Demonstration of capability of SIFT-MS to measure volatile carbonyl compounds in e-cigarettes.

Louise Bishop, GR&D, British American Tobacco

CORESTA SSPT2021

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The problem – Carbonyls!

Open Access Review

Carbonyl Compounds Generated from Electronic Cigarettes

by Kanae Bekki [1], Shigehisa Uchiyama [1,*], Kazushi Ohta [2], Yohei Inaba [1], Hideki Nakagome [2] and Naoki Kunugita [1]

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ADDITION / CORRECTION This article has been corrected. View the notice.

Selected Harmful and Potentially Harmful Constituents Levels in Commercial e-Cigarettes

Maxim Belushkin, Donatien Tafin Djoko, Marco Esposito, Alexandra Korneliou, Cyril Jeannet, Massimo Lazzerini, and Guy Jaccard*

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Abstract

A broad range of commercially available electr… and potentially harmful constituents (HPHC), … formaldehyde. The tobacco-specific nitrosamin… the elements arsenic, cadmium, chromium, lea… The results show that except for the levels of ca… levels for HPHCs were generally not quantifiab… Overall, the lowest levels of formaldehyde were… in yields in comparison with cigarette smoke. F… formaldehyde levels across different brands we… results for variable-power devices operated at t… differences in puffing regimes. Furthermore, o… range of testing conditions (with minimal varia… some products exhibit high variability in emiss… related contributions to HPHC levels to avoid r… consistently across the full e-liquid depletion c… cigarettes is emphasized.

Supporting Information

The Supporting Information is available free of cha…

- List of devices and liquids used in the projec…

1 of 1

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Tobacco Control • Open Access • Volume 23, Issue 2, Pages 133 - 139 • March 2014

Levels of selected carcinogens and toxicants in vapour from electronic cigarettes

Goniewicz M.L.[a,b,c], Knysak J.[c], Gawron M.[c], Kosmider L.[c,d], Sobczak A.[c,d], Kurek J.[d], Prokopowicz A.[d], Jablonska-Czapla M.[e], Rosik-Dulewska C.[e], Havel C.[f], Jacob III P.[f], Benowitz N.[f]

Save all to author list

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…and Population Sciences, Roswell Park …

… London, London, United Kingdom …ersity of Silesia, Sosnowiec, Poland …d Environmental Health, Sosnowiec, Poland

…tes, are devices designed to imitate …out combusting tobacco. They are … to be a safer alternative to regular …med to evaluate the chemical nature of … was to screen e-cigarette vapours for …ic compounds: carbonyls, volatile …erials and methods: Vapours were …e product, the medicinal nicotine …g machine. The selected toxic …quid phase and analysed with … found that the e-cigarette vapours …nts were 9-450 times lower than in …h trace amounts found in the reference …e idea that substituting tobacco …osure to selected tobacco-specific …g smokers unwilling to quit, warrants

CORRESPONDENCE

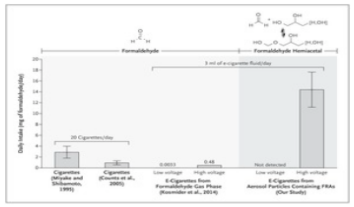
Hidden Formaldehyde in E-Cigarette Aerosols

338 Citing Articles | Letters

TO THE EDITOR:

E-cigarette liquids are typically solutions of propylene glycol, glycerol, or both, plus nicotine and flavorant chemicals. We have observed that formaldehyde-containing hemiacetals, shown by others to be entities that are detectable by means of nuclear magnetic resonance (NMR) spectroscopy,[1] can be formed during the e-cigarette "vaping" process. Formaldehyde is a known degradation product of propylene glycol that reacts with propylene glycol and glycerol during vaporization to produce hemiacetals (Figure 1). These molecules are known formaldehyde-releasing agents that are used as industrial biocides.[5] In many samples of the particulate matter (i.e., the aerosol) in "vaped" e-cigarettes, more than 2% of the total solvent molecules have converted to formaldehyde-releasing agents, reaching concentrations higher than concentrations of nicotine. This happens when propylene glycol and glycerol are heated in the presence of oxygen to temperatures reached by commercially available e-cigarettes operating at high voltage. How formaldehyde-releasing agents behave in the respiratory tract is unknown, but formaldehyde is an International Agency for Research on Cancer group 1 carcinogen.[4]

Figure 1.



Daily Exposures to Formaldehyde Associated with Cigarettes and E-Cigarettes.

Here we present results of an analysis of commercial e-liquid vaporized with the use of a "tank system" e-cigarette featuring a variable-voltage battery. The aerosolized liquid was collected in an NMR spectroscopy tube (10 50-ml puffs over 5 minutes; 3 to 4 seconds per puff). With each puff, 5 to 11 mg of e-liquid was consumed, and 2 to 6 mg of liquid was collected. At low voltage (3.3 V), we did not detect

January 22, 2015
N Engl J Med 2015; 372:392-394
DOI: 10.1056/NEJMc1413069
Metrics

Related Articles

CORRESPONDENCE APR 16, 2015
More on Hidden Formaldehyde in E-Cigarette Aerosols

Most Viewed

ORIGINAL ARTICLE DEC 31, 2020

Conflicting evidence

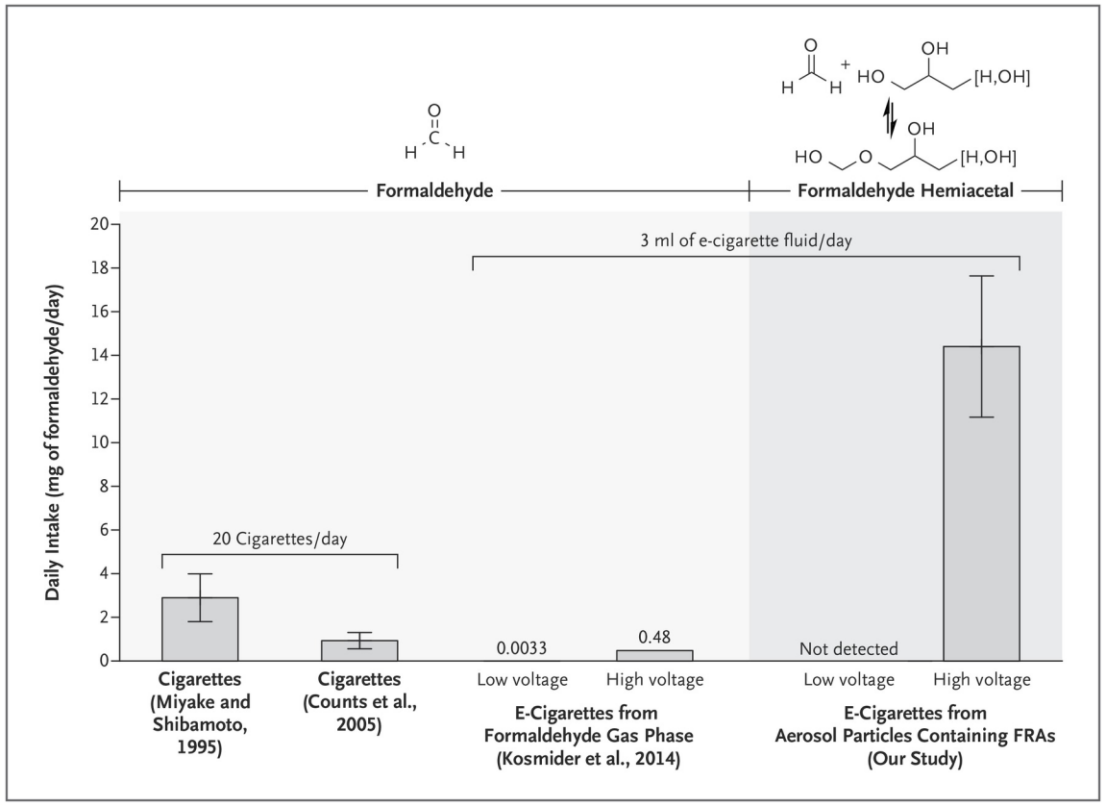


Figure 1[a]

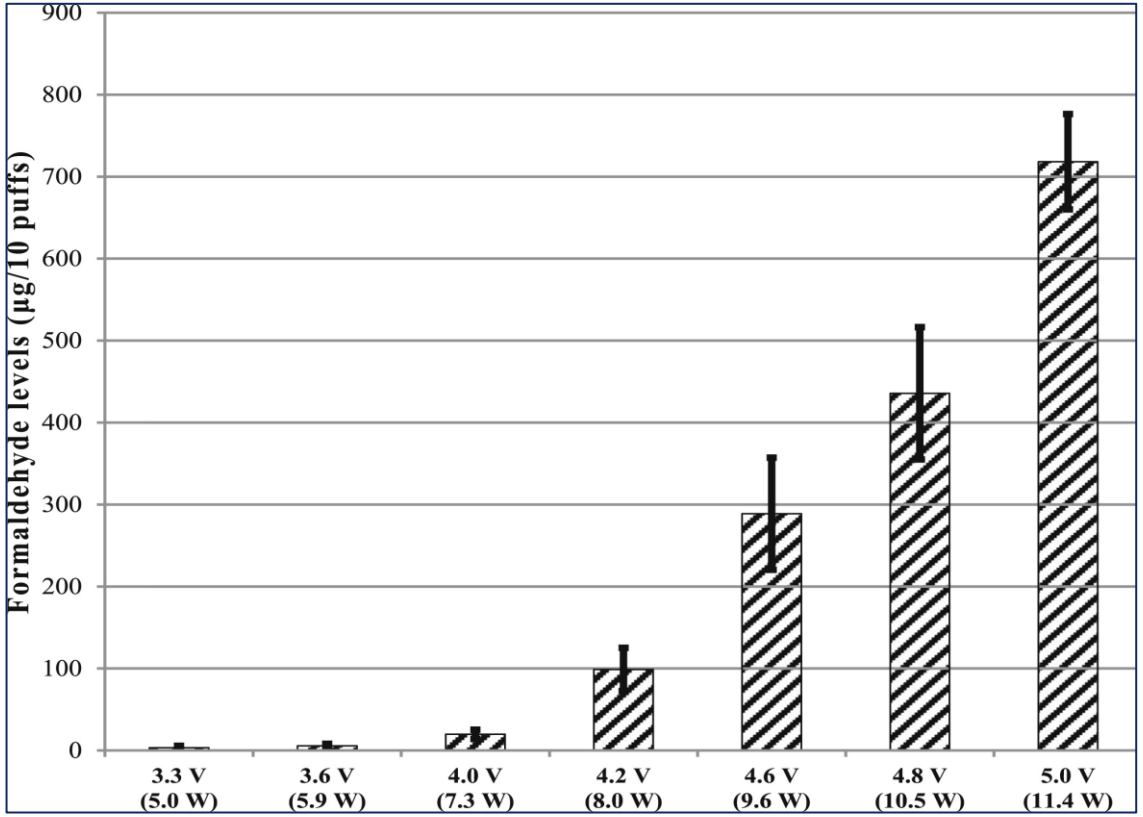


Figure 2[b]

a- Hidden formaldehyde in E-cigarette Aerosols, R. P. Jenson et al, New England Journal of Medicine 373, 4, 392-394
b-E-cigarettes emit very high formaldehyde levels only in conditions that are aversive to users: A replication study under verified realistic use conditions, K. E. Farsalinos et al, Food and Chemical Toxicology, Vol 109, 2017 90-94

Further studies tell a more complex story

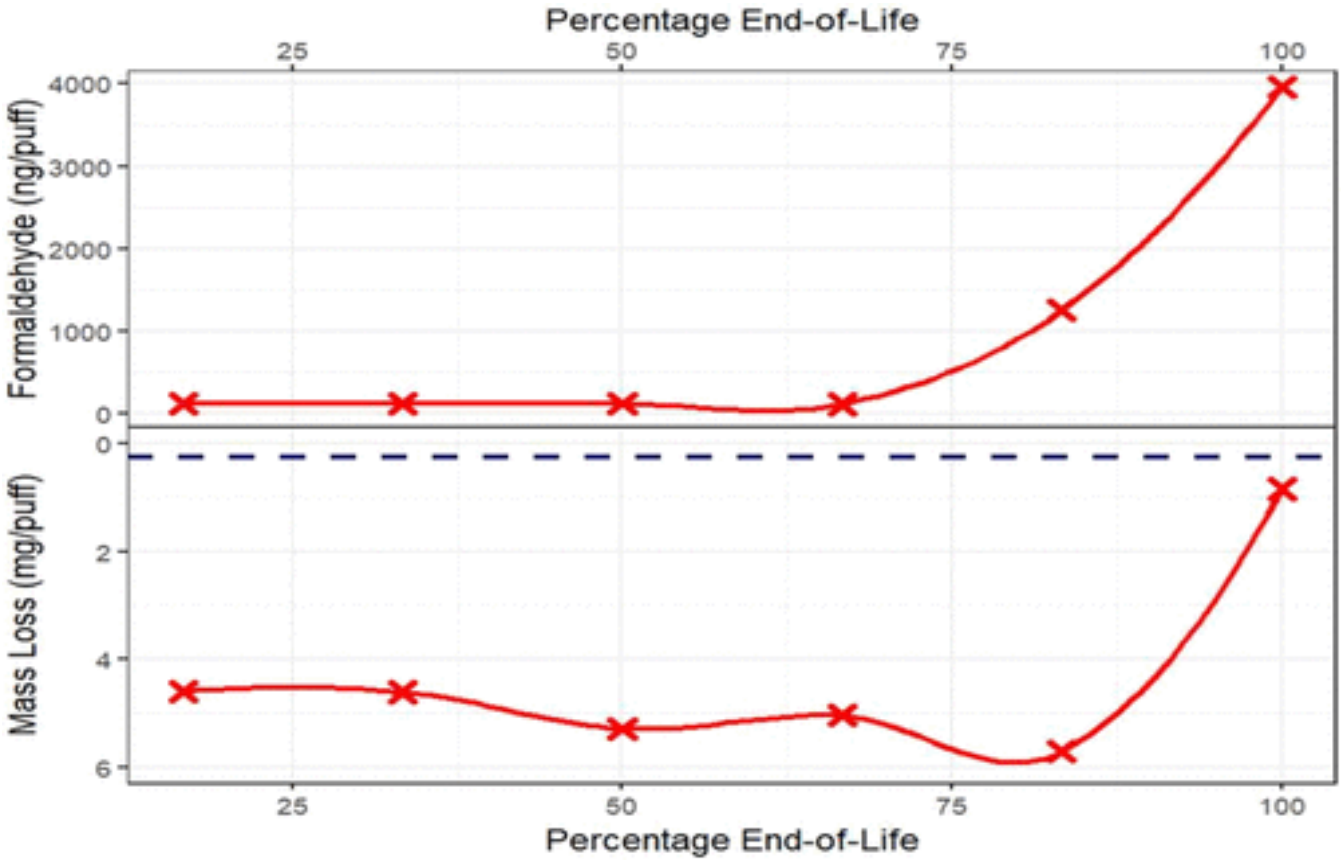
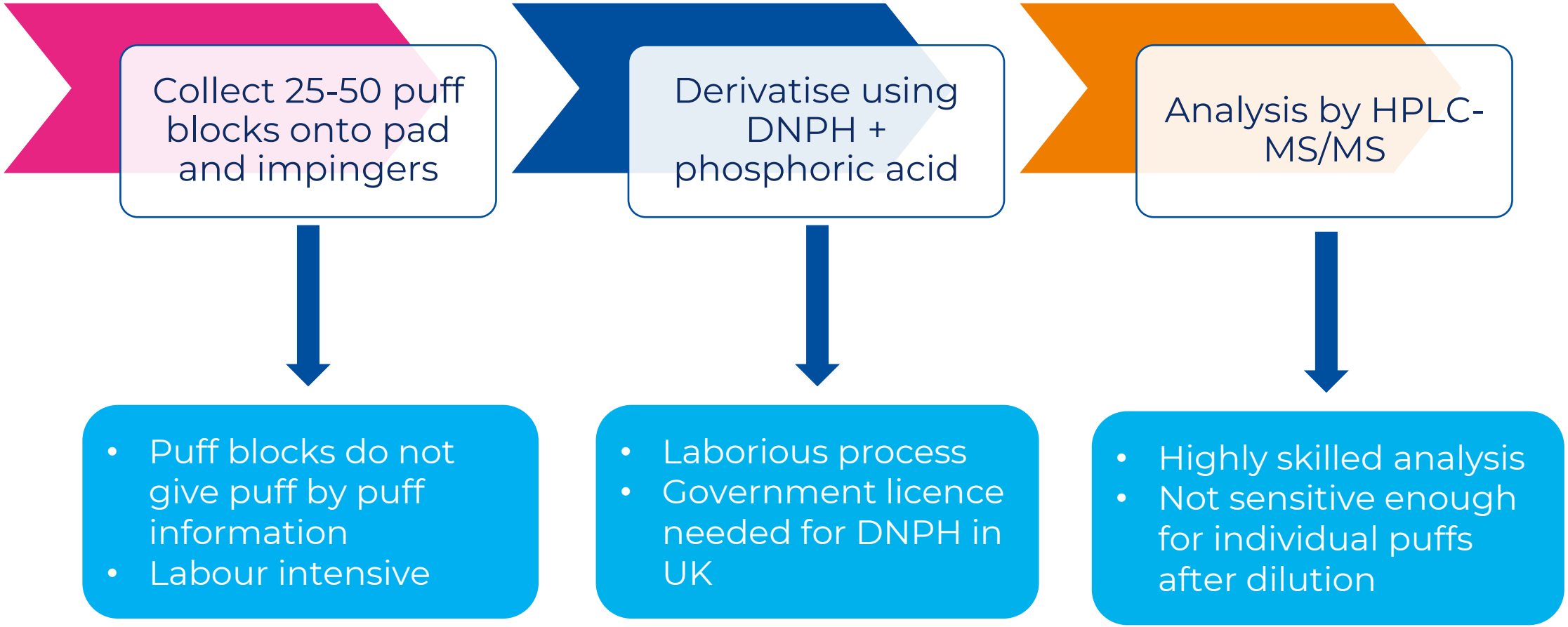


Figure 2[c]

c- Selected Harmful and Potentially Harmful Constituents Levels in Commercial e-Cigarettes , Belushkin, M et al, JO - Chem. Res. Toxicol., 2020, 33,2,657-668

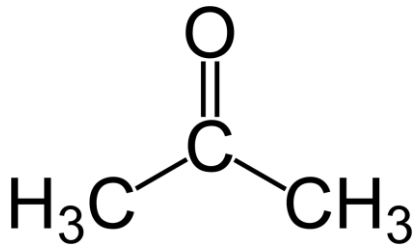
Current methodology

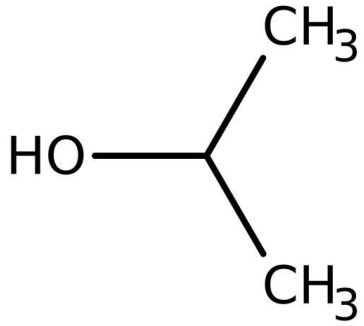


Possible Solution: New technique - SIFT-MS

- Selected Ion Flow Tube Mass Spectrometry (SIFT-MS)
- Direct, instantaneous analysis technique for gases and volatile compounds
- Wide linear range and sub ppb quantification (by volume)
- Ultra soft chemical ionisation providing high sensitivity and selectivity
- Easy to use
- Portable and low maintenance
- No sample preparation

Selectivity: Acetone and Propanal Isomers





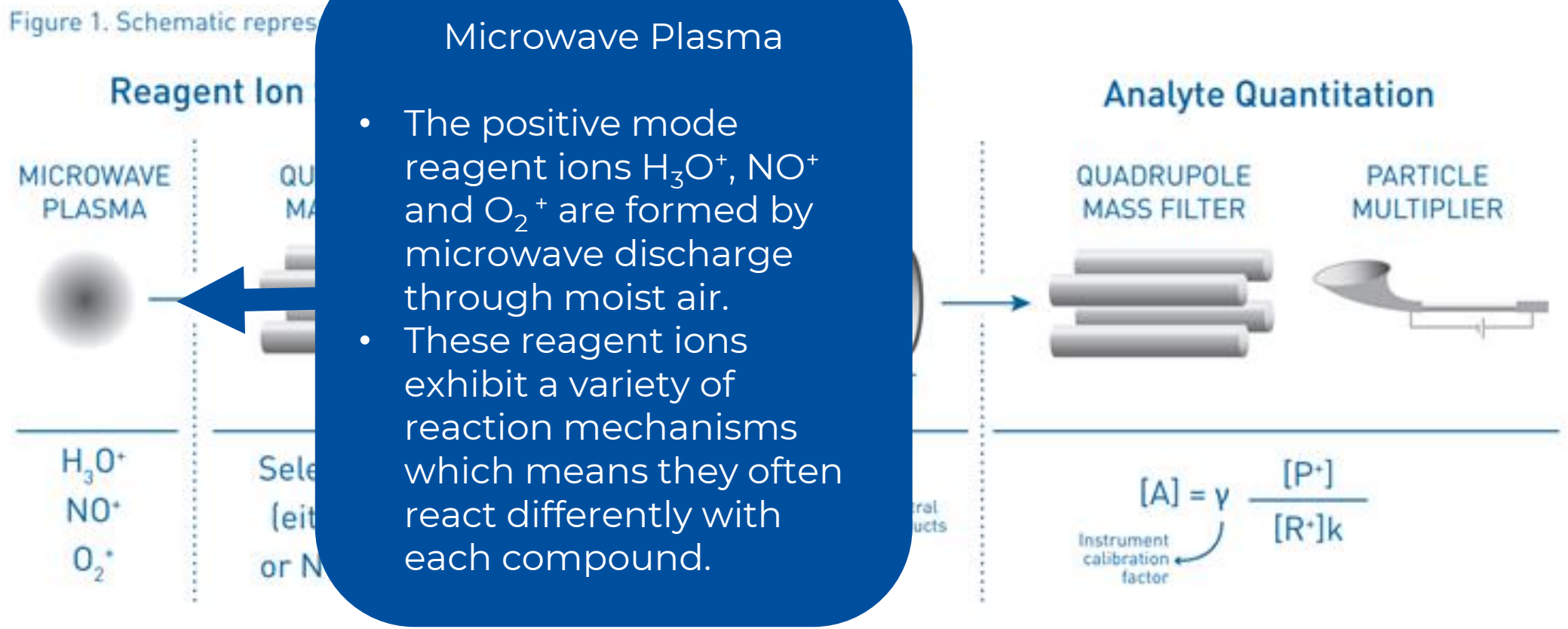
Reagent Ion	Acetone product ion (m/z)	Propanal product ion (m/z)
H_3O^+	$(CH_3)_2COH^+$ (59)	$CH_3CH_2CHOH^+$ (59)
NO^+	$(CH_3)_2CONO^+$ (88)	$CH_3CH_2CO^+$ (57)
O_2^+	$(CH_3)_2CO^+$ (58)	$CH_3CH_2CHO^+$ (58)
	CH_3CO^+ (43)	$CH_3CH_2CO^+$ (57)

SIFT-MS product ions of acetone and propanol

SIFT-MS dominant reaction mechanisms:

- H_3O^+: proton transfer
- NO^+: charge transfer, association, hydride abstraction
- O_2^+: charge transfer, dissociative charge transfer.

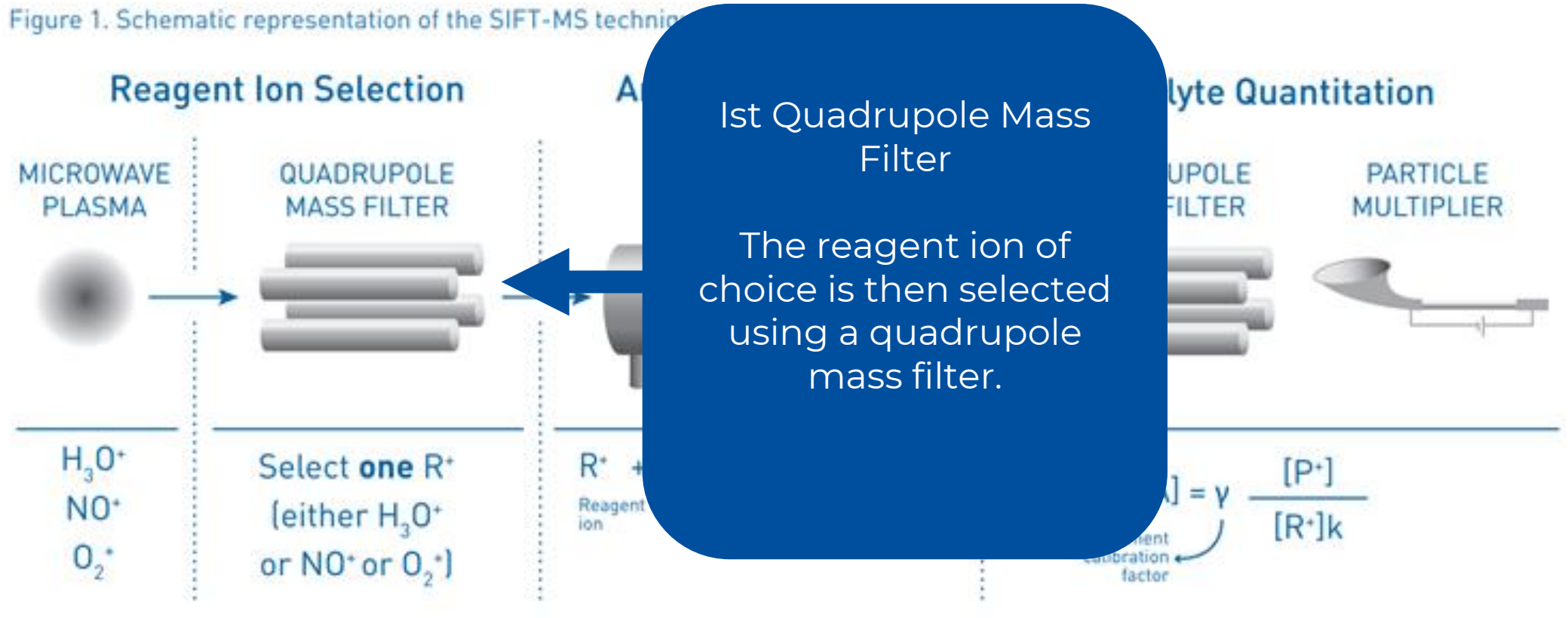
How SIFT-MS Works



Microwave Plasma

- The positive mode reagent ions H_3O^+, NO^+ and O_2^+ are formed by microwave discharge through moist air.
- These reagent ions exhibit a variety of reaction mechanisms which means they often react differently with each compound.

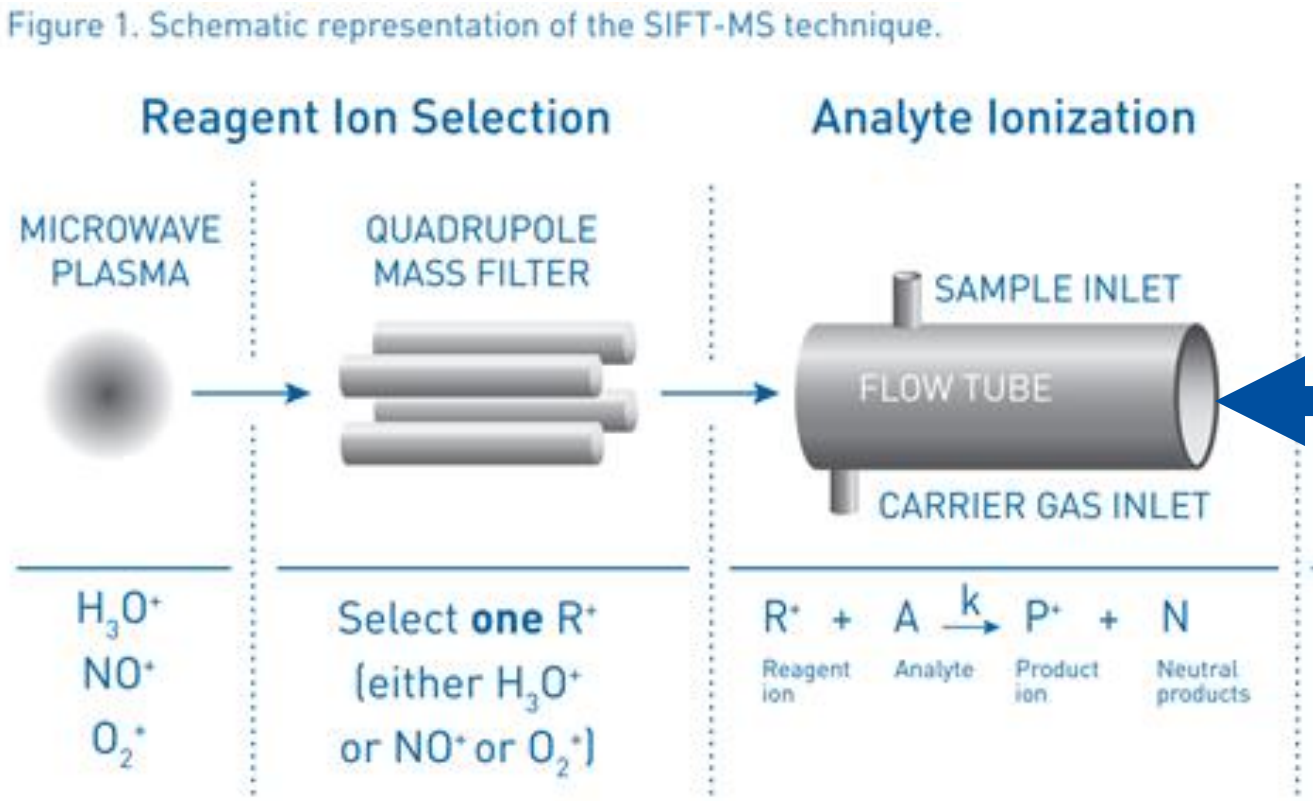
How SIFT-MS Works



Ist Quadrupole Mass Filter

The reagent ion of choice is then selected using a quadrupole mass filter.

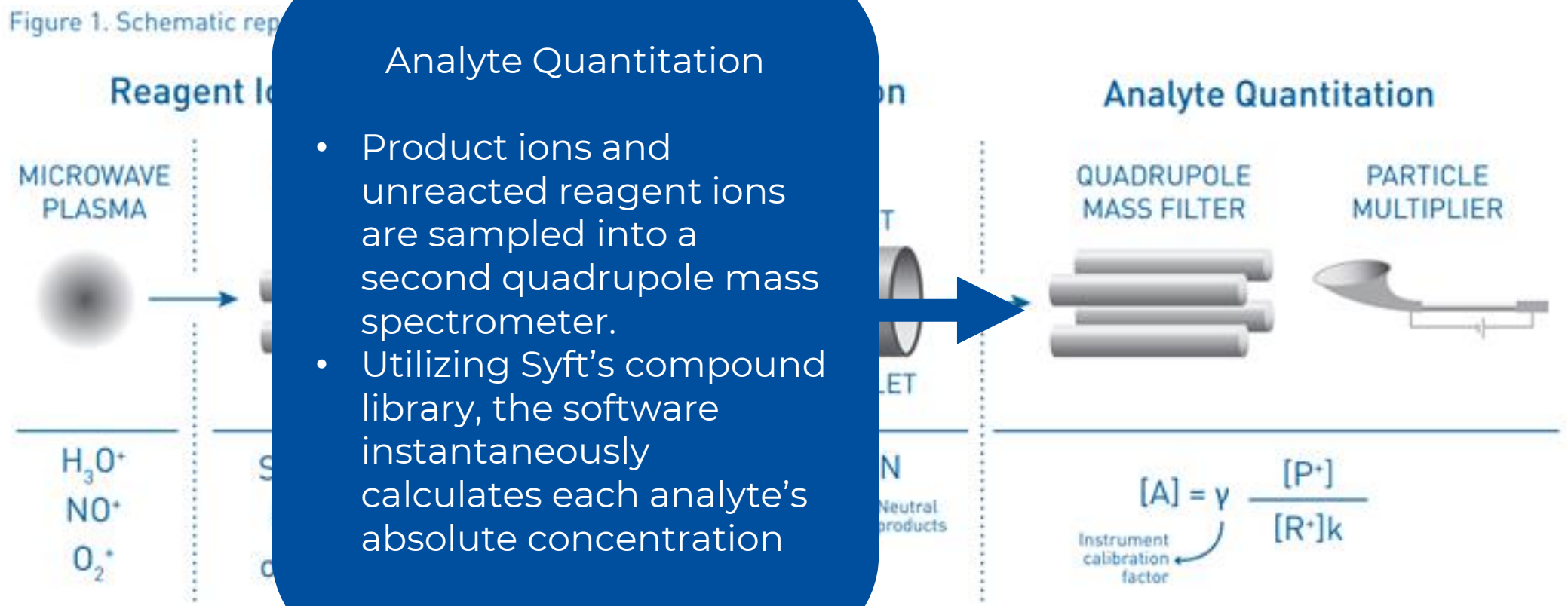
How SIFT-MS Works



Analyte Ionisation

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

How SIFT-MS Works

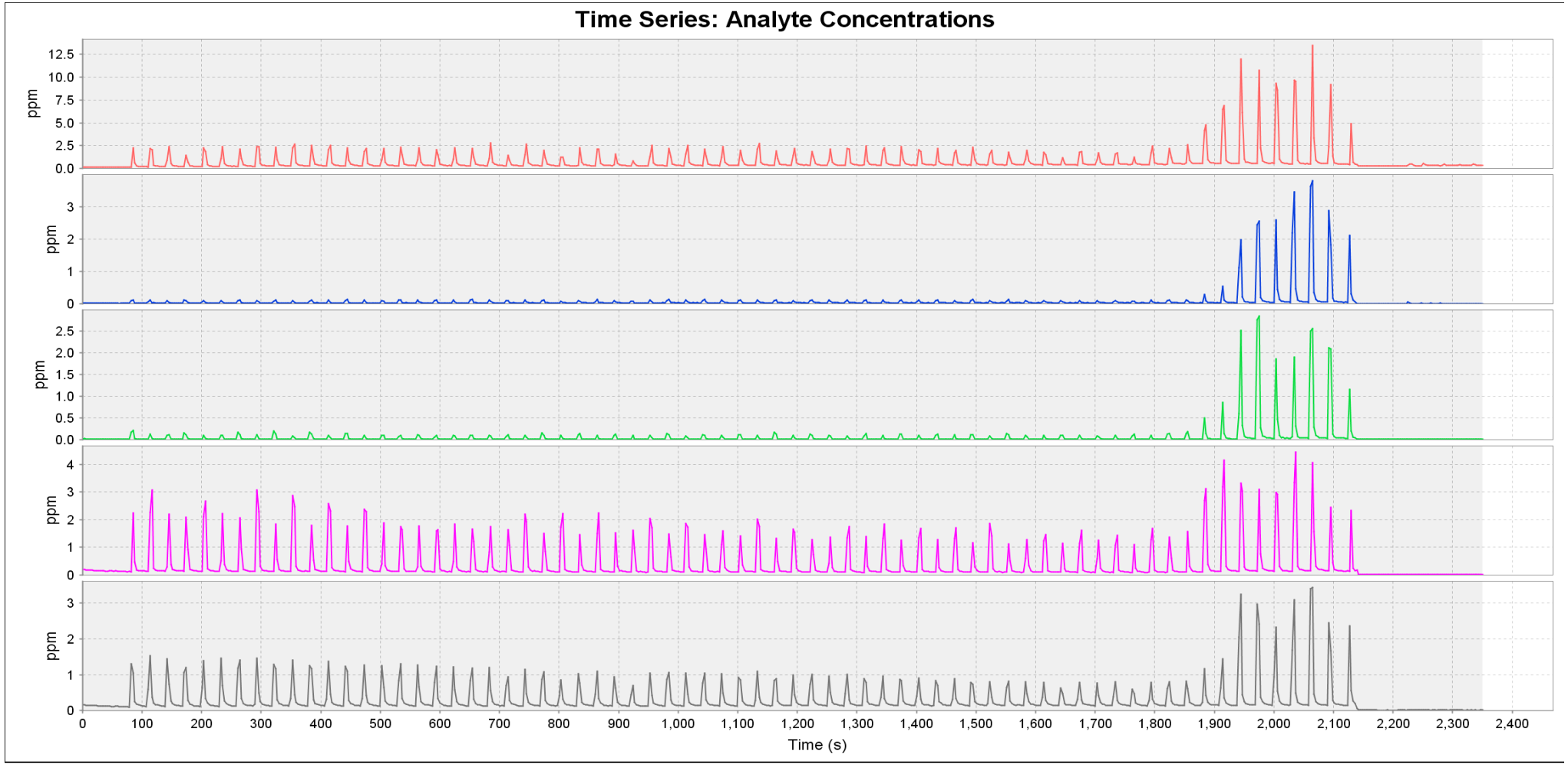


Analyte Quantitation

- 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

www.syft.com

Results for e-Cig device



Acetaldehyde

CH_3CHOH^+

Acetone

$C_3H_6OH^+$

Acrolein

$C_3H_4OH^+$

Formaldehyde

CH_2OH^+

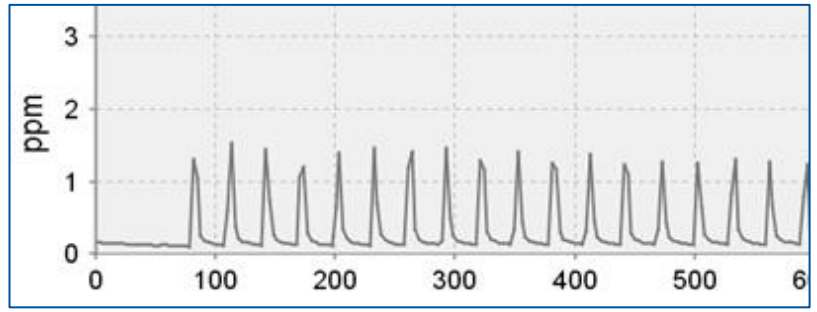
Propanal

$C_2H_5CHOH^+$

400:1 dilution Cirro (12 mg/ml nicotine, 80:20 gly:PG) half filled, puffed to dryness, 60+ puffs

Investigation of test rig to slow down puff

Figure 1 - Concentration Propanal



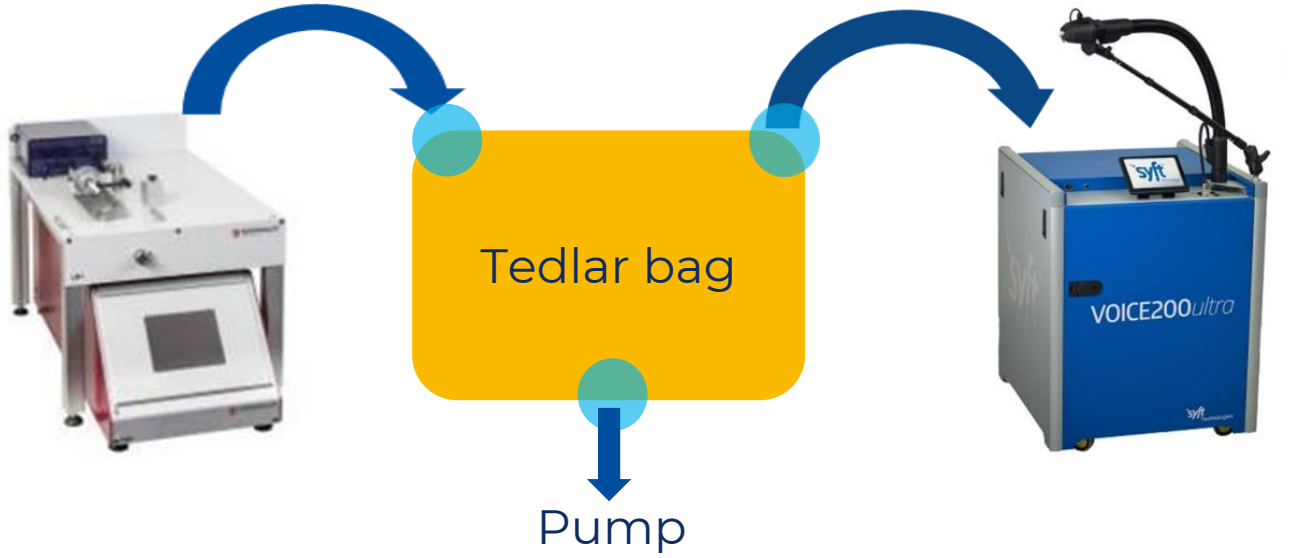
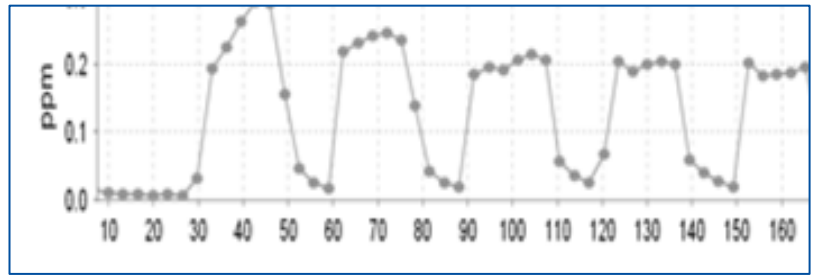


Figure 2 - Concentration Propanal



Connection to PM10 Syringe with Test rig

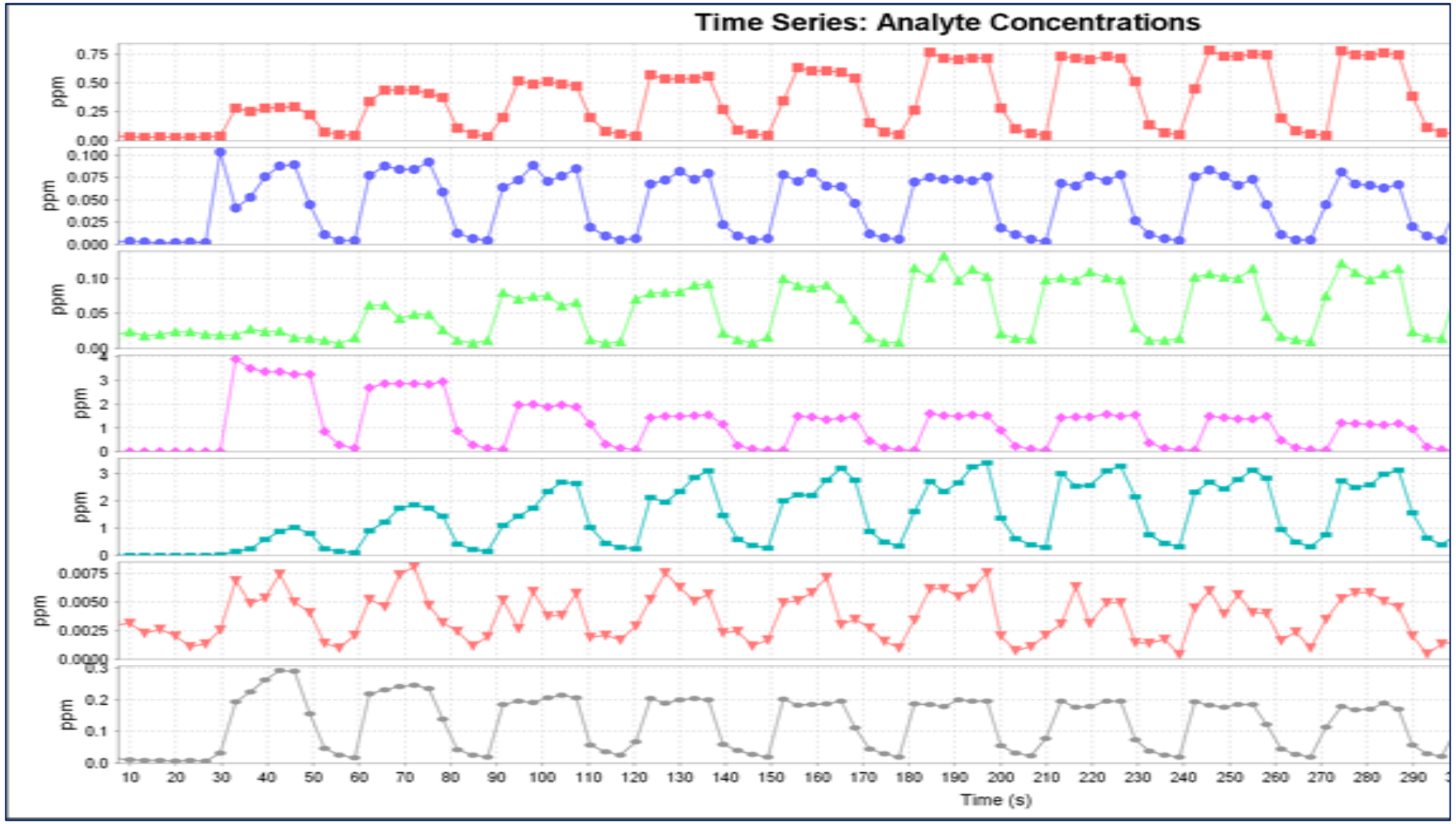
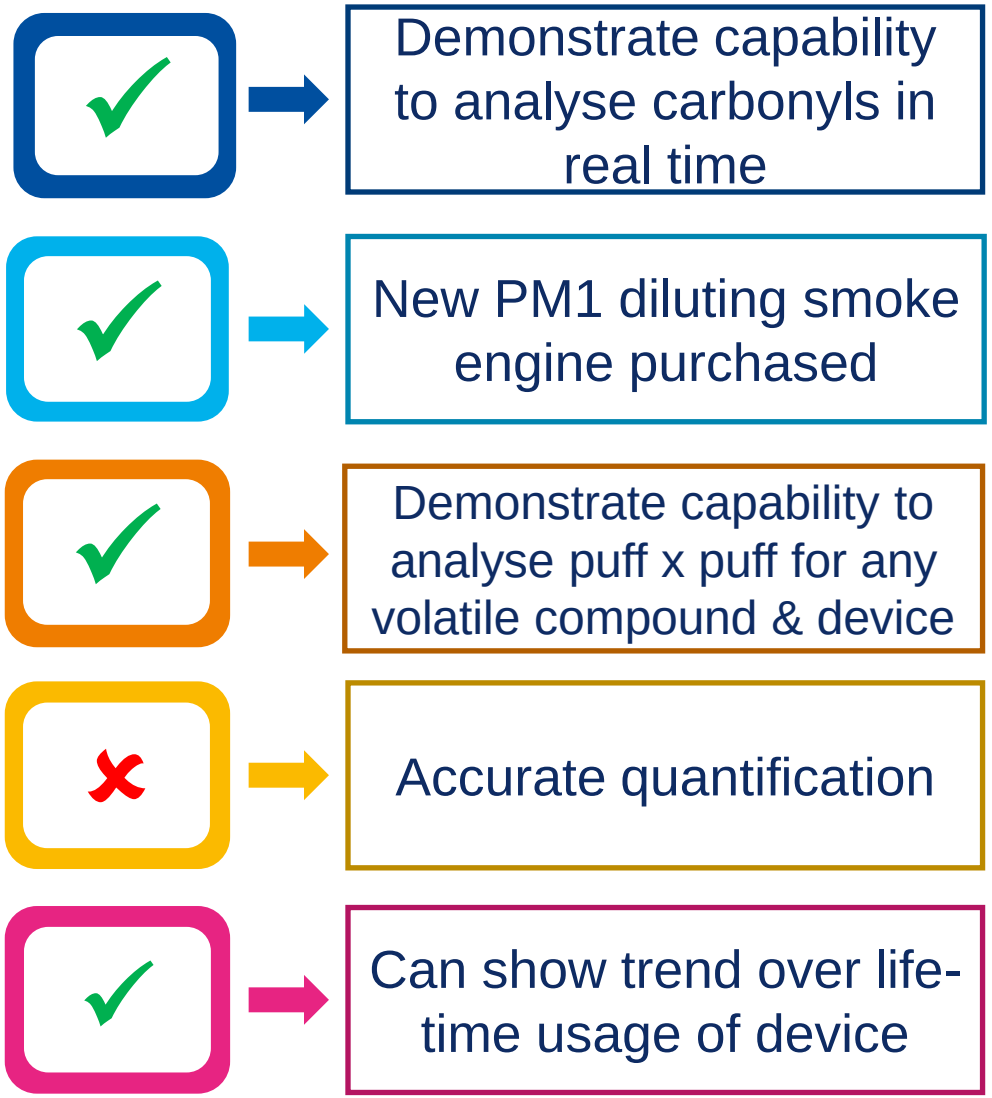


Figure 3 Sampling with PM10 with test rig

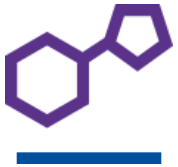
The Story continues...



✓ Demonstrate capability to analyse carbonyls in real time	Dilution is needed. Also need to slow down the puff to provide accurate analysis.
✓ New PM1 diluting smoke engine purchased	Smoke engine has not been validated due to COVID-19 restrictions, planned next step.
✓ Demonstrate capability to analyse puff x puff for any volatile compound & device	Semi-volatile compounds, such as nicotine, may not be suitable. Carryover of some flavours, such as menthol, needs resolving
✗ Accurate quantification	Gas standards required for validation of methods. Investigation into gas permeation tubes
✓ Can show trend over life-time usage of device	Gas standards may not be required for product development.

Summary – Use SIFT-MS for Puff x Puff Analysis

- Real time analysis
- Simple to use
- No sample preparation



- Analysis of wide range of volatiles
- Sub ppb detection

- Direct quantitation

- Connect to smoke engine
- Use for all devices
- Dilution required for e-cigs

- Also use for breath analysis

Thanks for Listening!
Any questions?

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