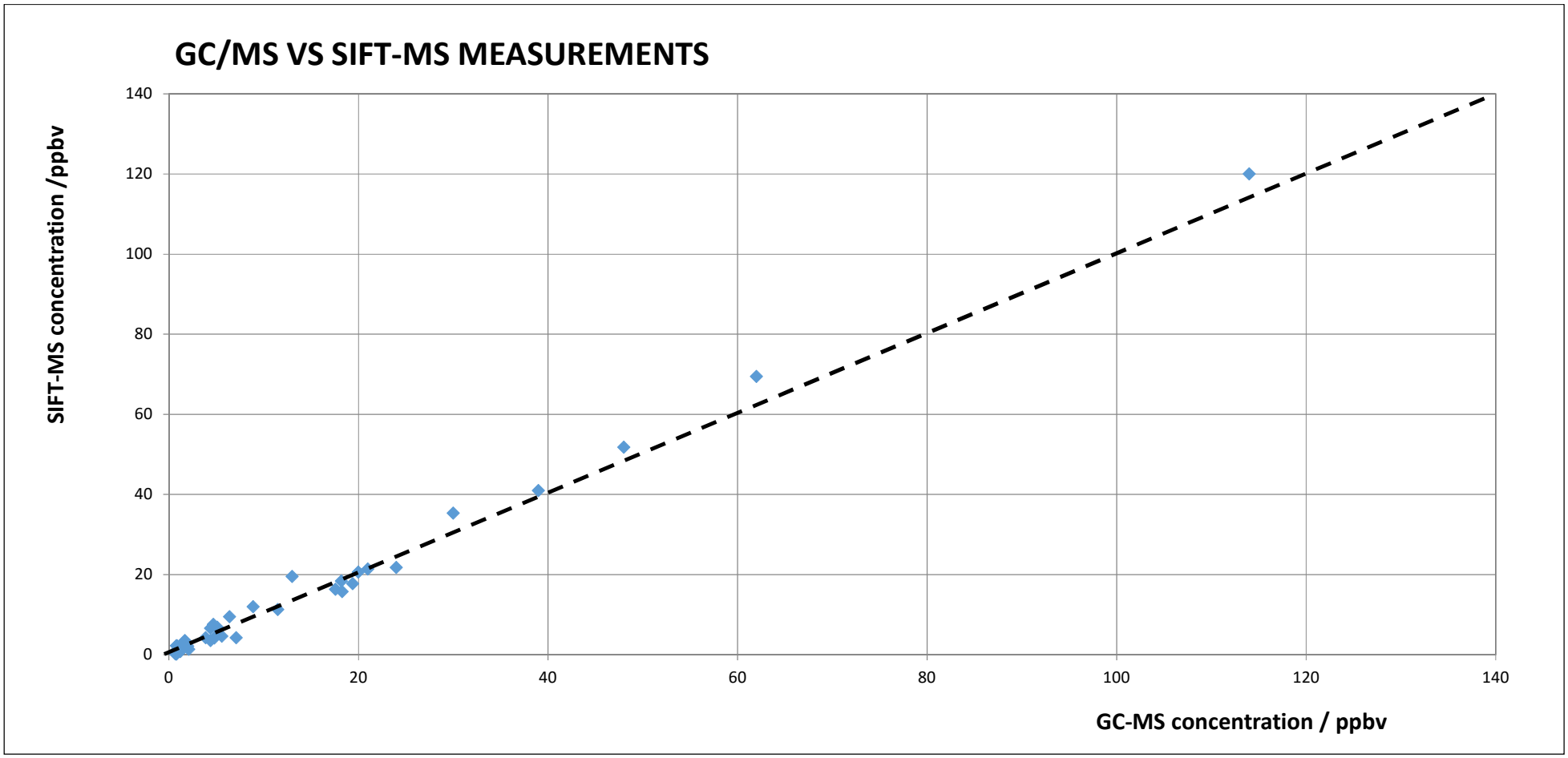
$PH_3 + O_2^-$ X *no reaction*

acetaldehyde vs hydrocarbons (m/z = 44)

$C_2H_4O + O^- \rightarrow O + C_2H_4O^-$ *m/z = 44*

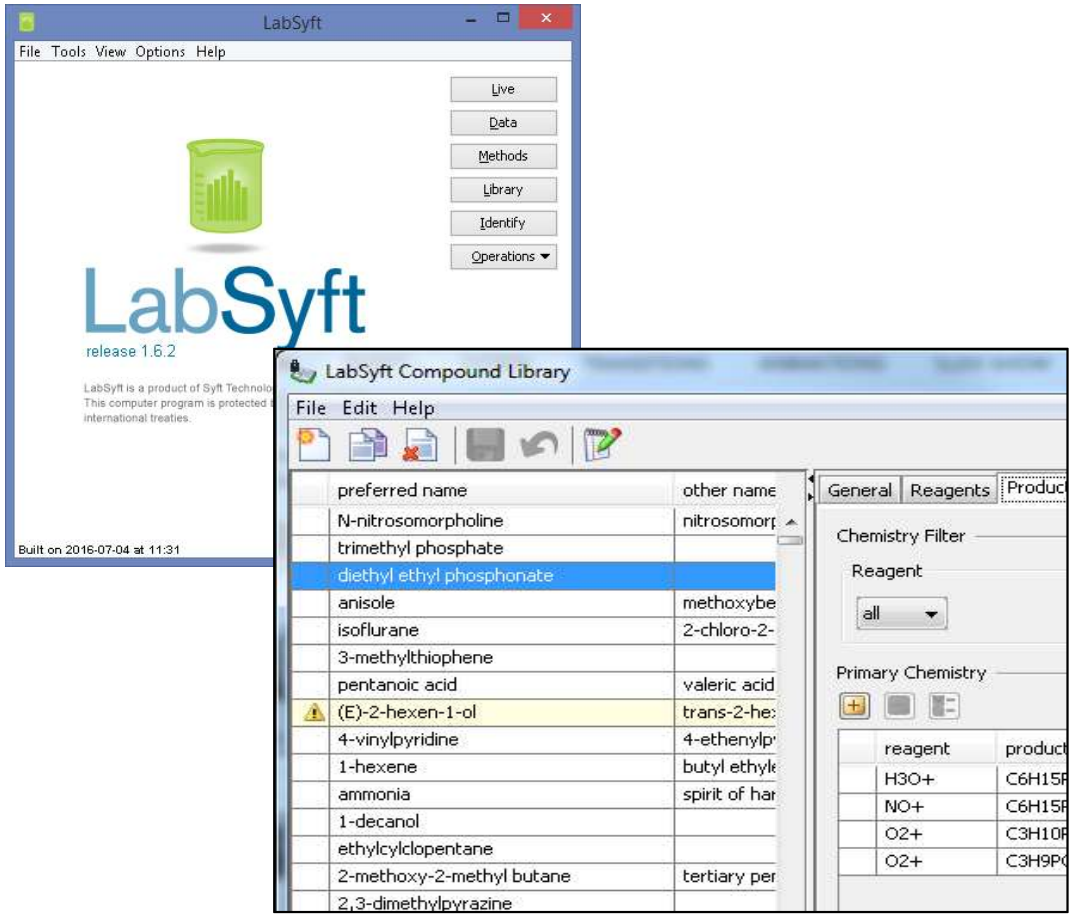
$C_3H_8 + O^- \rightarrow C_3H_7 + OH^-$ *m/z = 17*

Comparable quantitation – Calibrated GC/MS and SIFT-MS



Key characteristics of SIFT-MS for all-in-one air analysis

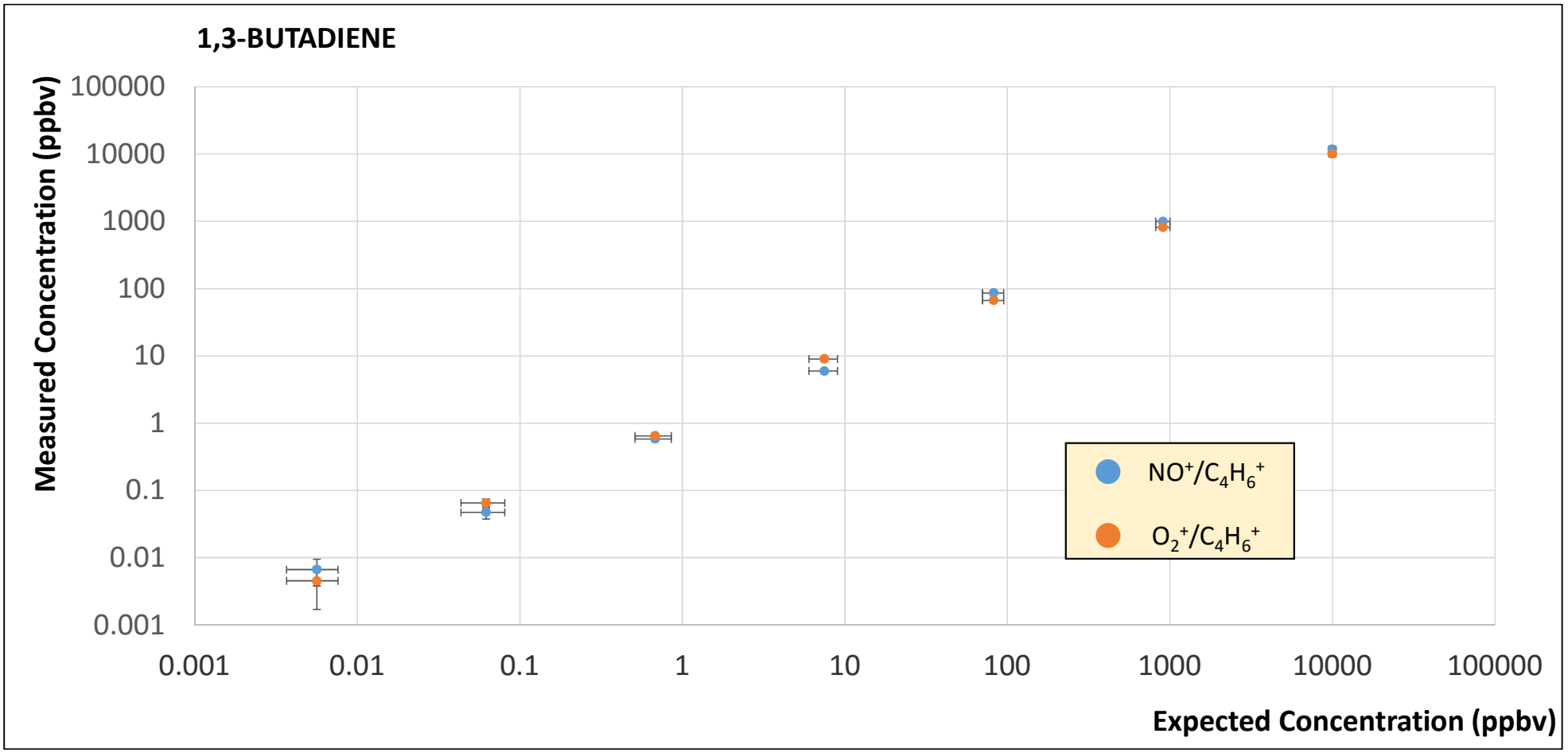
Syft's compound library is chiefly responsible for the variety of deployment



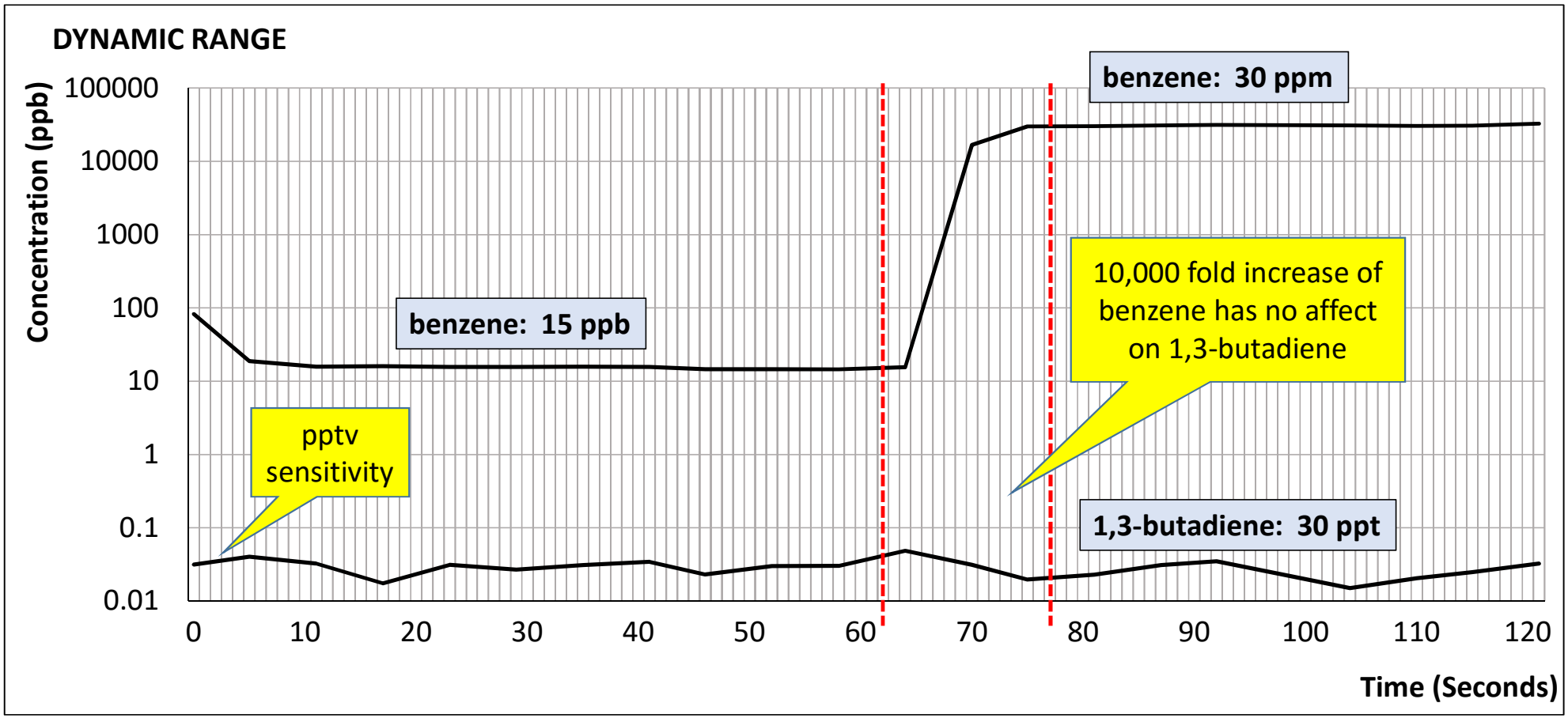
The predictability that comes for the highly controlled nature of the SIFT ionization process results in quantitative measurements without compound-specific calibrations using Syft's compound library.

The library contains over one thousand compounds and new target species can be routinely added.

SIFT-MS linearity spans over five orders of magnitude



SIFT-MS is extremely sensitive and has a dynamic range of 6 orders of magnitude

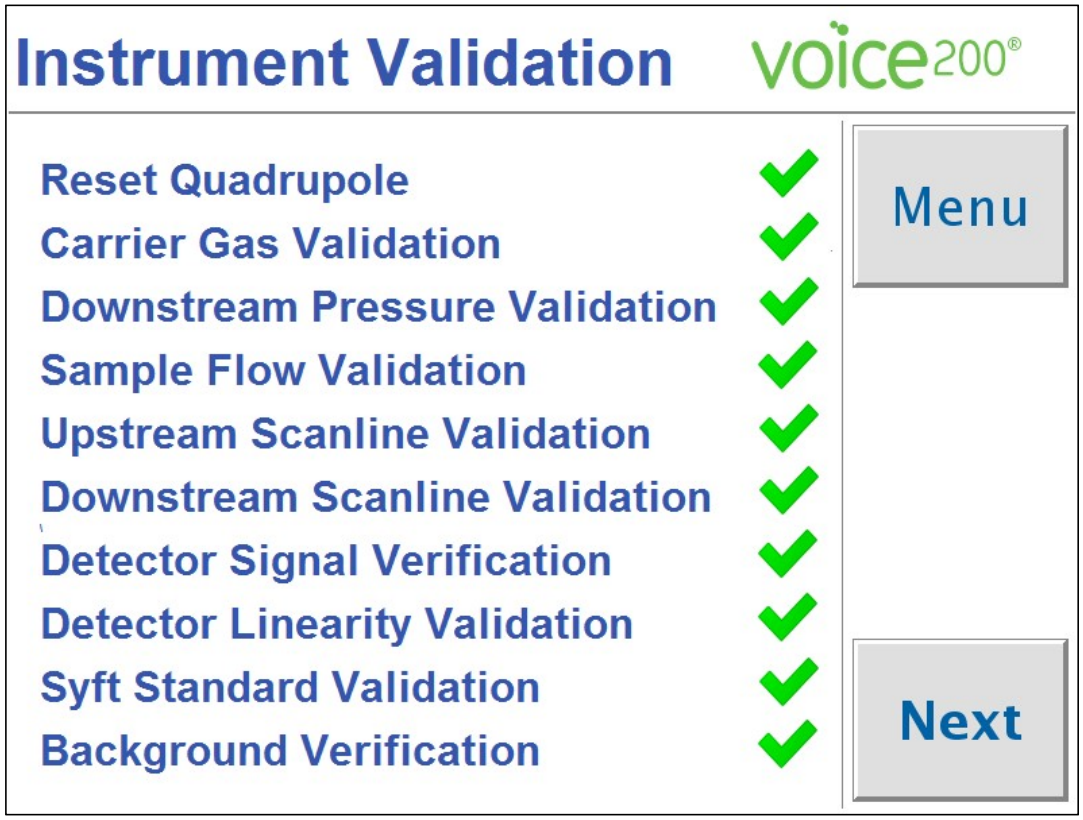


A Voice200 is robust and can be operated by non-technical users

Syft instruments have been deployed in industrial environments for nearly a decade and operated by non-technical, front-line staff.

Instruments can be placed at the point of testing, allowing faster response times.

Built-in Automatic 10-point Instrument Validation



Syft's instruments automatically run a battery of tests at regularly scheduled intervals, which constitute the Instrument Validation consists

The Instrument Validation tests all aspects of the instrument performance and culminates in the measurement of a certified analytical standard, which provide and end-to-end test of the overall instrument performance.

The Instrument Validation provides an assurance of the quality of the data collecting by the Syft system.

Syft's Voice200 can be operated and suported remotely

The Voice200 can be operated continuously and remotely.

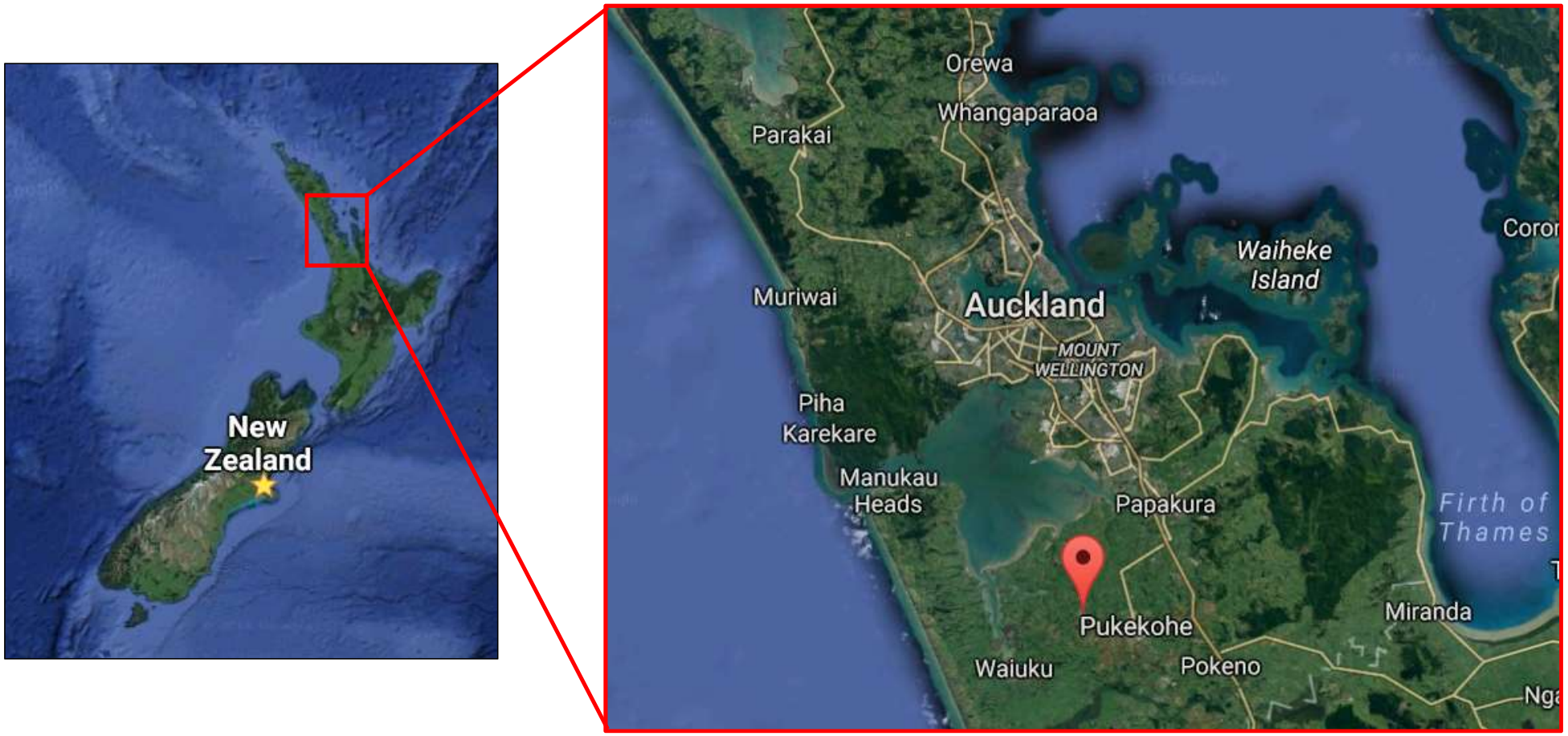
Syft's unique operating characteristics ensure a high confidence with the date through the following:

- Automatic validation
- Stable, consistent data
- Integration into existing systems
- Very easy to operate

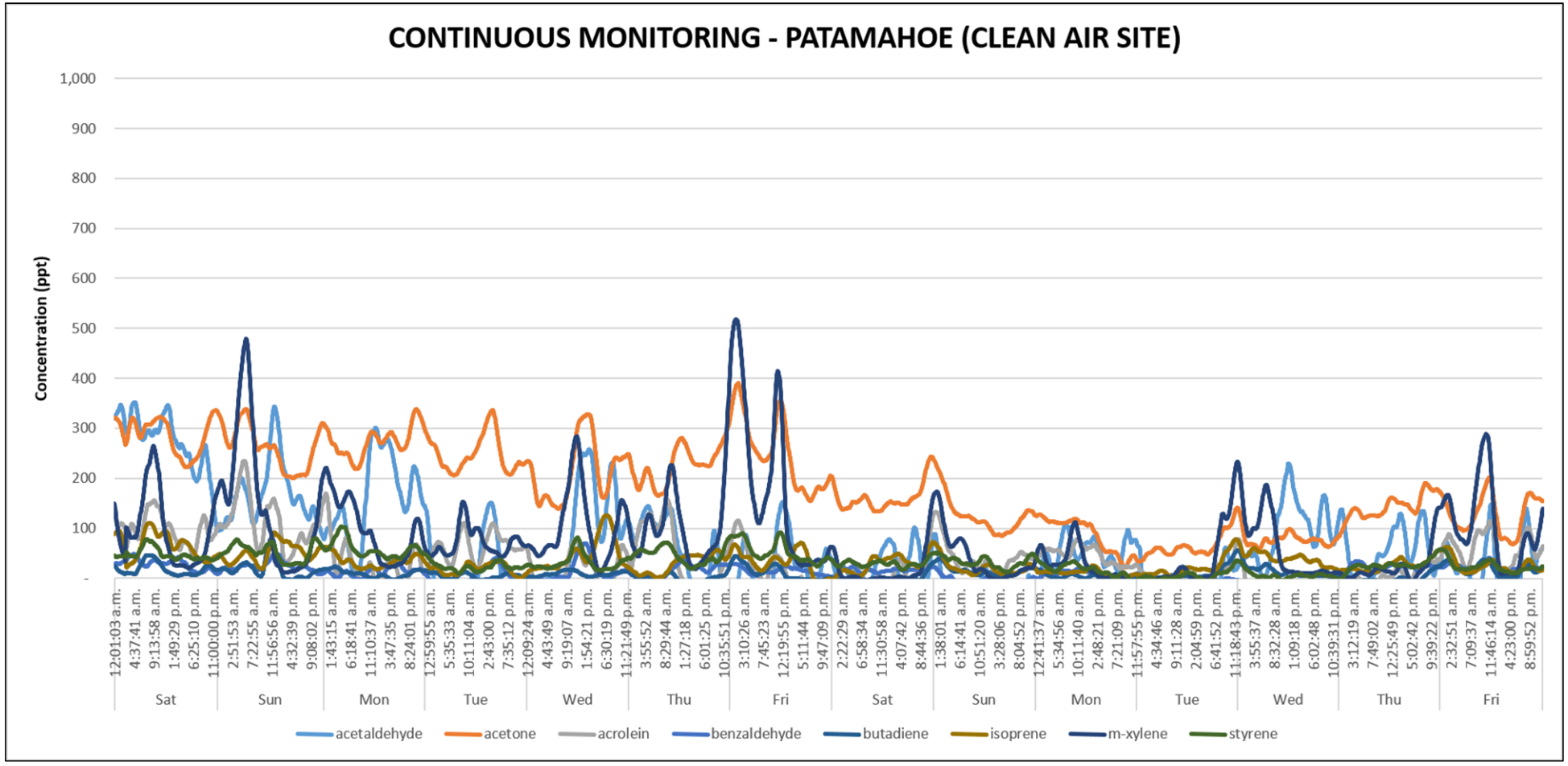
Syft can also provide remote support.

Application 1
Continuous air quality monitoring

Continuous Clean Air monitoring – Auckland City Council



Continuous Clean Air monitoring – Auckland City Council



Application 2
Stack emissions

Stack Monitoring

Butanone	Methyl isobutyl alcohol
Isobutyl alcohol	Butanal
Propanal	Butyl acetate
Pentanal	Propanoic acid
Hydrogen sulfide	Ammonia
Xylenes	Toluene
Styrene	Butanoic acid
Dimethyl disulfide	Acetaldehyde
Formaldehyde	Methyl mercaptan
Trimethyl amine	3-Methylbutanoic acid
Sulfur dioxide	Sulfur trioxide
Carbon dioxide	Hydrogen chloride
Hydrogen fluoride	Benzene

SIFT-MS has enhanced selectivity for important environmental VOCs

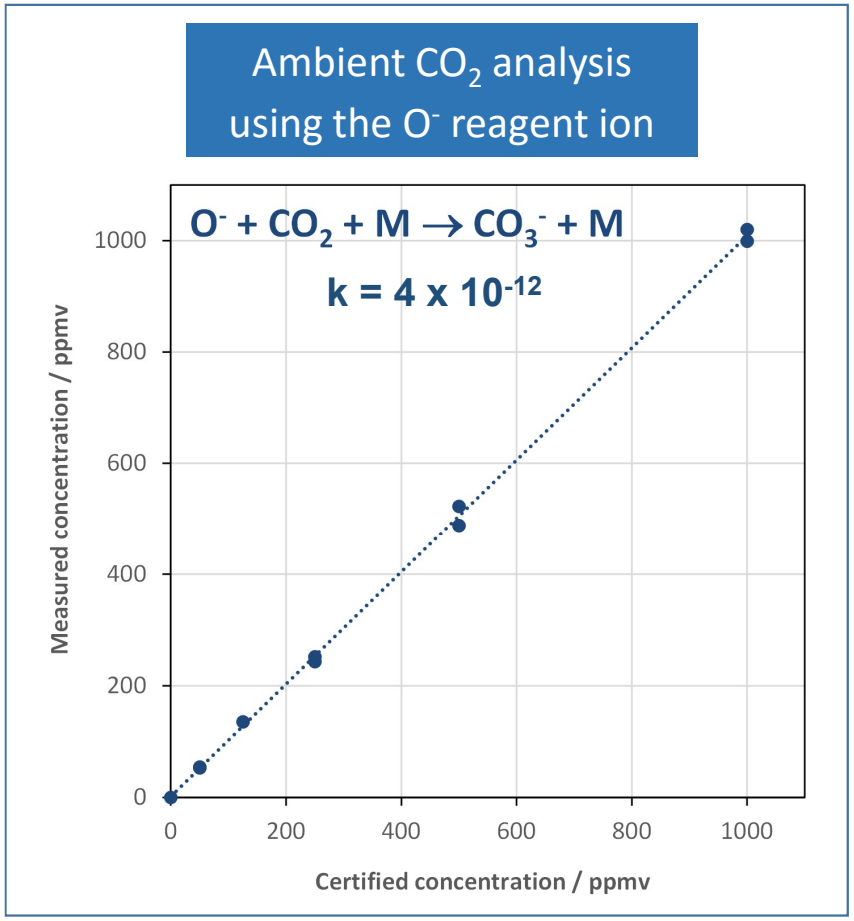
Compound	Positive Reagent Ions		Negative Reagent Ions	
	Reagent ion	Product ion	Reagent ion	Product ion
Benzene	H_3O^+	$C_6H_7^+$ m/z 79	O-	$C_6H_4^-$ m/z 76 $C_6H_5^-$ m/z 77
	NO^+	$C_6H_6^+$ m/z 78 $C_6H_6.NO^+$ m/z 108		
Toluene	H_3O^+	$C_7H_9^+$ m/z 93	O^-	$C_7H_7^-$ m/z 91
	NO^+, O_2^+	$C_7H_8^+$ m/z 92	OH^-	$C_7H_7^-$ m/z 91
Formaldehyde	H_3O^+	$C_2H_5O^+$ m/z 31	O^-	HCO_2^- m/z 45
			OH^-	HCO_2^- m/z 45
Acetaldehyde	H_3O^+	$C_2H_5O^+$ m/z 45	O-	$C_2H_2O^-$ m/z 42 $C_2H_3O^-$ m/z 43
	NO^+	$C_2H_3O^+$ m/z 43	OH^-	$C_2H_3O^-$ m/z 43
Acrolein	H_3O^+	$C_3H_5O^+$ m/z 57	O^-	$C_3H_3O_2^-$ m/z 71
	NO^+	$C_3H_3O^+$ m/z 55 $C_2H_4O.NO^+$ m/z 86	OH-	$C_3H_3O^-$ m/z 55

Negative reagent Ions also allow detection of inorganic gases

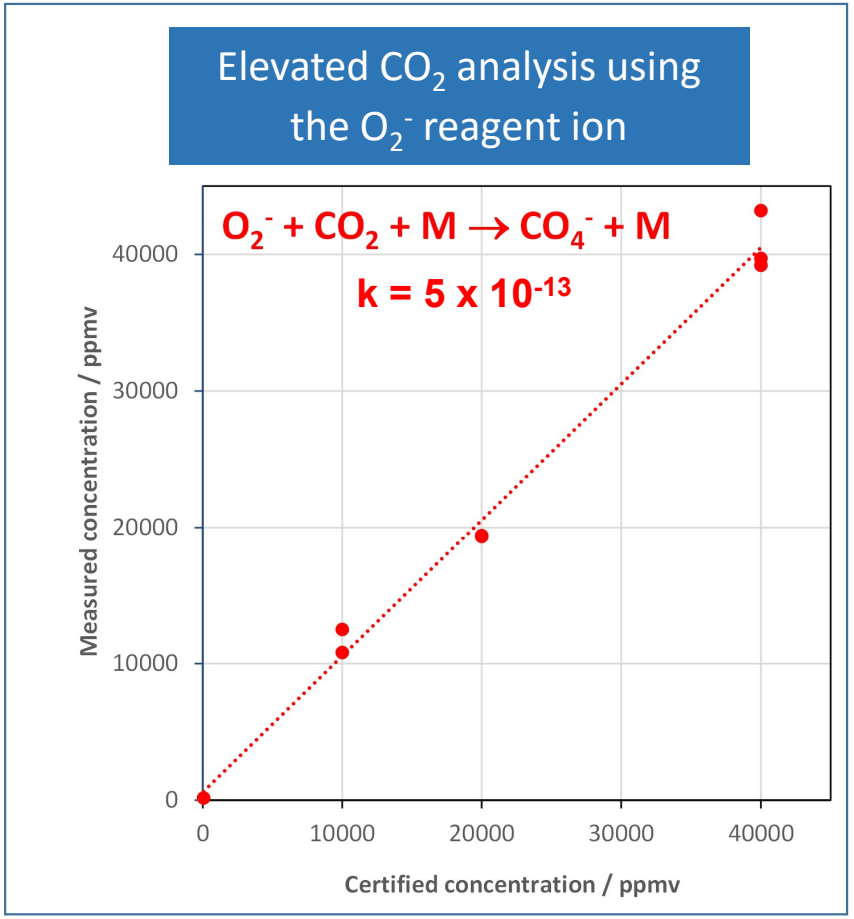
Compound	Reagent ion	Product ion
Ozone	O^-, OH^-,O_2^-	O_3^- m/z 48
Sulfur dioxide	OH^-	$SO_2.OH^-$ m/z 81
	O_2^-	SO_2^- m/z 64
Sulfur trioxide	O^-	SO_3^- m/z 80
		SO_2^- m/z 64
	OH^-, O_2^-	SO_3^- m/z 80
	NO_2^-, NO_3^-	SO_4^- m/z 96
Carbon dioxide	O^-	CO_3^- m/z 60
	OH^-	CO_3H^- m/z 61
	O_2^-	CO_4^- m/z 76
Nitrous oxide	O^-	NO^- m/z 30
Hydrogen chloride	O^-, OH^-	Cl^- m/z 35, 37
Hydrogen fluoride	O^-, OH^-	F^- m/z 19

Exploiting ion chemistry – CO_2 measurement over a very wide dynamic range

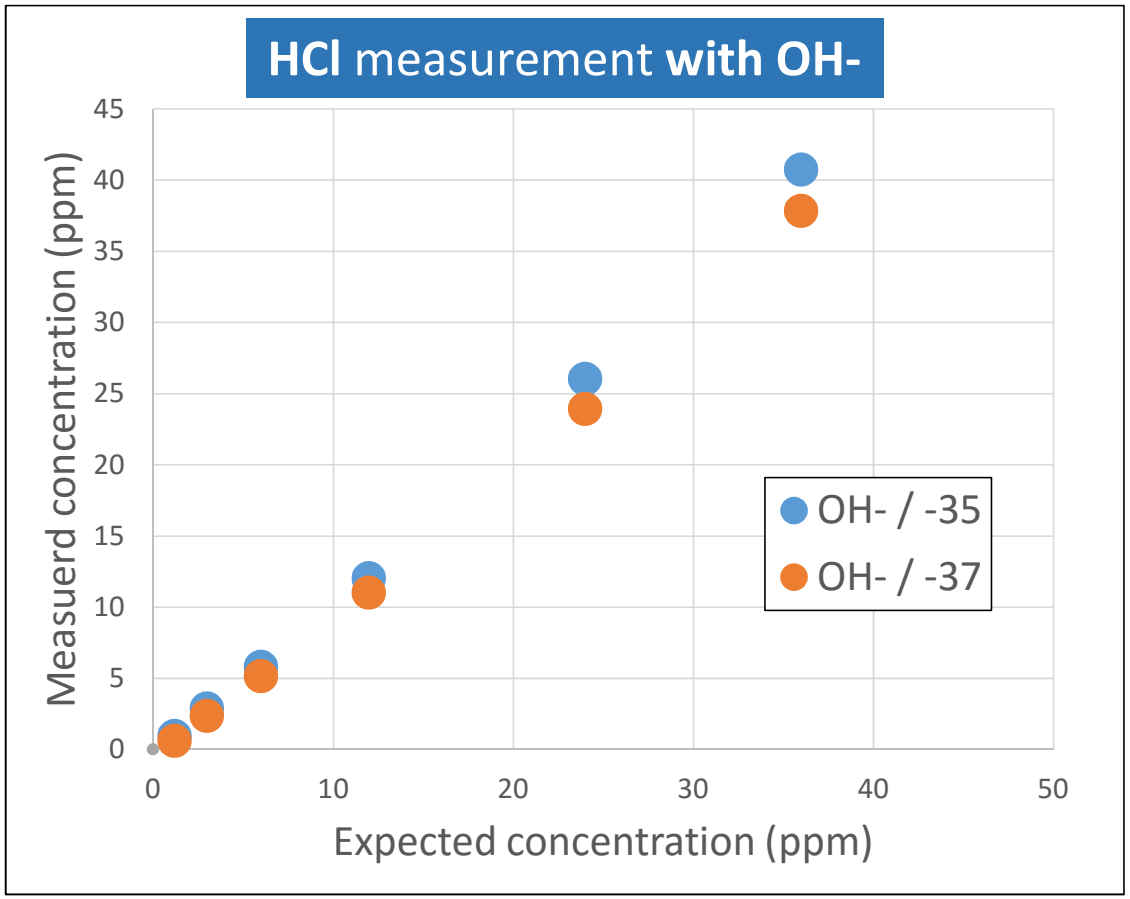
Ambient CO_2 analysis using the O^- reagent ion



Elevated CO_2 analysis using the O_2^- reagent ion



Sample delivery is key for detection of HF and HCl



HF and HCl can both be detecting using a wide range of the negative reagent ions.

HF needs special sample handling to prevent corrosion but the lack of a column means you can just use the correct inert material.

Syft has a “Corrosive-gas inlet” for delivery of samples containing these compounds.

Application 3
High-throughput analysis

Integration of autosampler with SIFT-MS for high-throughput analysis

Simplest way to leverage high sample throughput from the rapid analysis provided by SIFT-MS

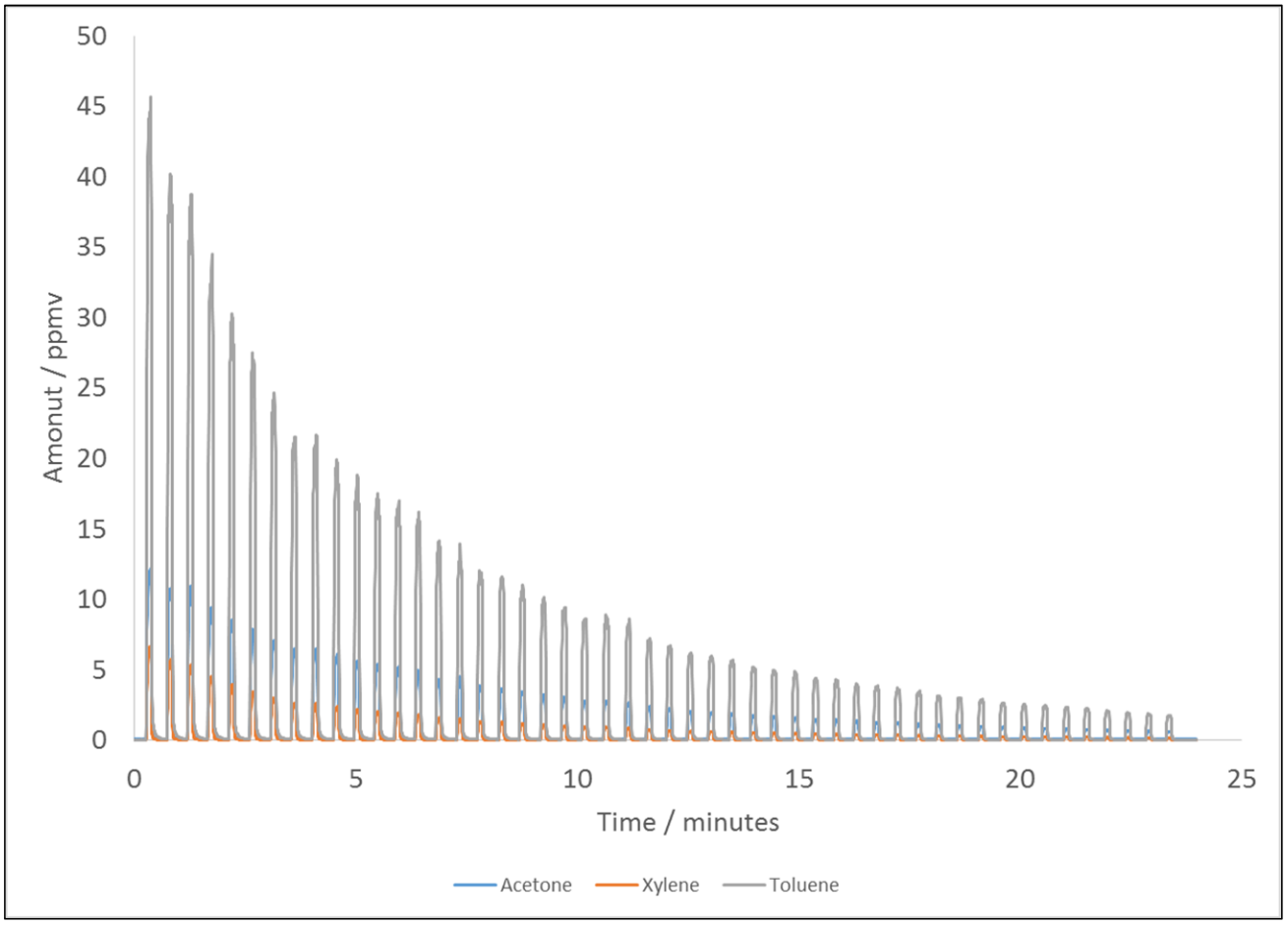
Better repeatability and reproducibility

Reduce labor costs

Analytical equipment:

- Syft Voice200 SIFT-MS
- Syft autosampler interface kit
- Syft LabSyft software package
- Gerstel MPS headspace autosampler
- Gerstel Maestro software
- Anatune 160-vial tray

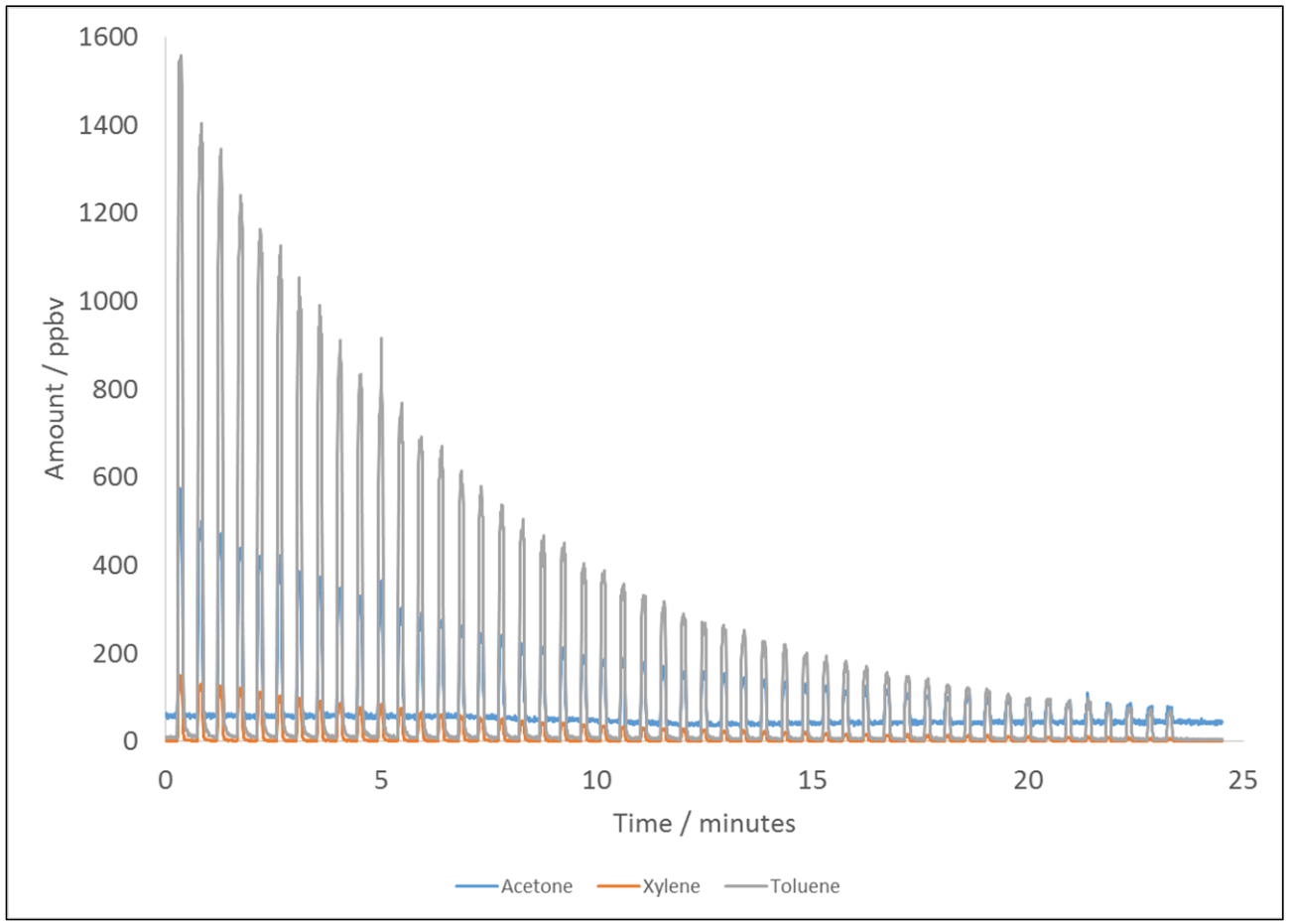
Automated sample handling coupled to fast SIFT-MS analysis give very fast cycle times



<u>20 mL headspace vial</u>

1. sample 2 mL @ 200 uL/sec
2. add 2 mL of air
3. repeat

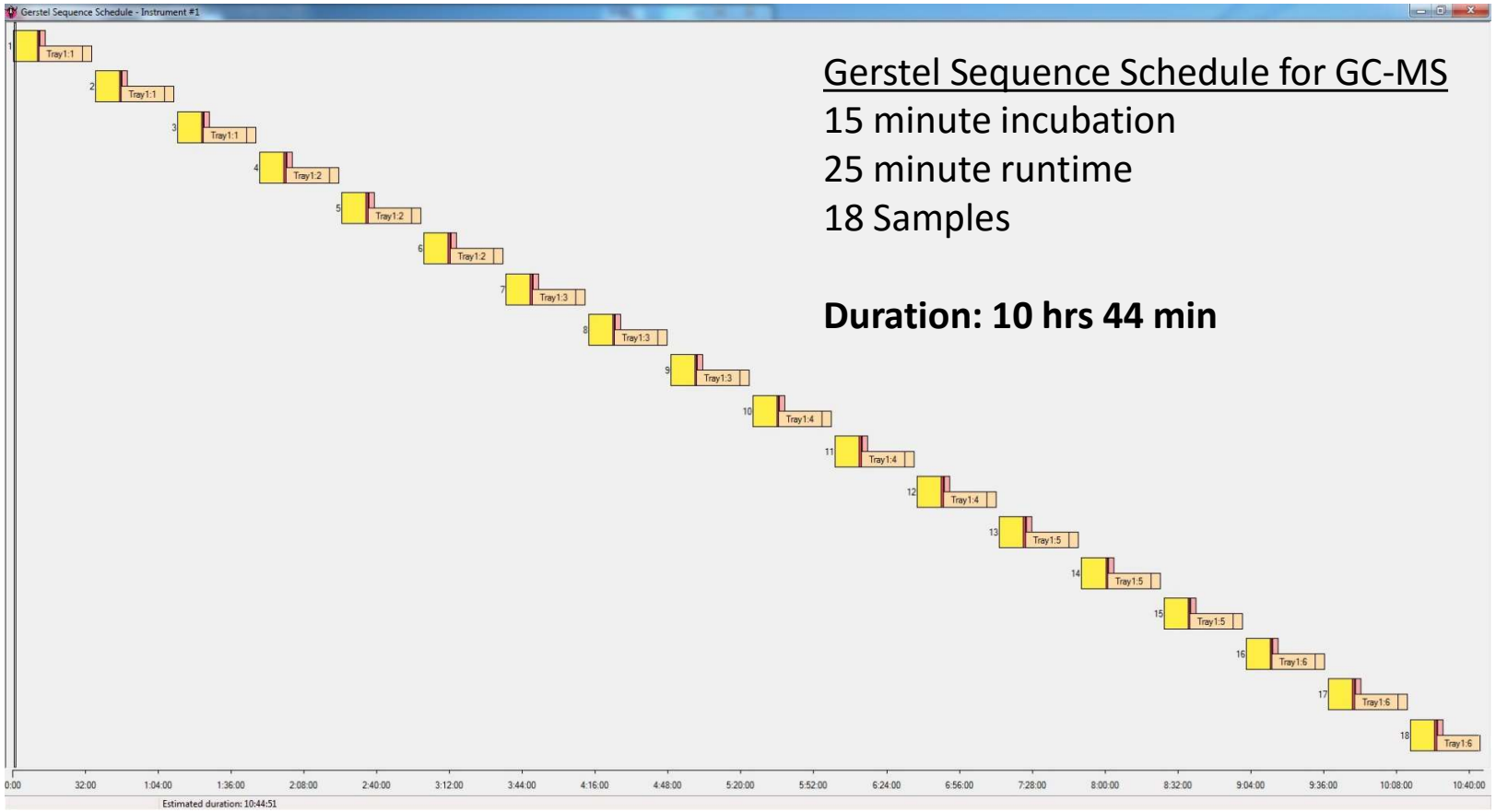
Integration of autosampler with SIFT-MS for high-throughput analysis



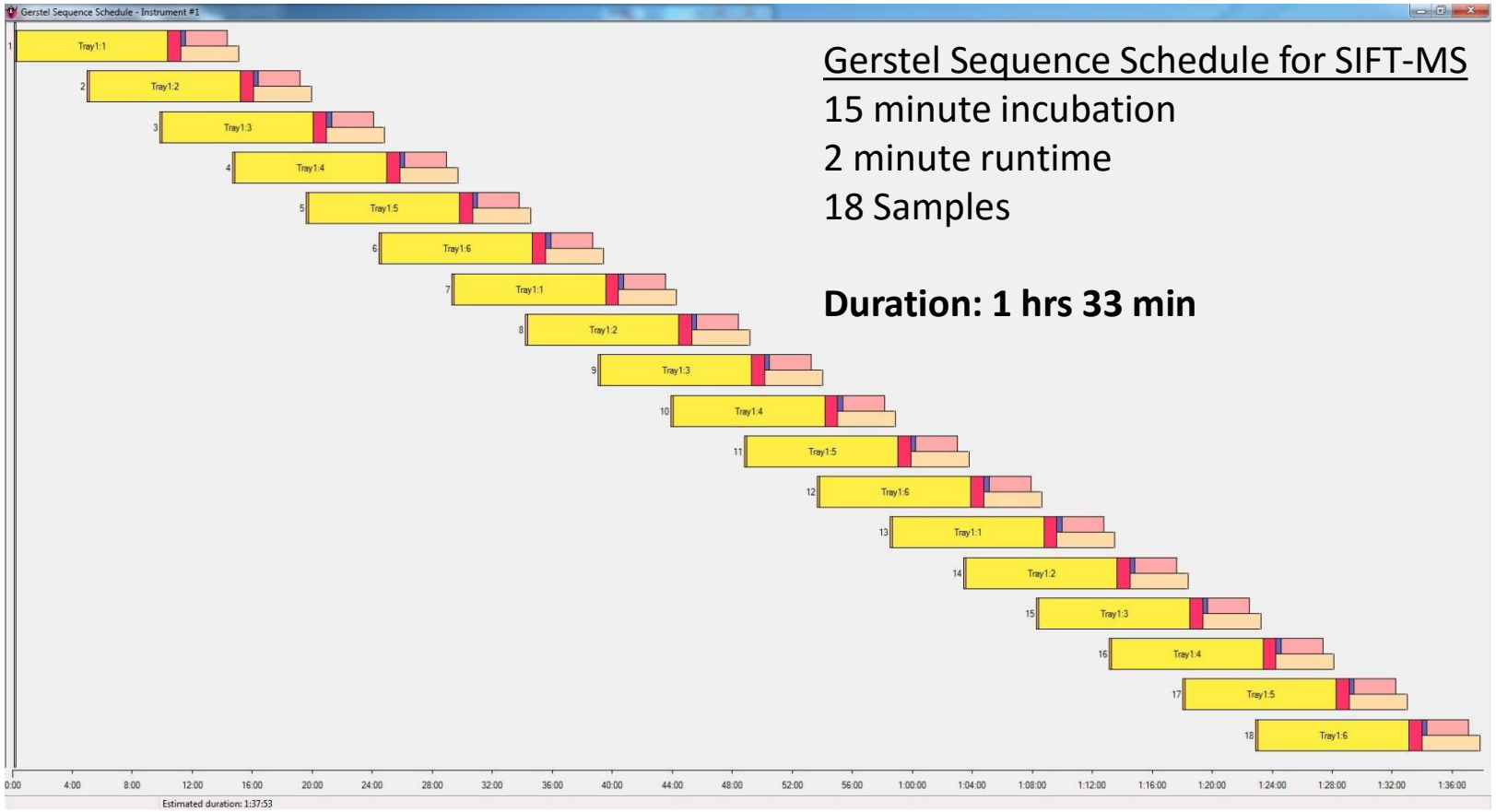
Continued…

100 analyses in 50 minutes!

GC-MS throughput is limited by GC run time



SIFT-MS throughput is limited by incubation time



Gerstel Sequence Schedule for SIFT-MS

15 minute incubation

2 minute runtime

18 Samples

Duration: 1 hrs 33 min

Summary

SIFT-MS uses chemical rather than physical separation

This is possible due to Ultra-Soft ionization and multiple reagent ions

The SIFT-MS technique provides a unique combination of selectivity, sensitivity and speed for a diverse range of chemical species

SIFT-MS is deployed in a number of demanding applications throughout the world

Acknowledgements

Nick Reid, Auckland City Council, Auckland, New Zealand

Mark Perkins, Anatune, Cambridge UK

syft™ Technologies

Questions?