Comparison of two sample inlet types for exhaled breath acetone determination using portable mass spectrometry

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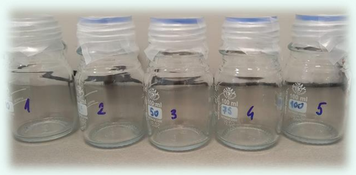
PURPOSE: Growing potential of breath analysis as approachable diagnostic tool initiates scientists from various fields to give their contribution to research and development of analytical methods development and their improvement. This is particularly the case for non-invasive disease diagnostics and personalized nutrition applications. Therefore, this research is focused on the development of a method for determination of food intake effects on levels of specific volatile organic compounds (VOCs) in exhaled human breath.

ACETONE STANDARDS PREPARATION

Preparation technique: Static dilution
Concentration levels (ppb): 10, 25, 50, 75, 100



Acetone calibration gas standards

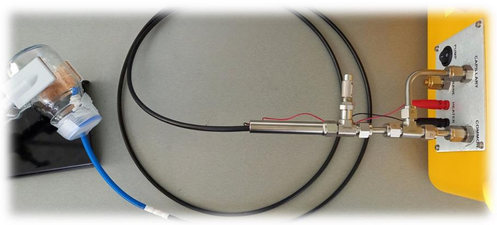
INSTRUMENTATION

Ion source: Electron impact (EI)
Mass analyzer: Single quadrupole (QMS 200)
Mass scan range (m/z): 0-200
System dimensions (LxHxW): 616x220x433mm

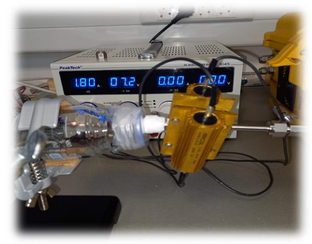
Portable mass spectrometer

EXPERIMENTAL: A choice of a sample inlets type is a crucial step for obtaining optimal sensitivity and resolution with a portable MS. This work compares two types of inlets – a commercially available fused silica capillary probe heated at 120◦C (FSCP) and an in-house made sheet membrane probe with silicone polymer membrane heated at 70◦C (SPM). Acetone gas standards were prepared by static dilution method in concentration range 10-100 ppb (v/v) and analyzed by a portable MS system for characteristic mass fragments (m/z=43 and m/z=58). Inlet performances were compared by observing signal current intensity (A), inlet response time (s) and resolution (FWHM) for a range of concentration levels.

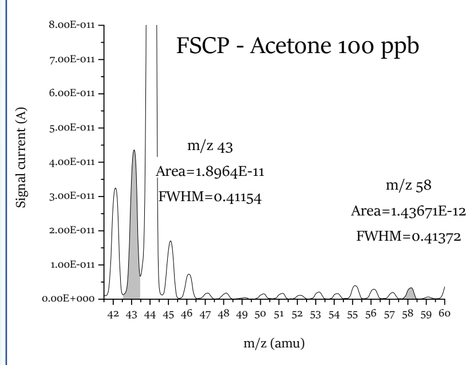
ACETONE GAS STANDARDS SAMPLING BY TWO INLET TYPES



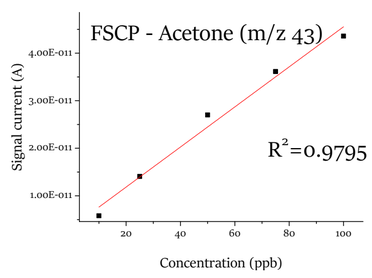
Fused silica capillary probe (FSCP)

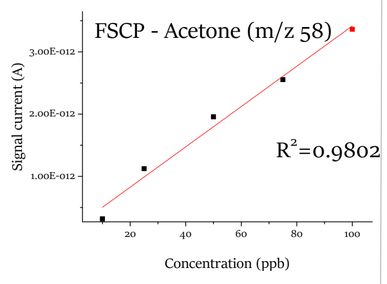


Sheet membrane probe (SMP)

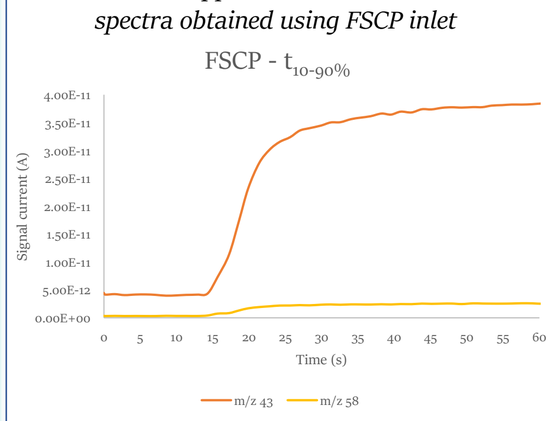


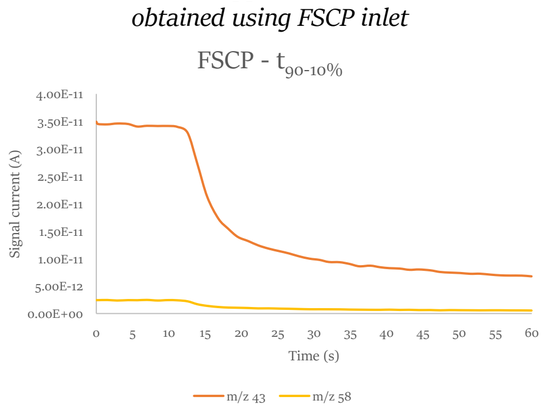
Acetone 100 ppb calibration level mass spectra obtained using FSCP inlet



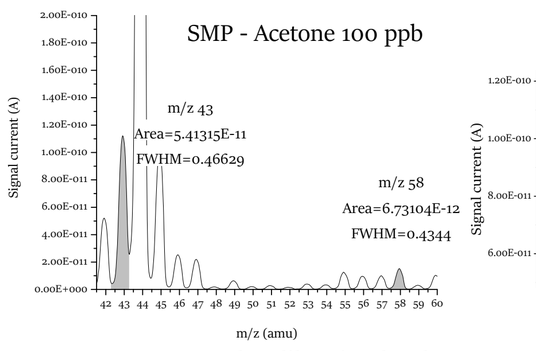


Acetone 10-100 ppb calibration curves obtained using FSCP inlet

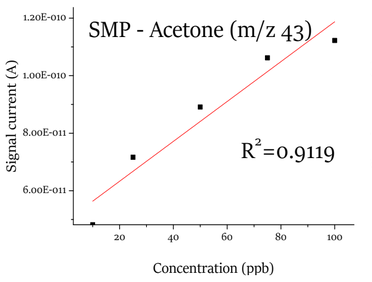


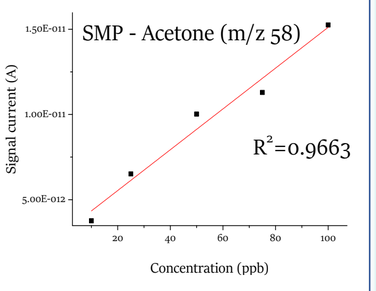


Acetone 100 ppb calibration level rise and fall response times obtained using FSCP inlet

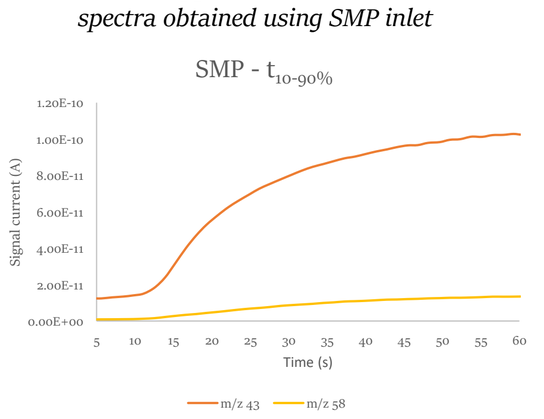


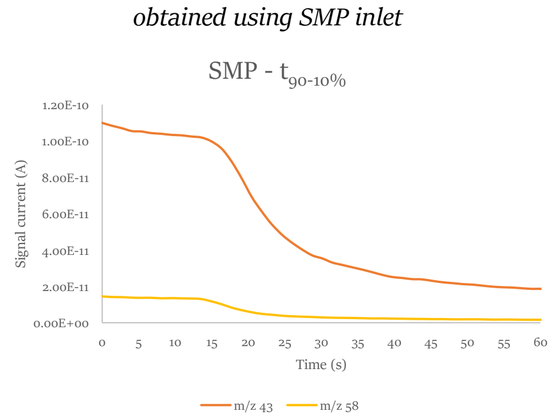
Acetone 100 ppb calibration level mass spectra obtained using SMP inlet





Acetone 10-100 ppb calibration curves obtained using SMP inlet





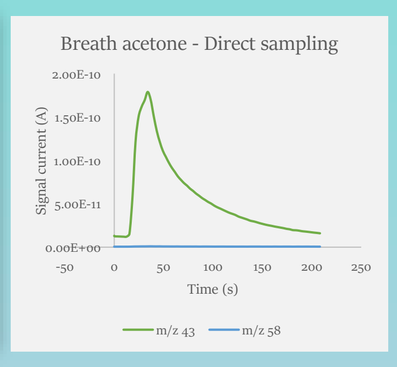
Acetone 100 ppb calibration level rise and fall response times obtained using SMP inlet

RESULTS:	Signal intensity (A)				Resolution (FWHM)				Rise time - $t_{10\text{-}90\%}$ (s)		Fall time - $t_{90\text{-}10\%}$ (s)	
Concentration	FSCP	SMP	FSCP	SMP	FSCP	SMP	FSCP	SMP	FSCP	SMP	FSCP	SMP
(ppb)	m/z 43		m/z 58		m/z 43		m/z 58		m/z 43		m/z 43	
10 ppb	5.80E-12	4.82E-11	3.17E-13	3.76E-12	0.6224	0.4791	0.4211	0.4419	20	29	25	25
25 ppb	1.41E-11	7.16E-11	1.12E-12	6.51E-12	0.4316	0.4681	0.3769	0.4516	18	47	21	71
50 ppb	2.70E-11	8.91E-11	1.96E-12	1.00E-11	0.4061	0.4679	0.4274	0.4511	17	17	17	17
75 ppb	3.61E-11	1.06E-10	2.55E-12	1.13E-11	0.4068	0.4686	0.4293	0.4689	15	15	18	18
100 ppb	4.36E-11	1.12E-10	3.36E-12	1.53E-11	0.4115	0.4663	0.4137	0.4344	19	19	34	34
					0.46	**0.47**	**0.41**	**0.45**	**18**	**25**	**23**	**33**

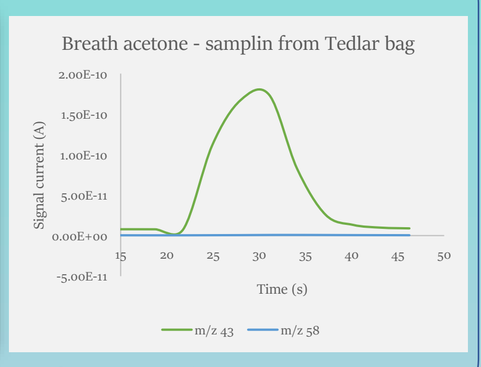
CONCLUSION: Results obtained indicate that SPM inlet type provides better sensitivity, while FSCP shows better response times. Considering that breath VOCs are present at ppb levels, greater sensitivity is always a desirable property. Therefore, SPM is chosen for our future research.

BREATH SAMPLING USING SHEET MEMBRANE PROBE

Direct breath sampling



Breath sampling from Tedlar bag



FUTURE RESEARCH:

Many breath VOCs which are related to digestion are structurally similar and produce common mass fragments (e.g. m/z 43 for acetone and isopropanol).
In order to enable diet impact determination and detection of these specific VOCs in one run, our main goal is to develop an in-house temperature-programmed desorption (TPD) system for separation of VOCs of interest.

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