

High-throughput soil and water contamination testing with automated SIFT-MS

PRESENTED BY

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Presentation outline

Approaches to soil and water analysis

Introduction to SIFT-MS

Water and soil testing with SIFT-MS

New possibilities; TD-SIFT-MS for purge and trap delivery



Soil and water contamination

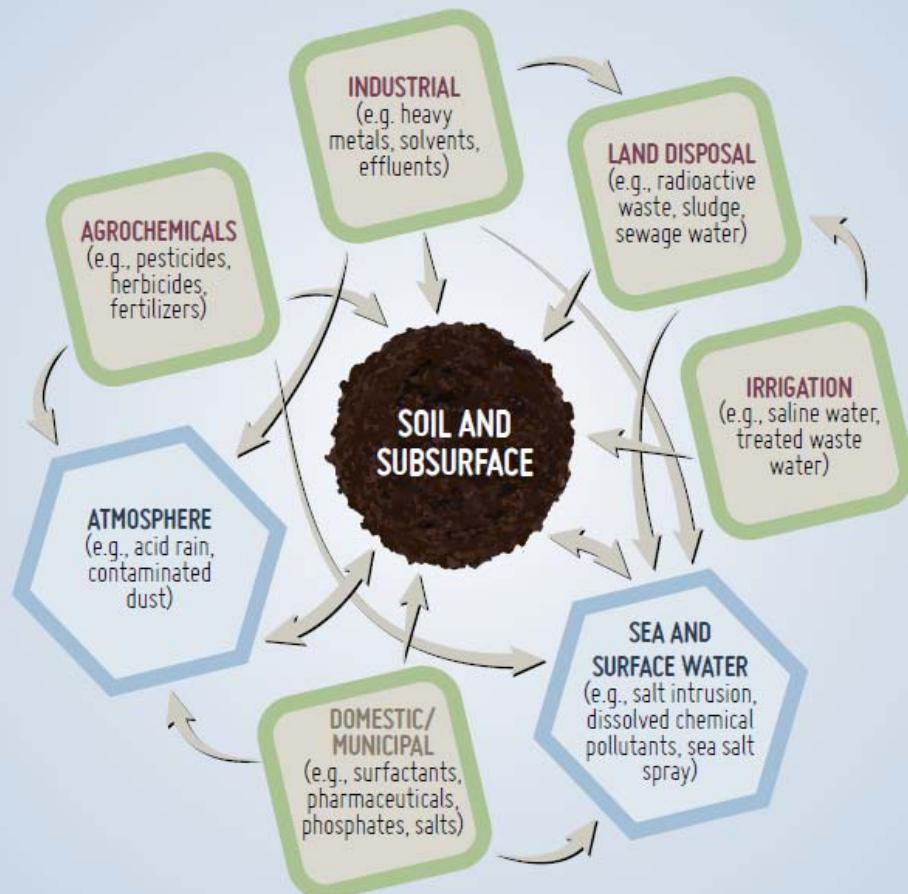


Image: Yaron, Dror and Berkowitz, 2012

VOC monitoring for soil and water



EPA 5035A (Soil), EPA 524.2 (surface water, ground water, drinking water), EPA 624 (wastewater)

Purge and trap methodology coupled with measurement by GC



54 commonly analyzed VOCs – BTEX, halogenates, oxygenates

Direct headspace approaches developed for improved throughput and screening

Approaches to soil and water testing

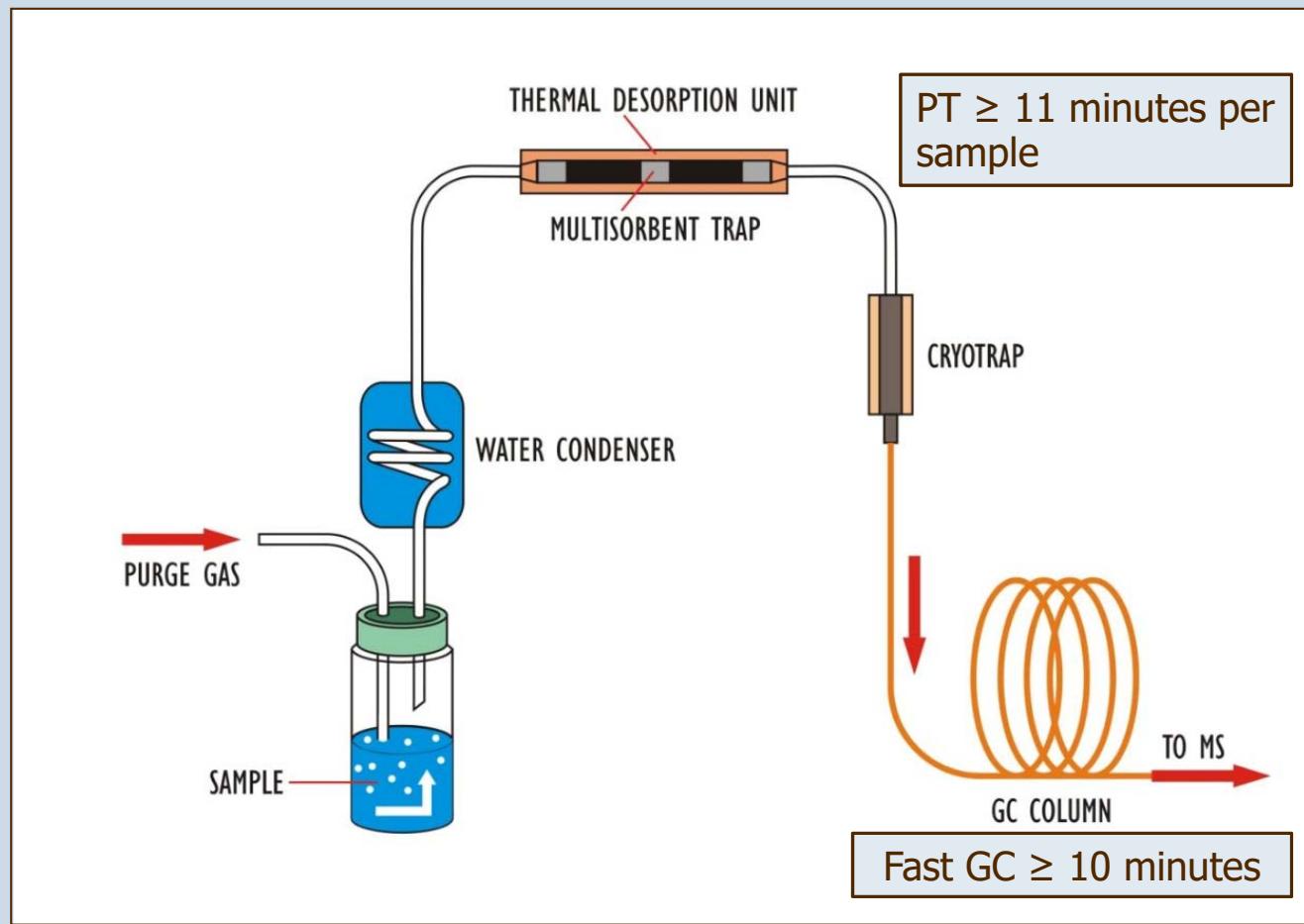


Image: Schmidt et al. Journal of Biomarkers 2015



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Approaches to soil and water testing

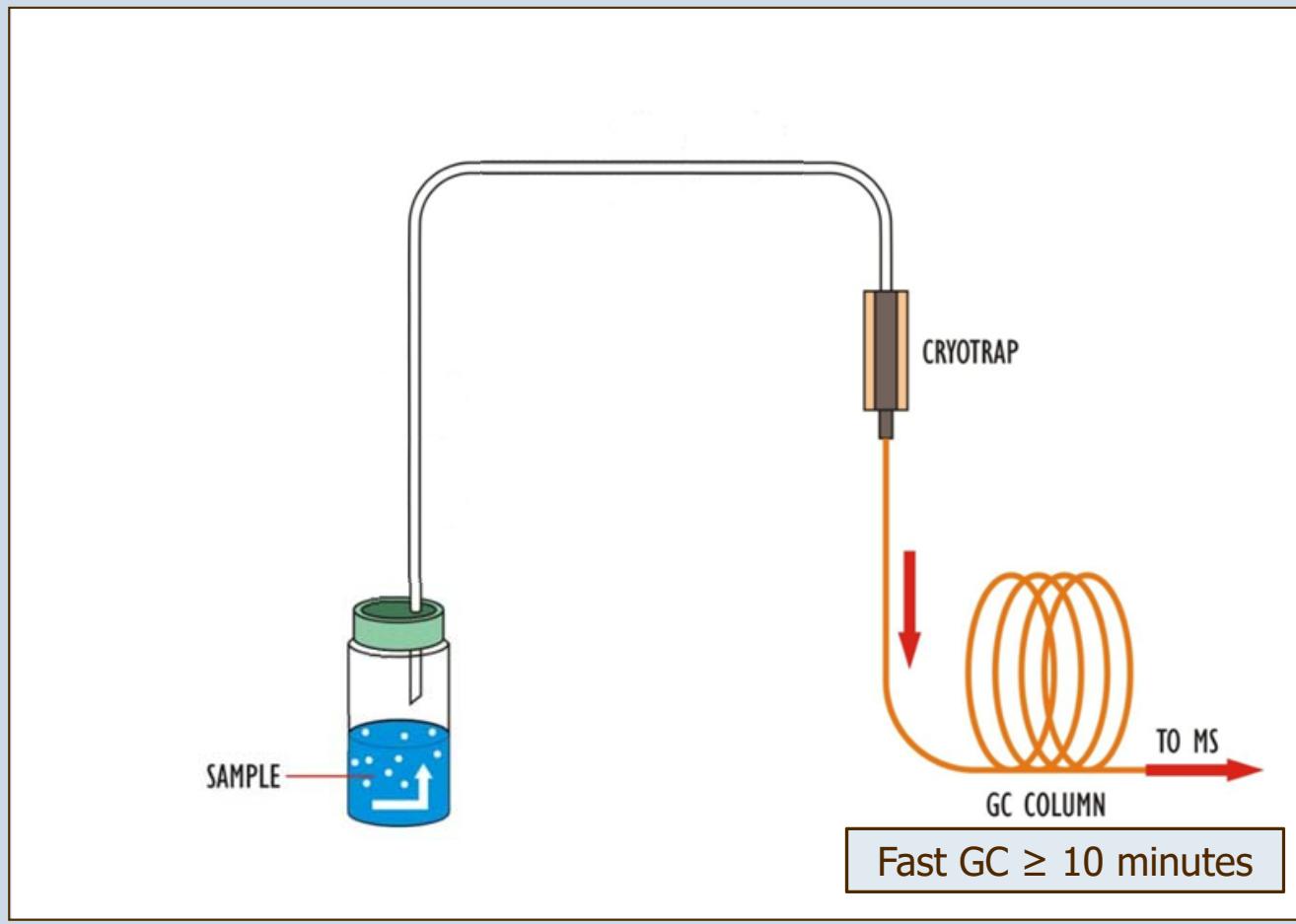


Image: Schmidt et al. Journal of Biomarkers 2015

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Approaches to soil and water testing

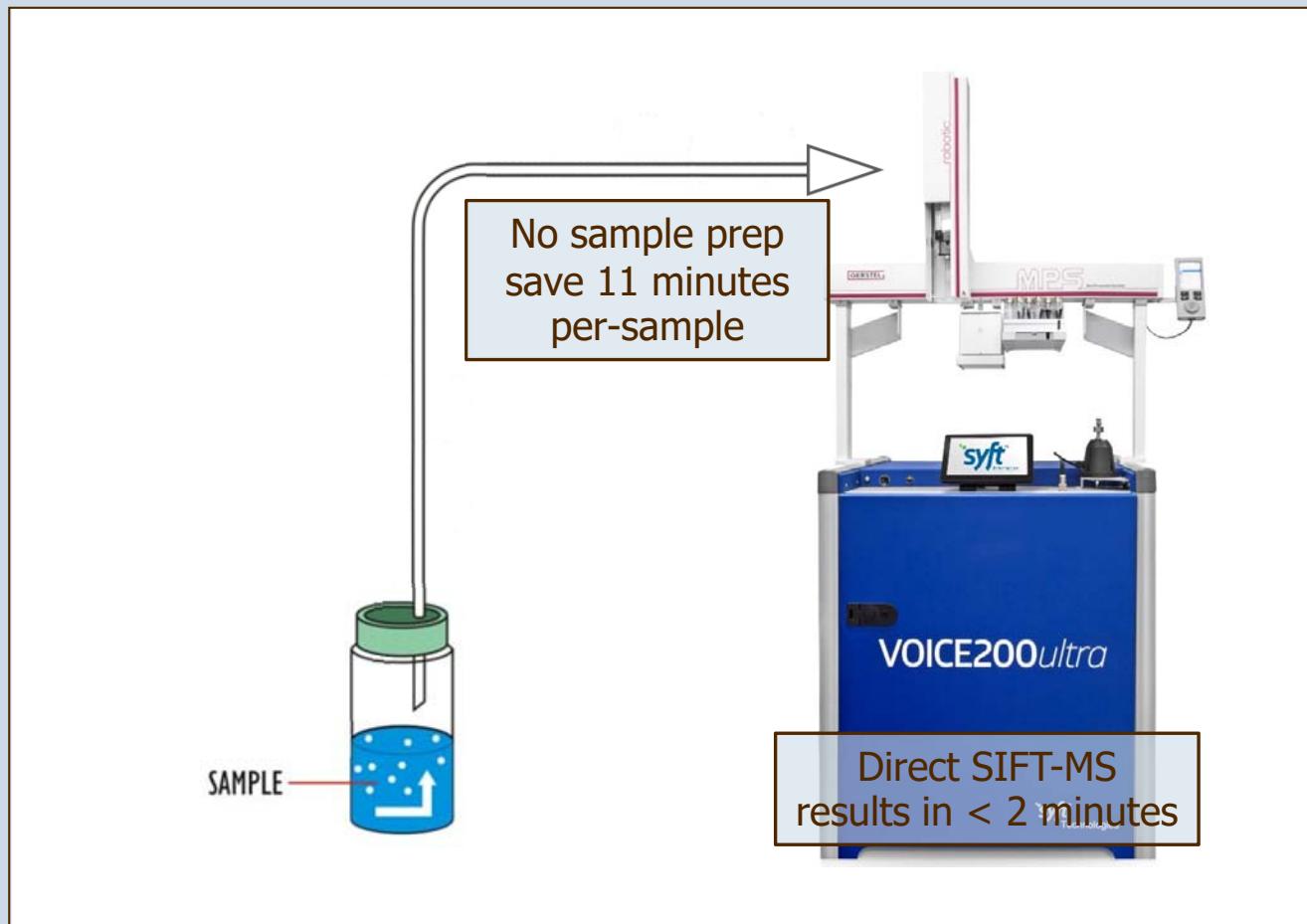


Image: Schmidt et al. Journal of Biomarkers 2015

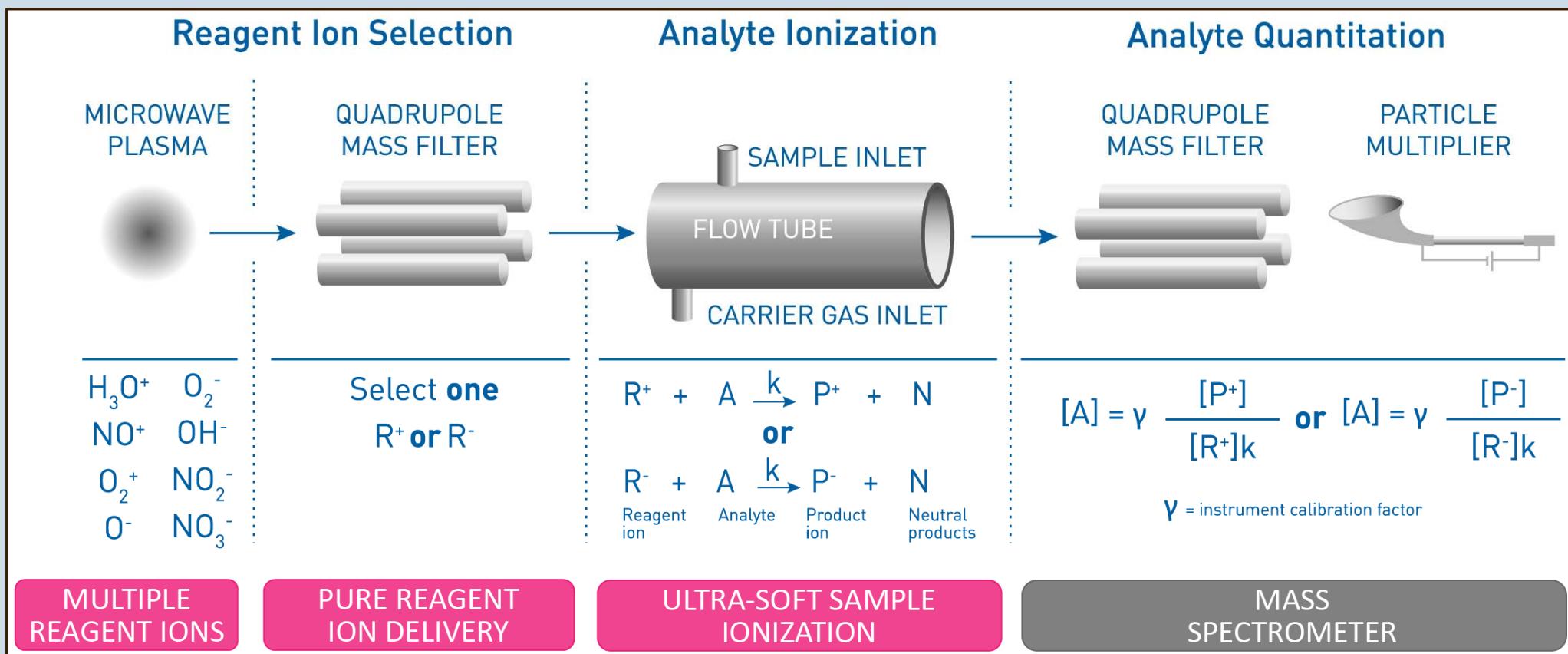


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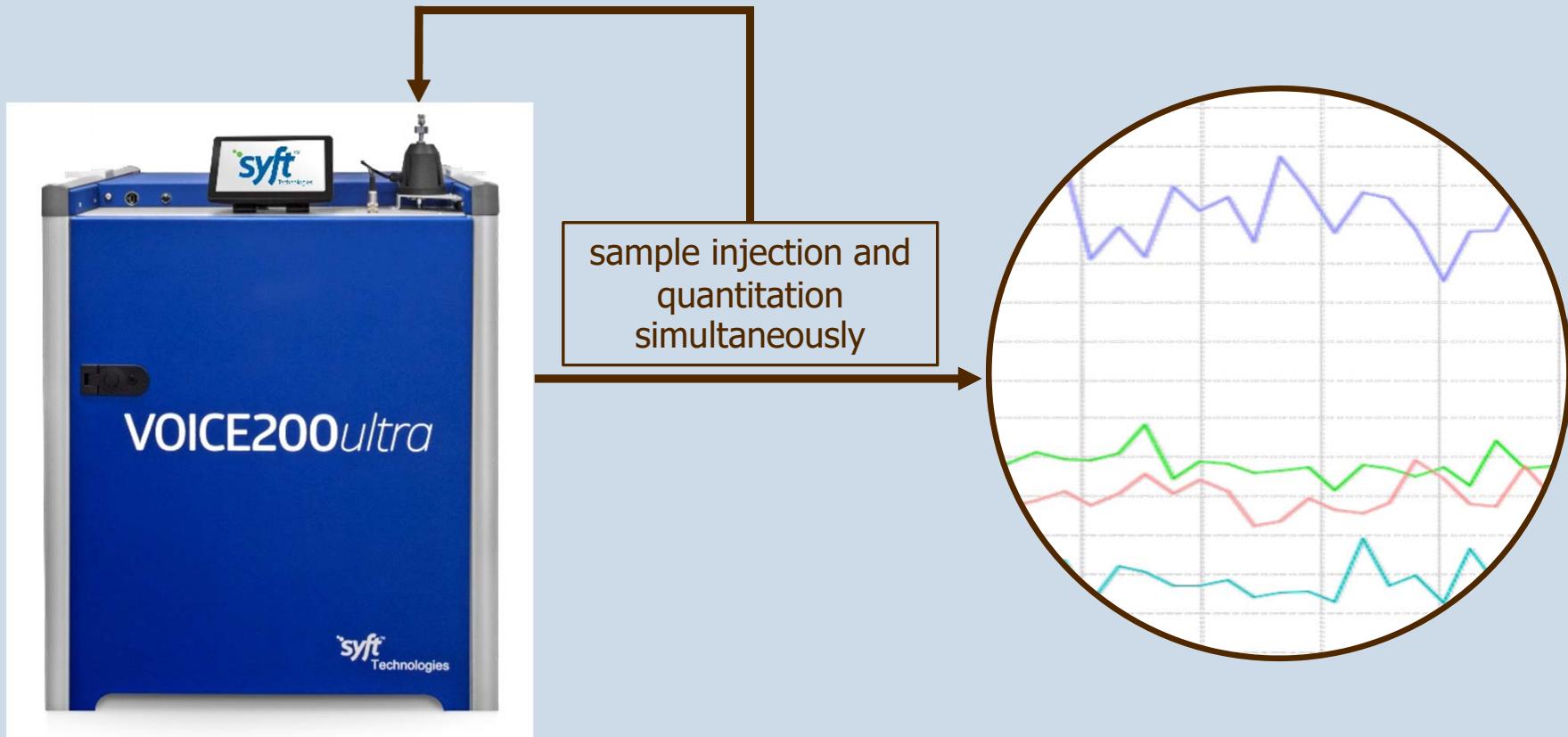
SIFT-MS; the science of speed and selectivity



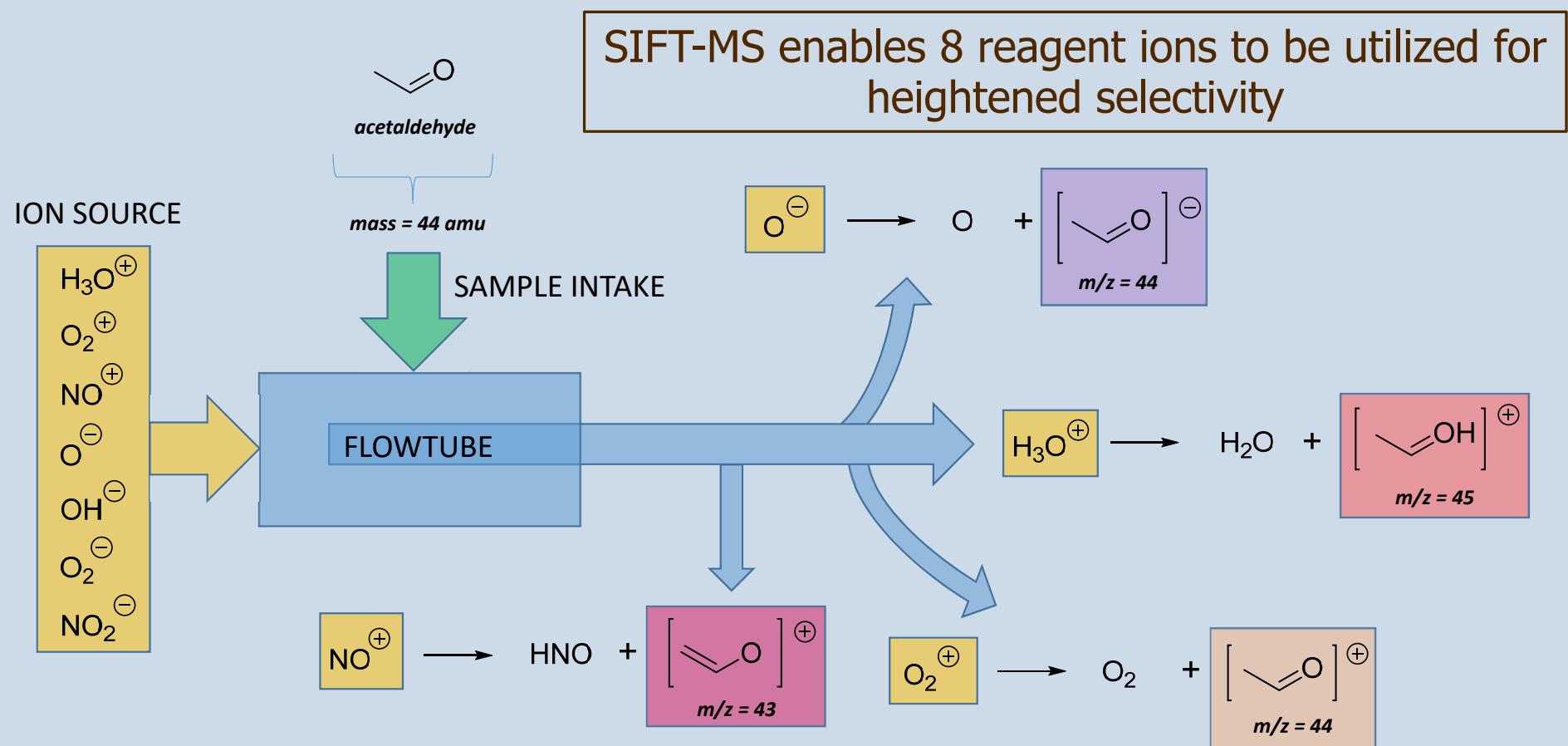
Selected Ion Flow-Tube Mass Spectrometry (SIFT-MS)



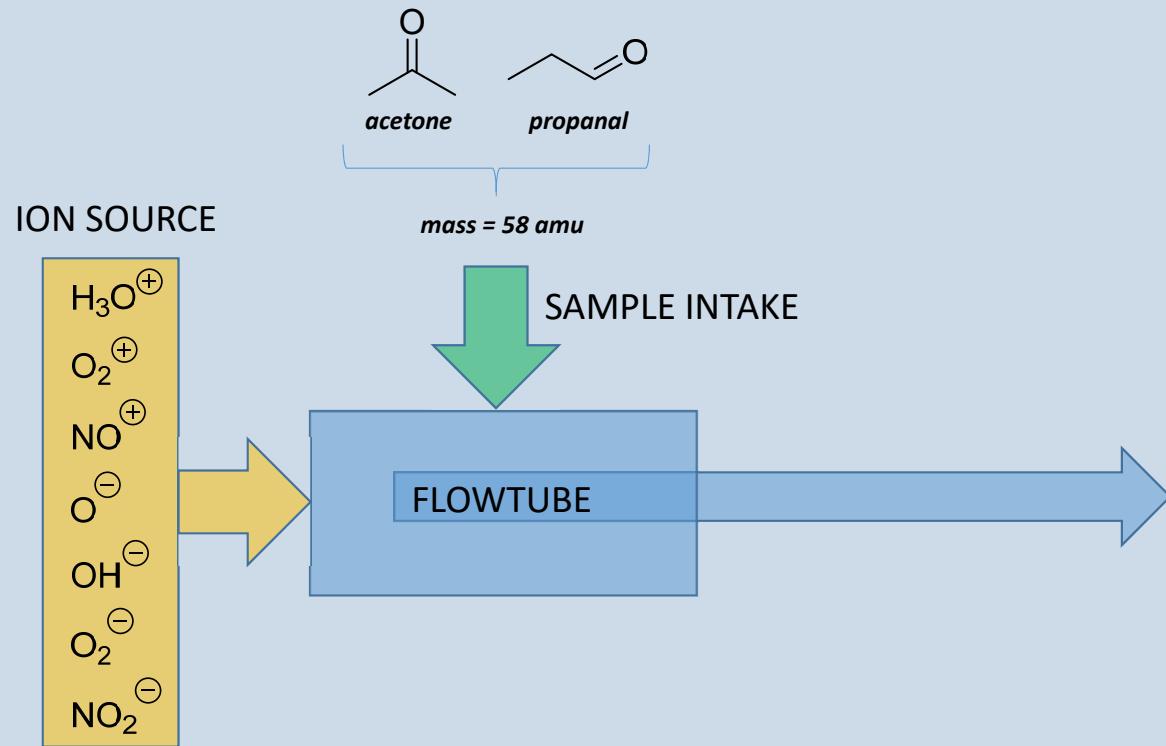
Direct MS for rapid analysis



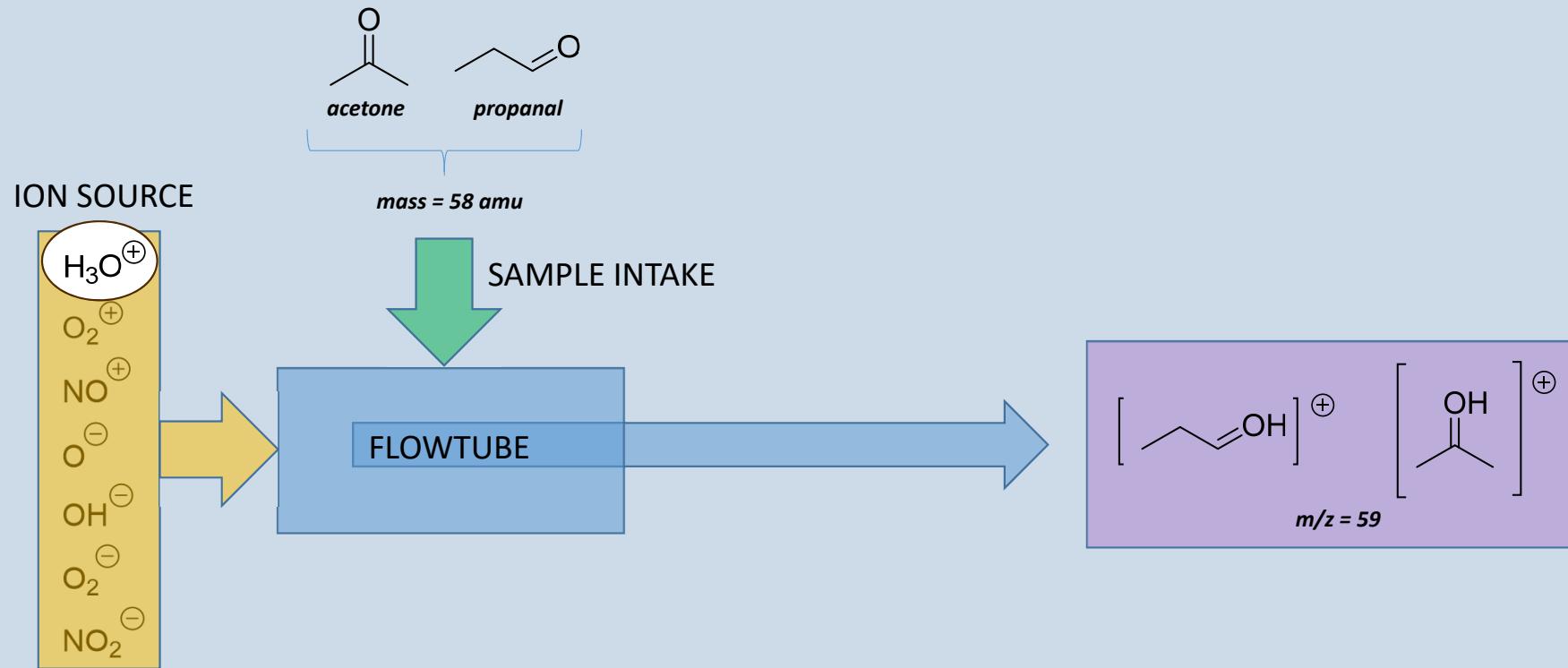
Ion-chemistry and mass spectrometry



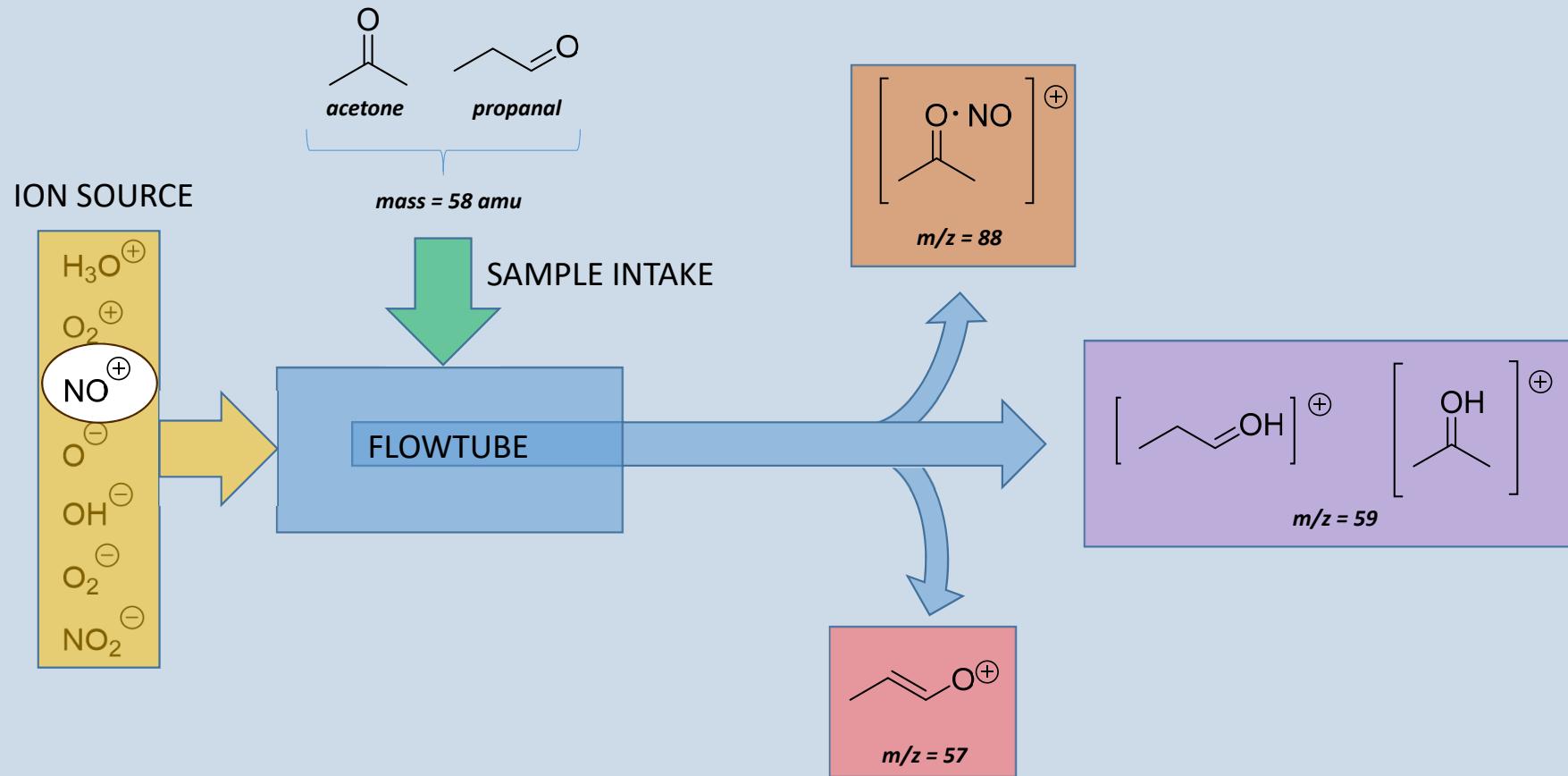
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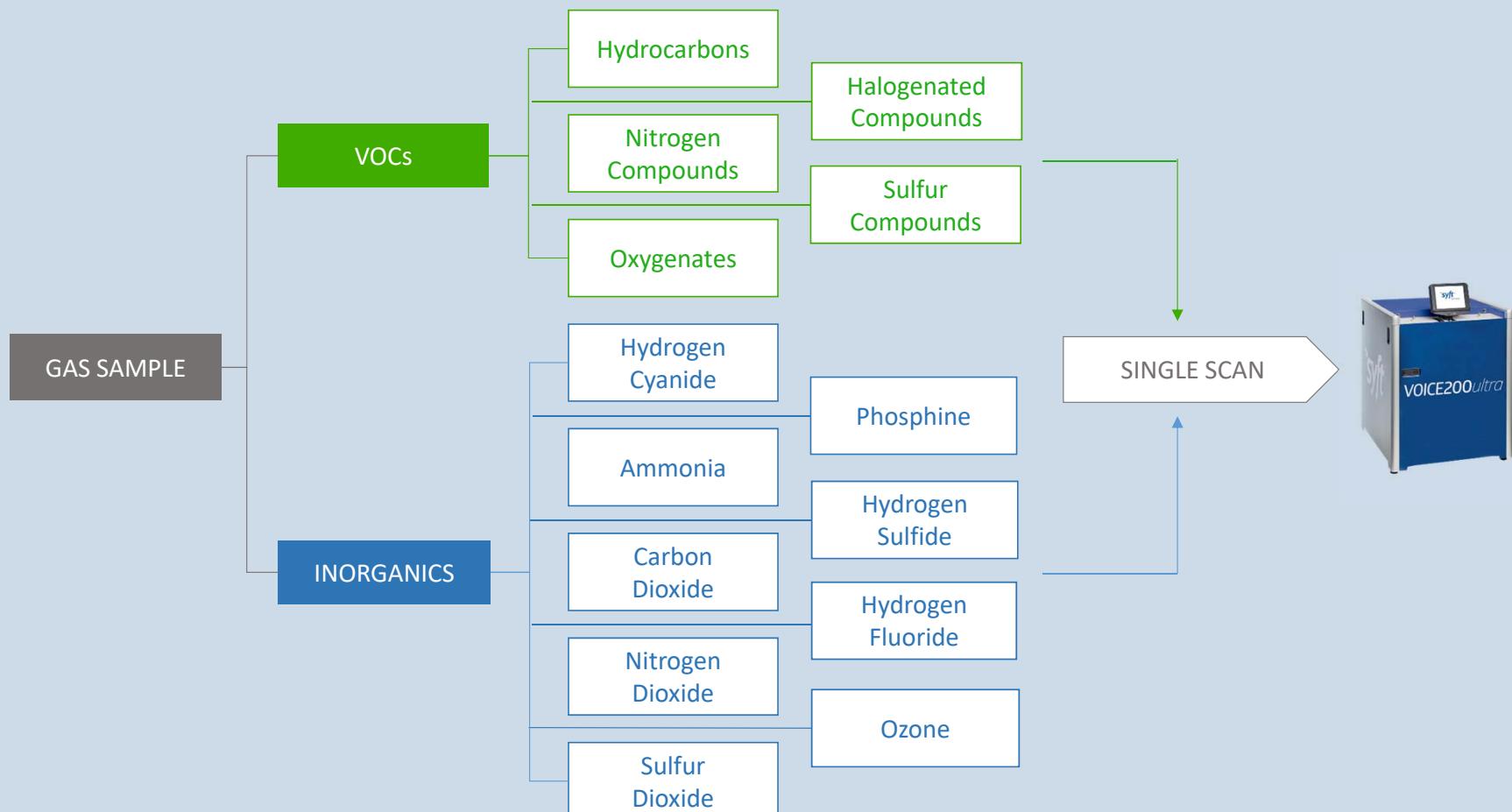
Ion-chemistry and mass spectrometry



Ion-chemistry and mass spectrometry



Analysis of diverse chemical targets



Throughput optimization with automated SIFT-MS



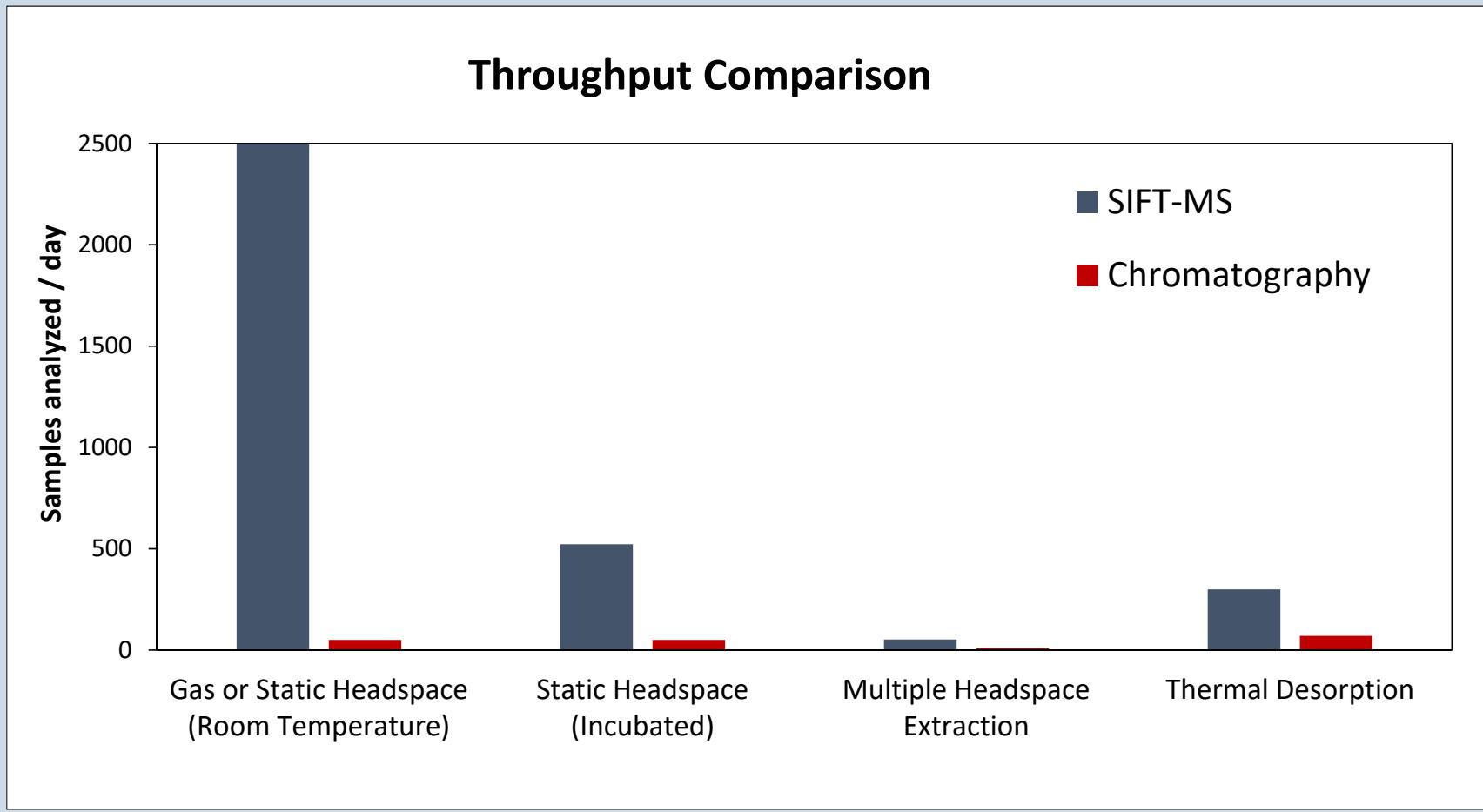
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Throughput optimization of SIFT-MS



Throughput optimization of SIFT-MS



VOC monitoring for soil and water



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Purge and trap methodology coupled with measurement by GC



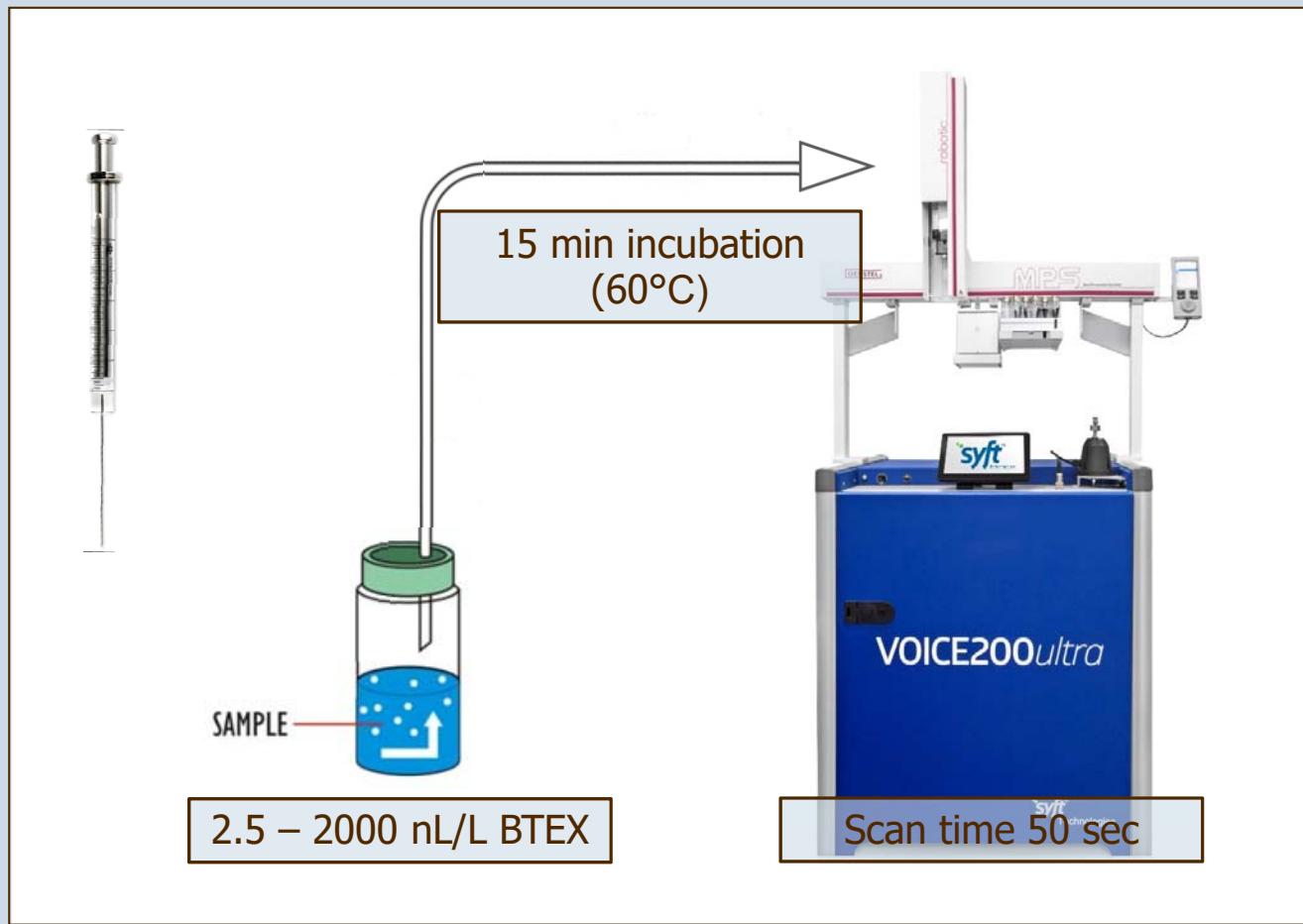
54 commonly analyzed VOCs – BTEX, halogenates, oxygenates

Direct headspace approaches developed for improved throughput and screening

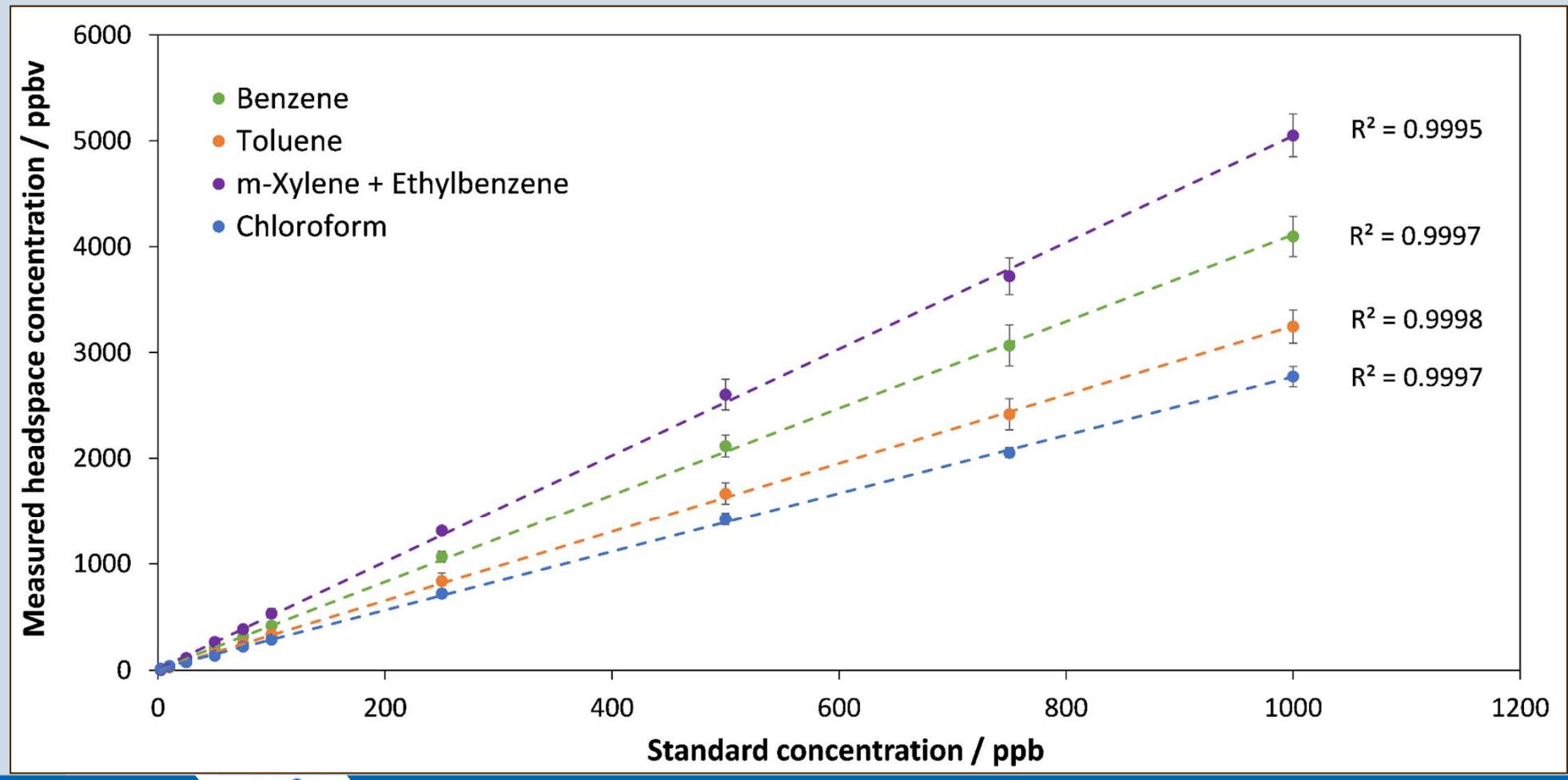
Automated water analysis using SIFT-MS



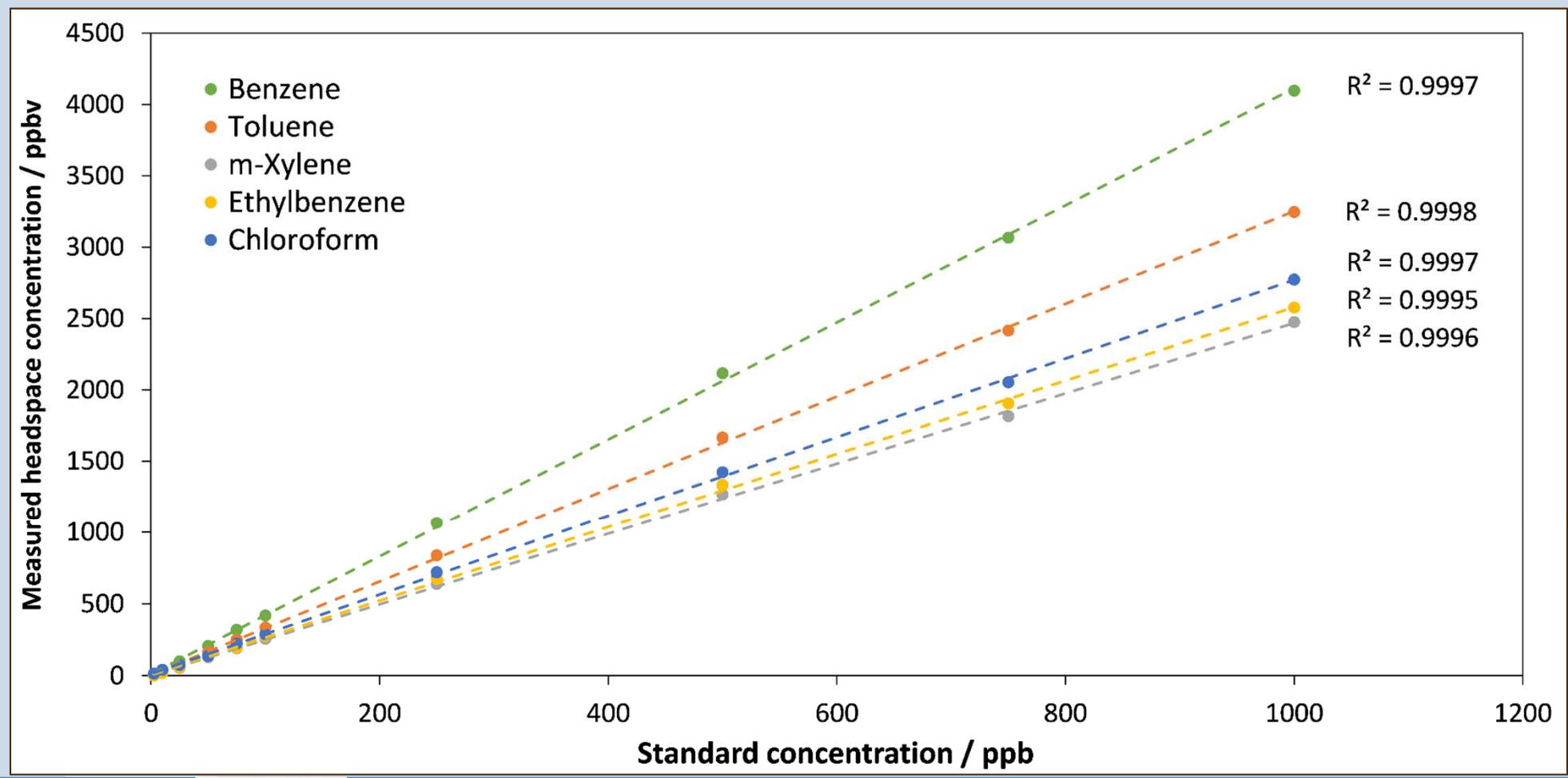
SIFT-MS water testing method validation



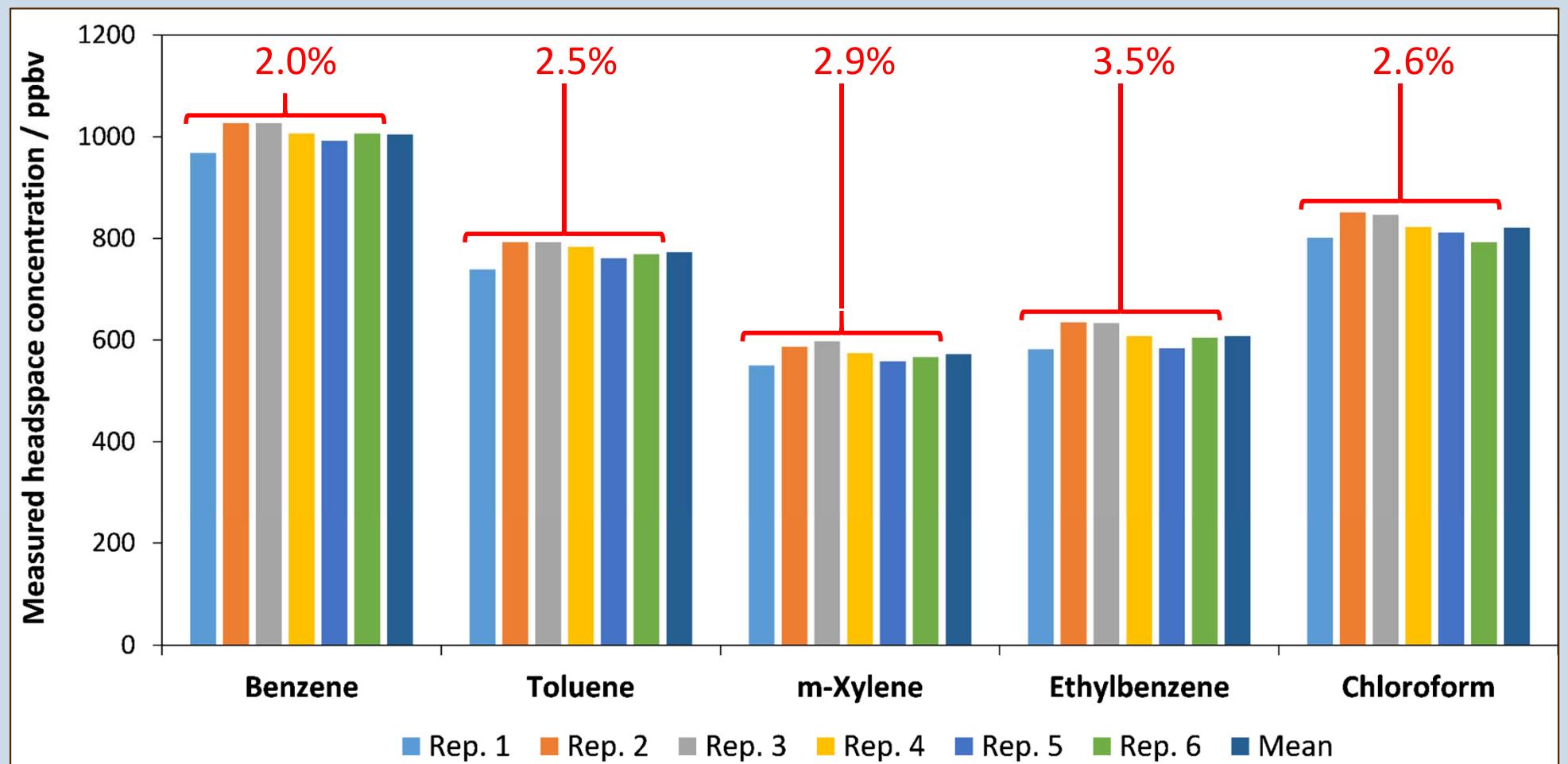
SIFT-MS water testing method validation



SIFT-MS water testing method validation



Repeatability



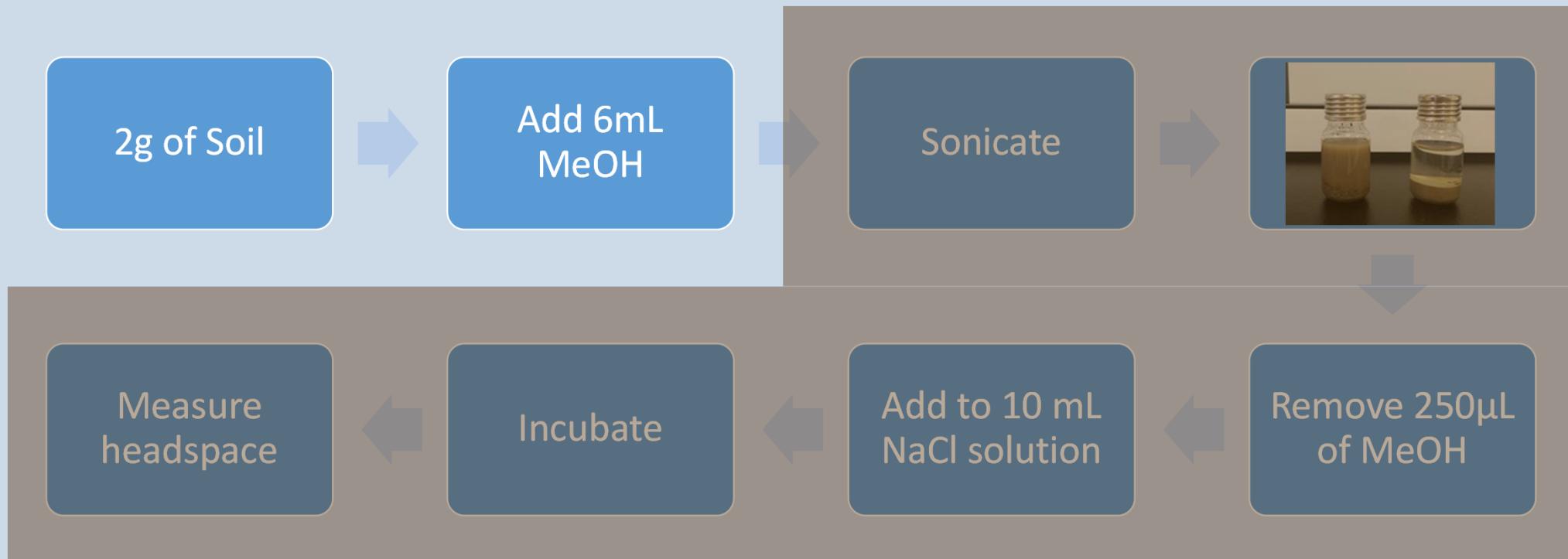
Repeatability

Parameter	Benzene	Toluene	m-Xylene	Ethylbenzene	Chloroform
Rep 1 / ppbv	968	739	550	582	802
Rep 2 / ppbv	1026	793	587	638	851
Rep 3 / ppbv	1026	793	598	634	847
Rep 4 / ppbv	1006	783	574	607	823
Rep 5 / ppbv	992	761	558	584	812
Rep 6 / ppbv	1006	767	567	605	793
Mean / ppbv	1004	773	572	608	821
SD / ppbv	20.1	19.2	16.4	21.1	21.6
% RSD	2.0	2.5	2.9	3.5	2.6

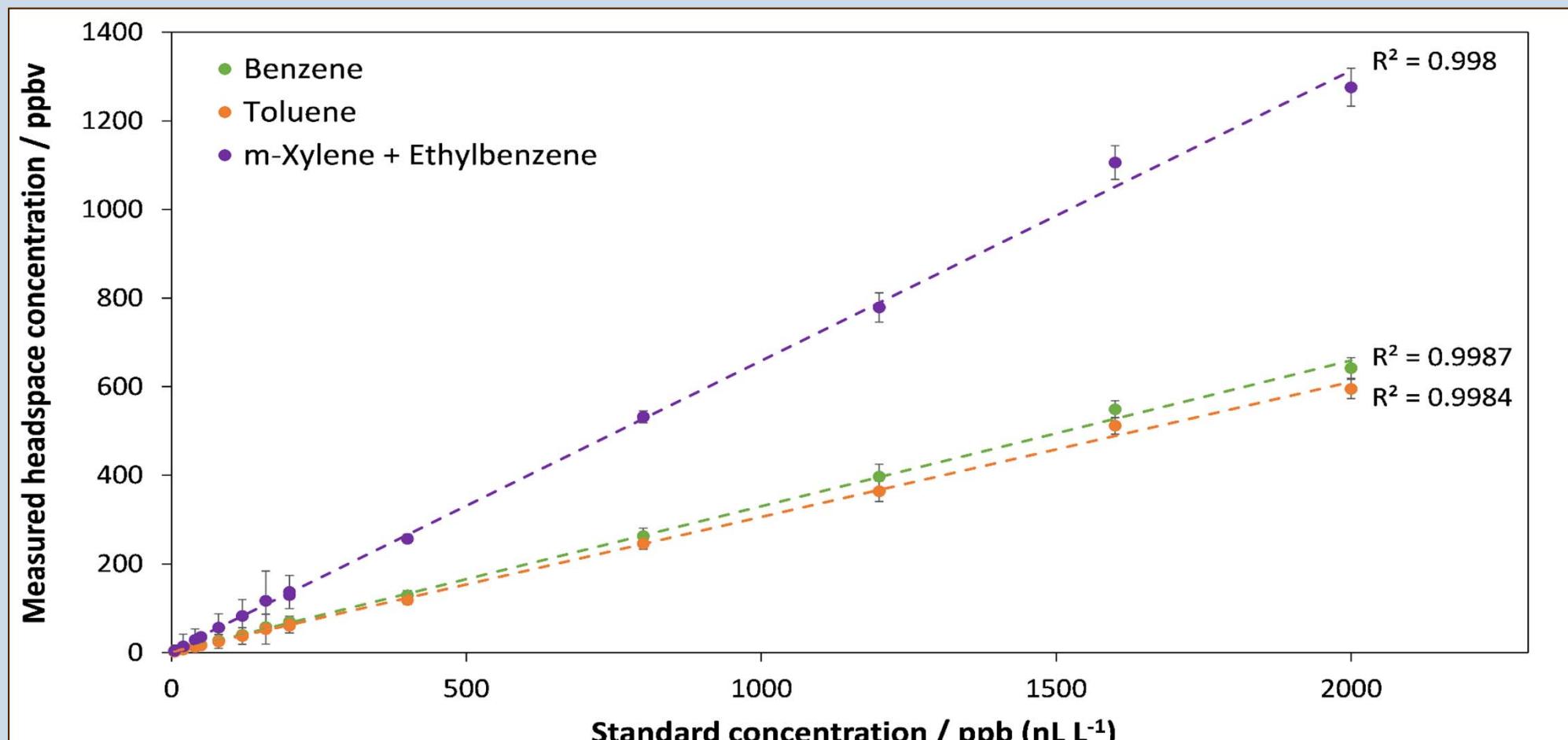
Automated soil analysis using SIFT-MS



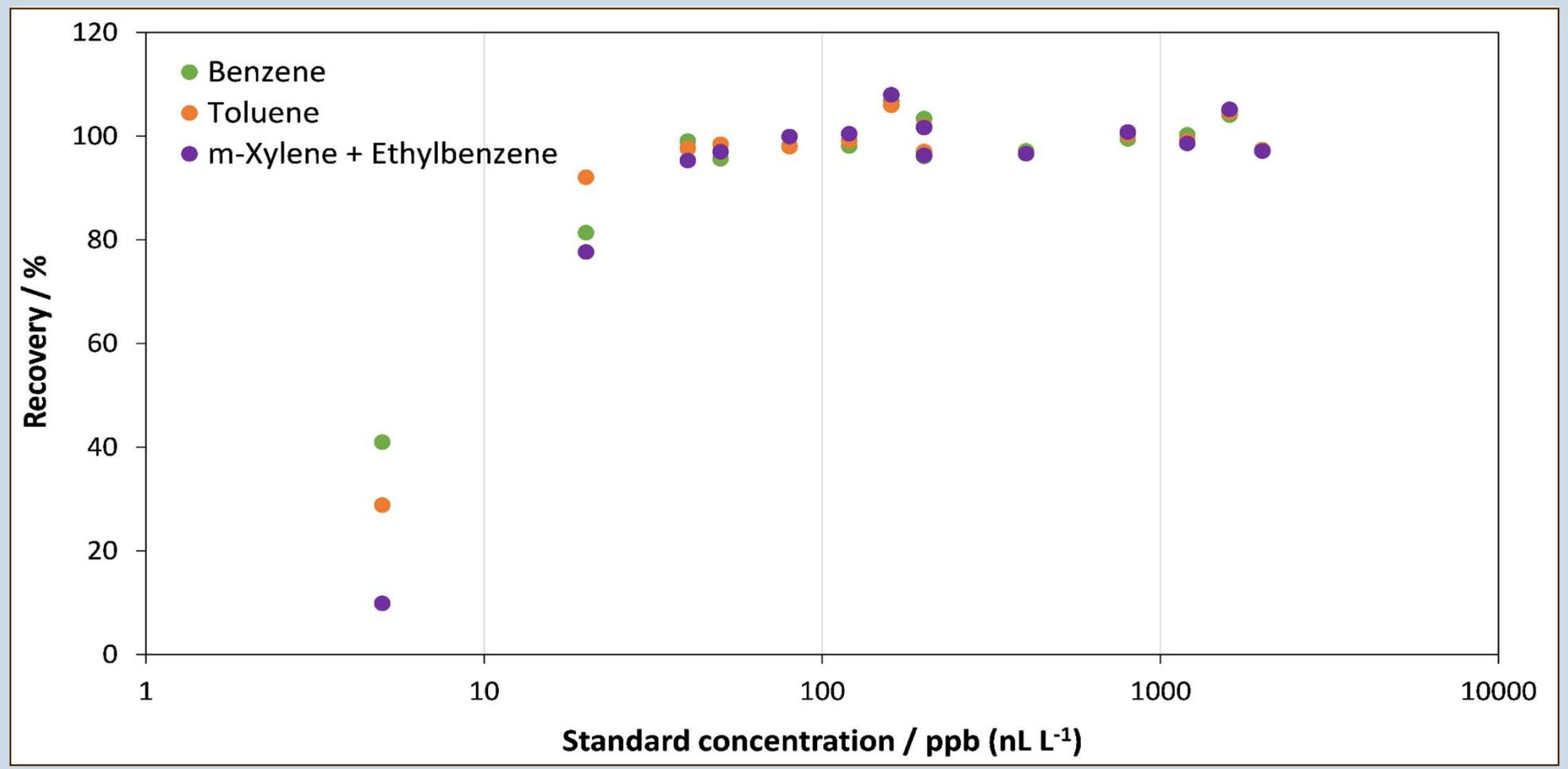
Methanolic extraction of soils



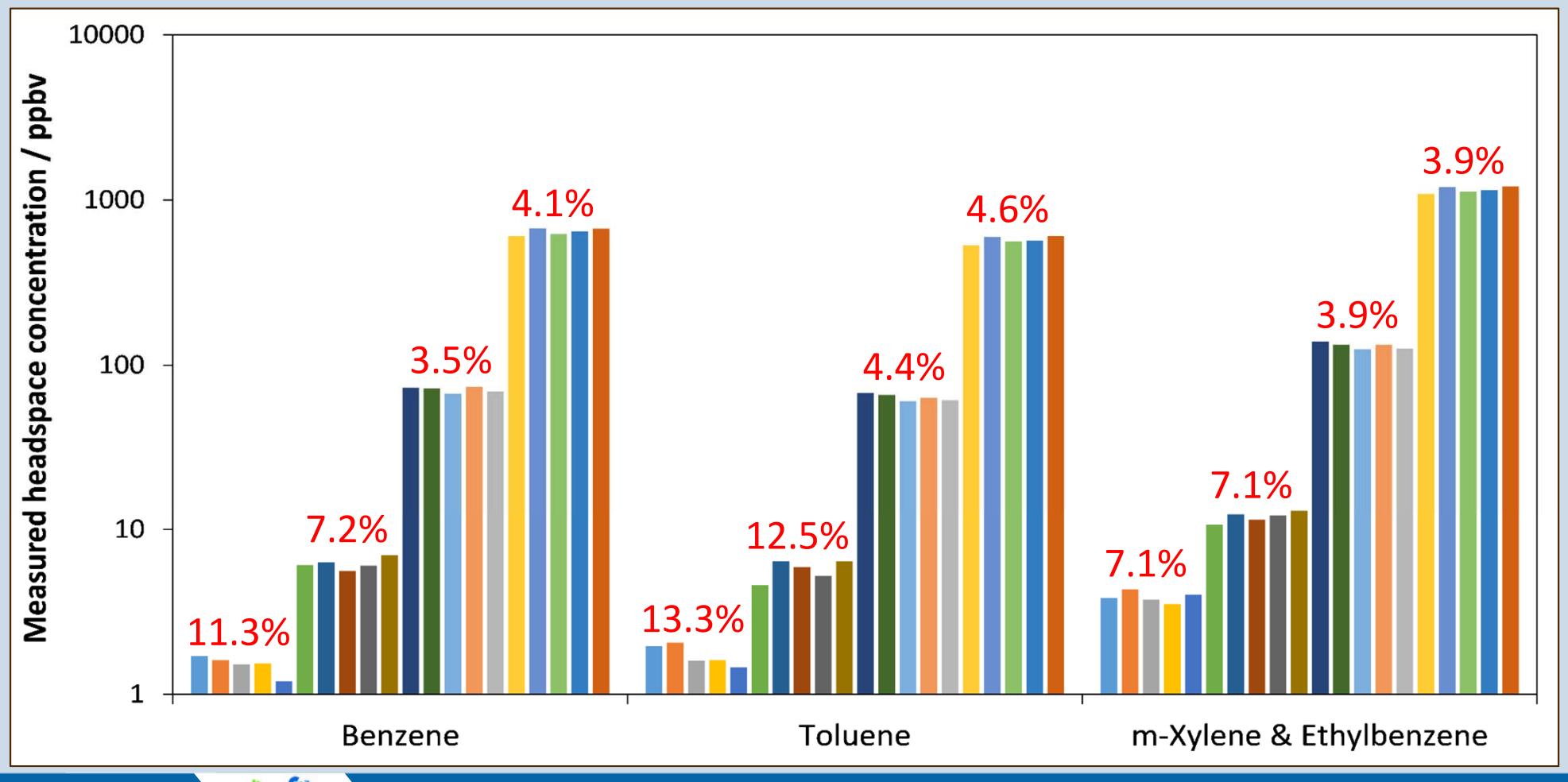
Linearity



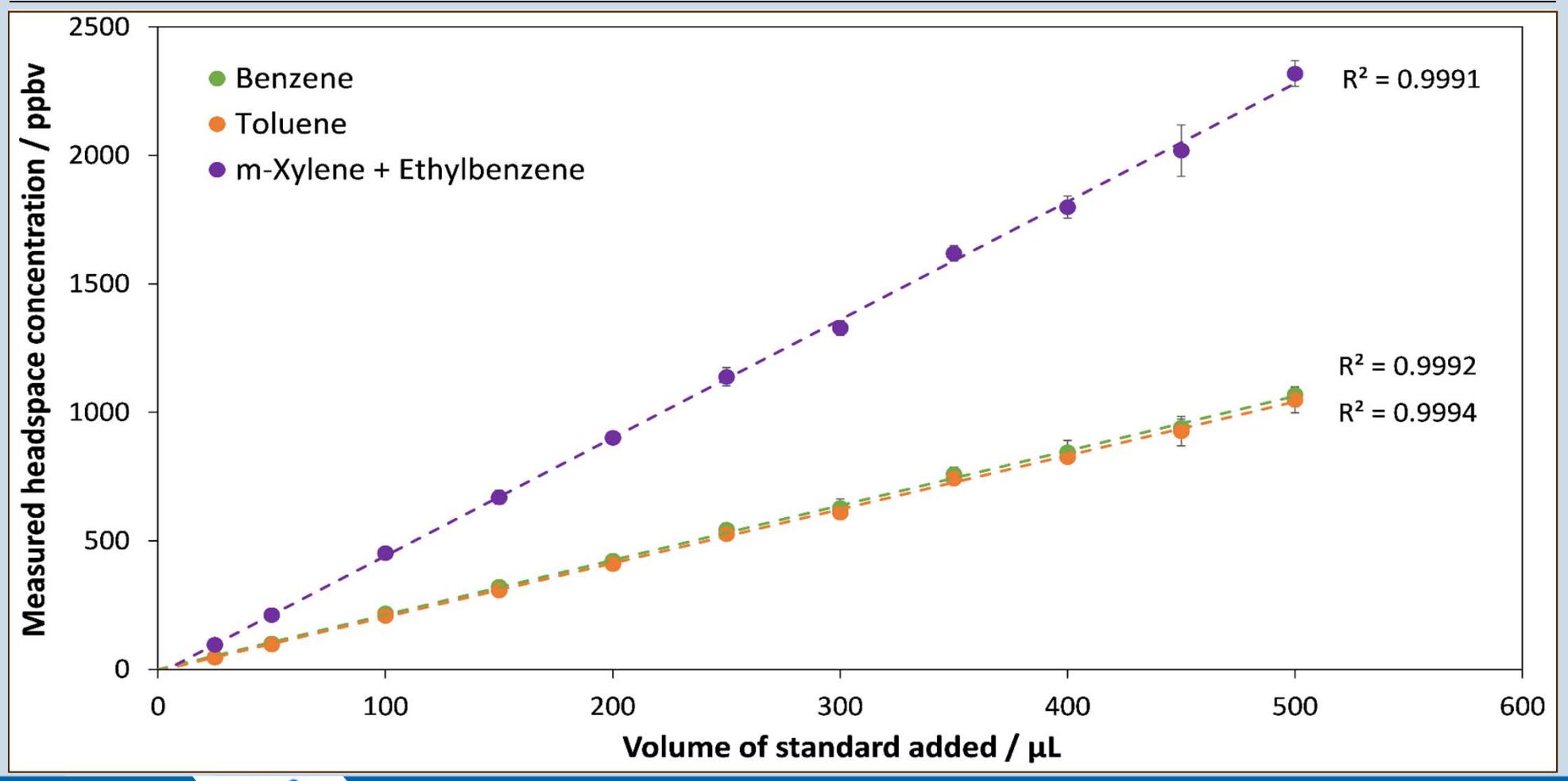
Linearity (recoveries)



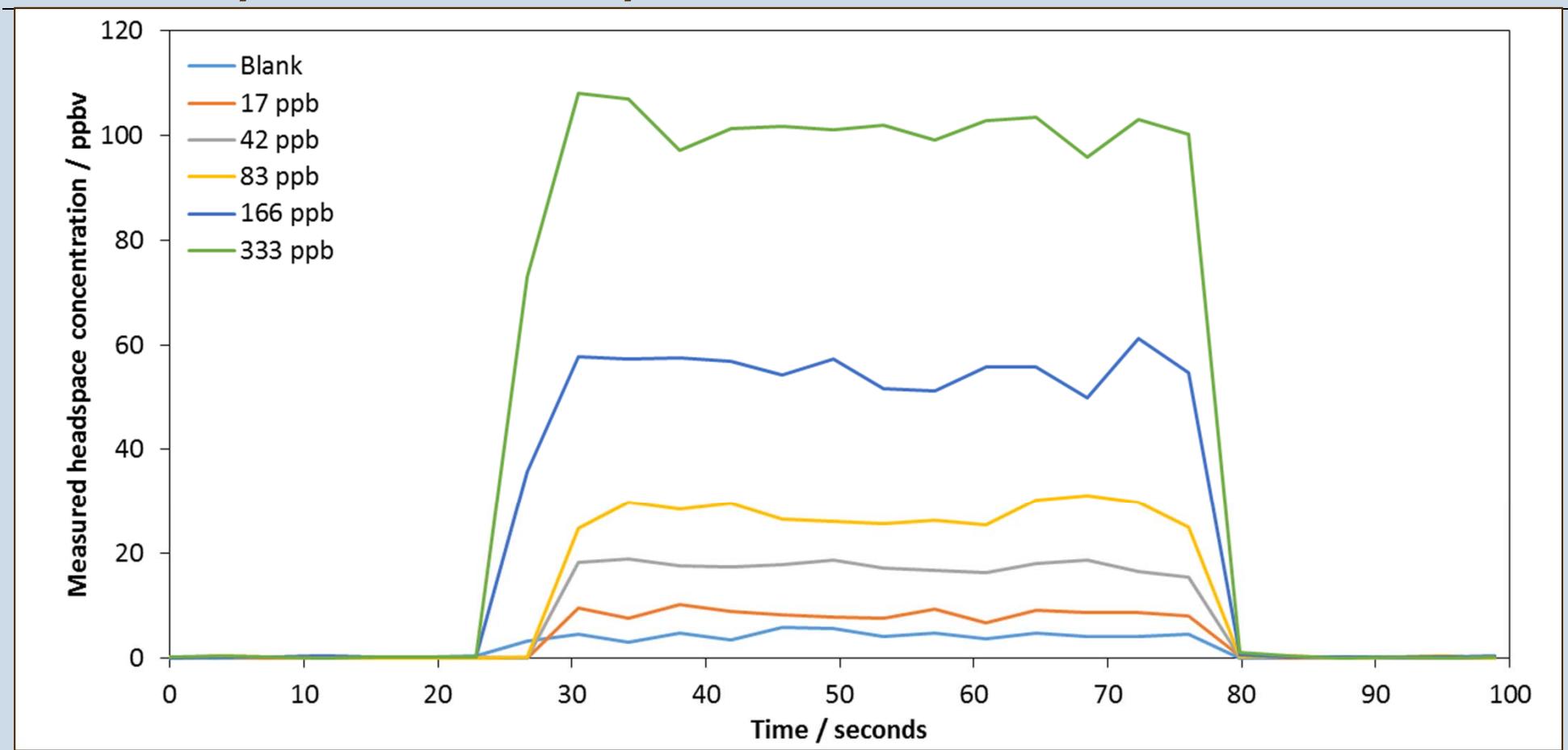
System precision



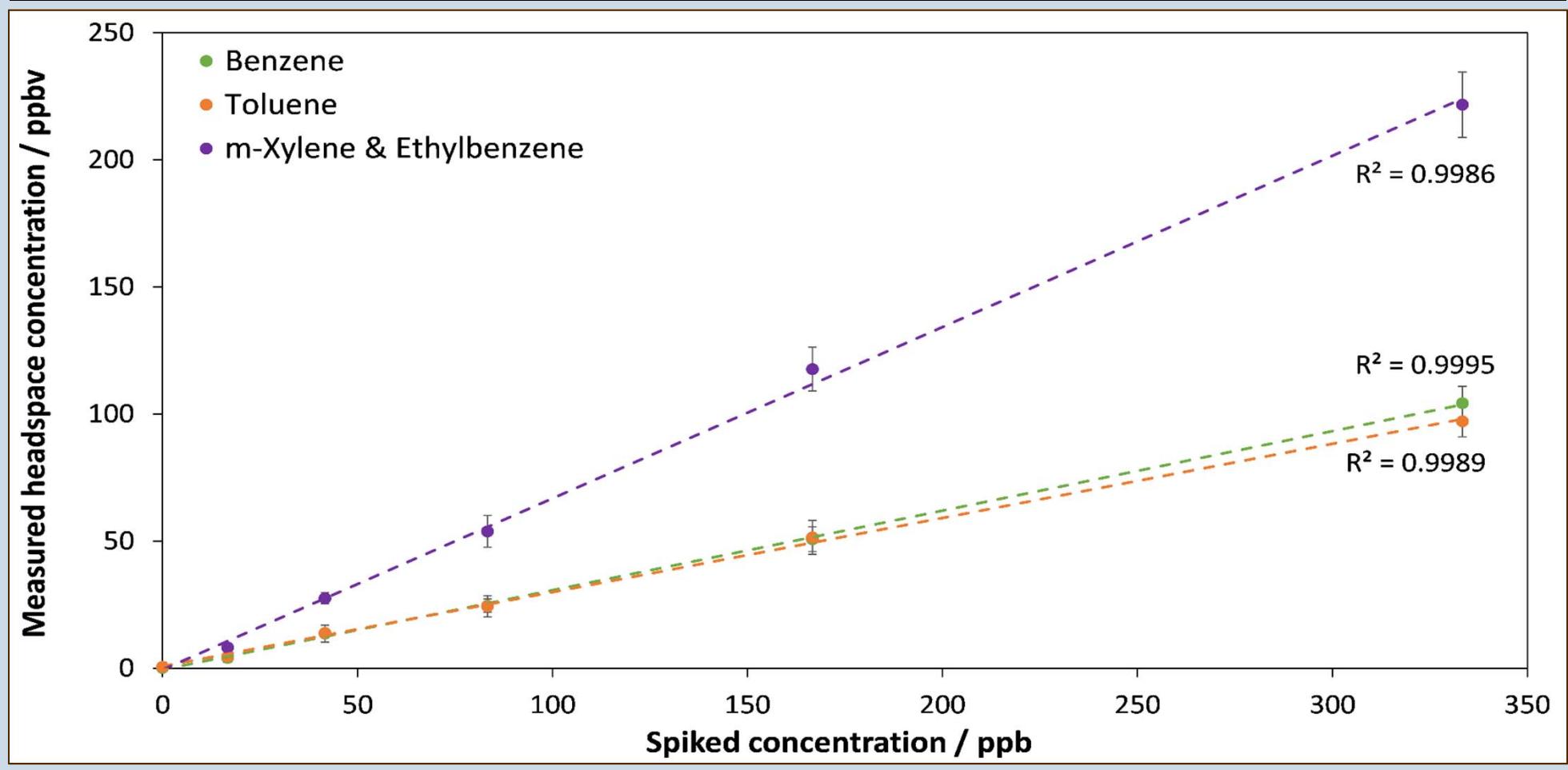
Volume of MeOH aliquot



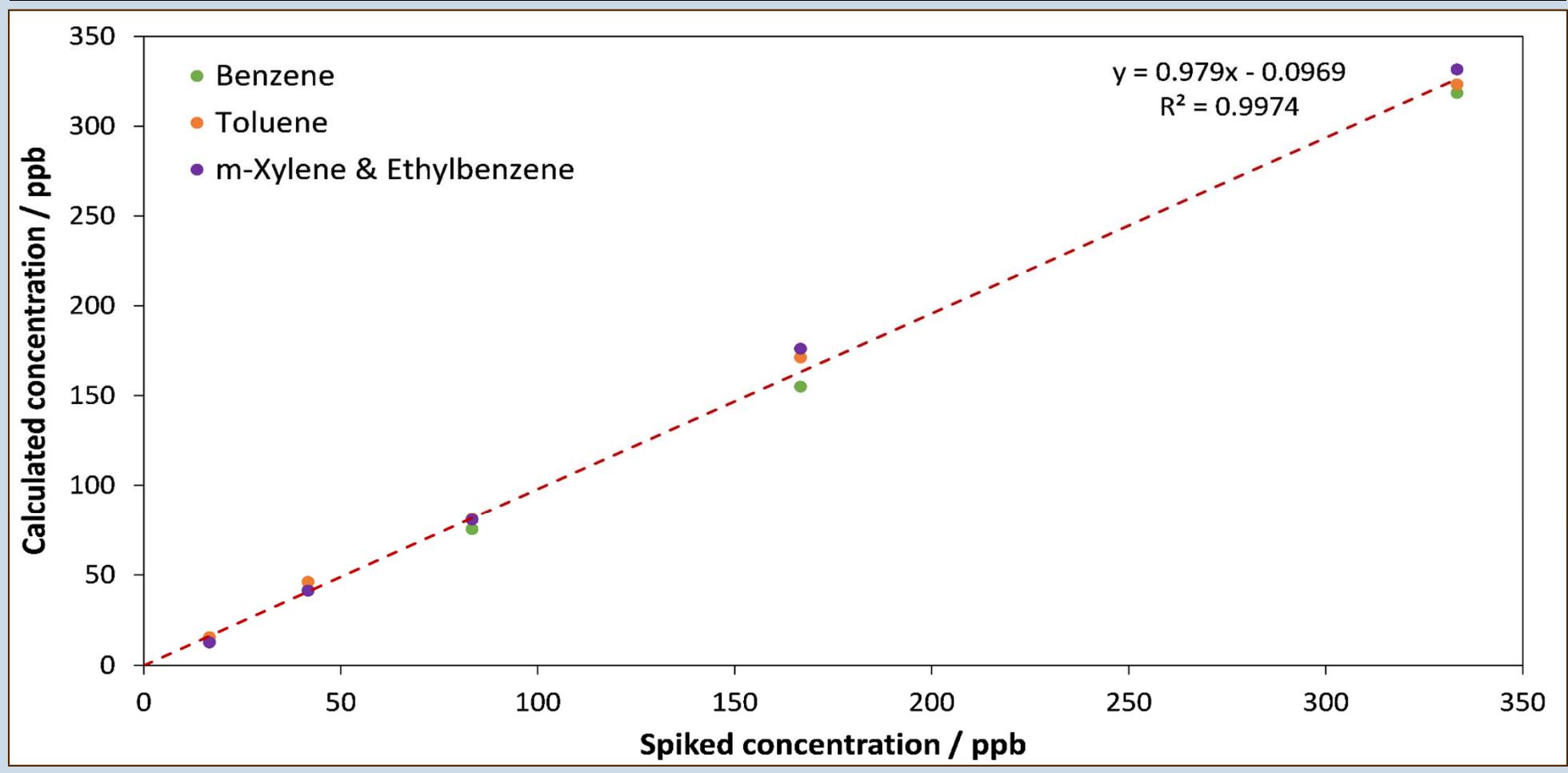
Accuracy and recovery - Toluene



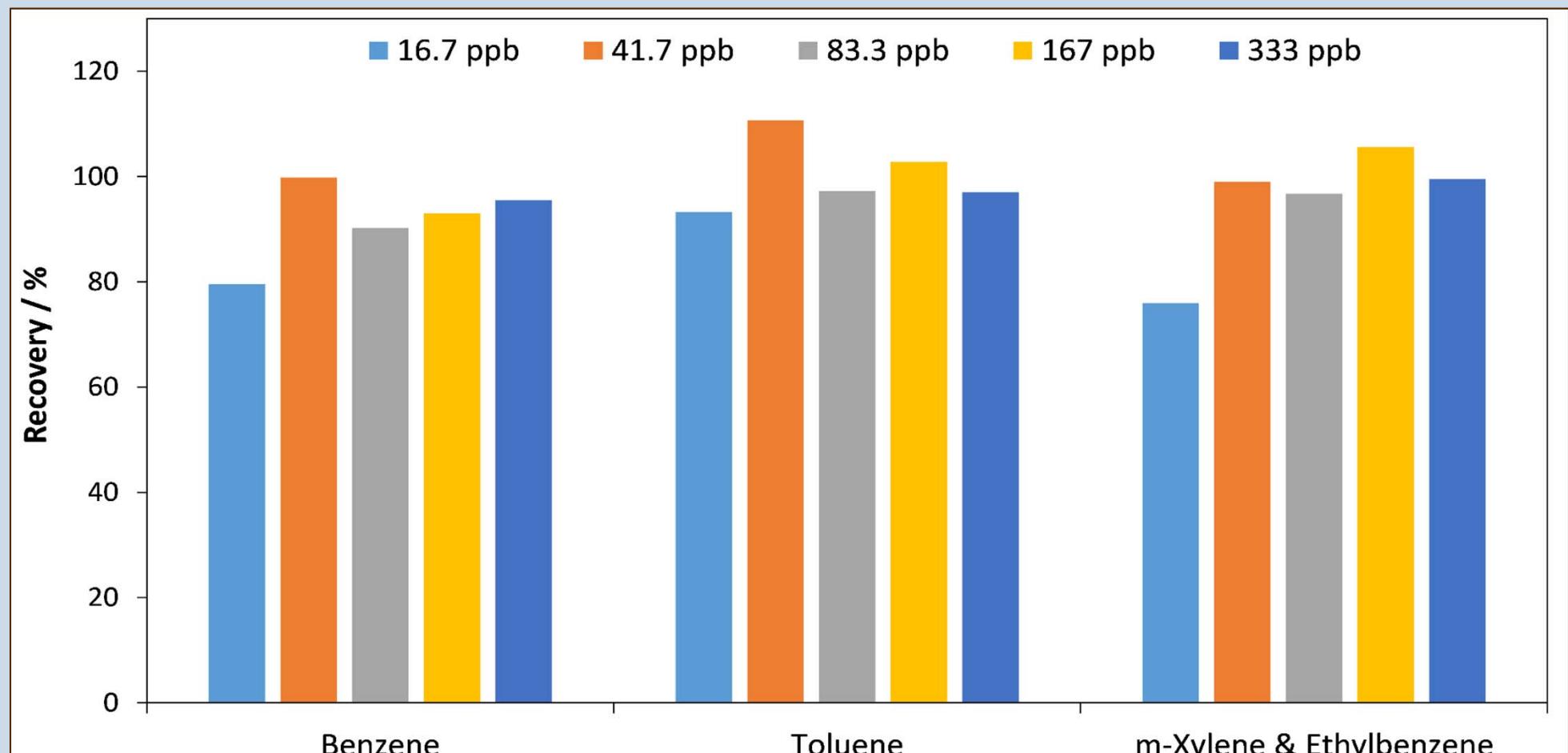
Accuracy and recovery



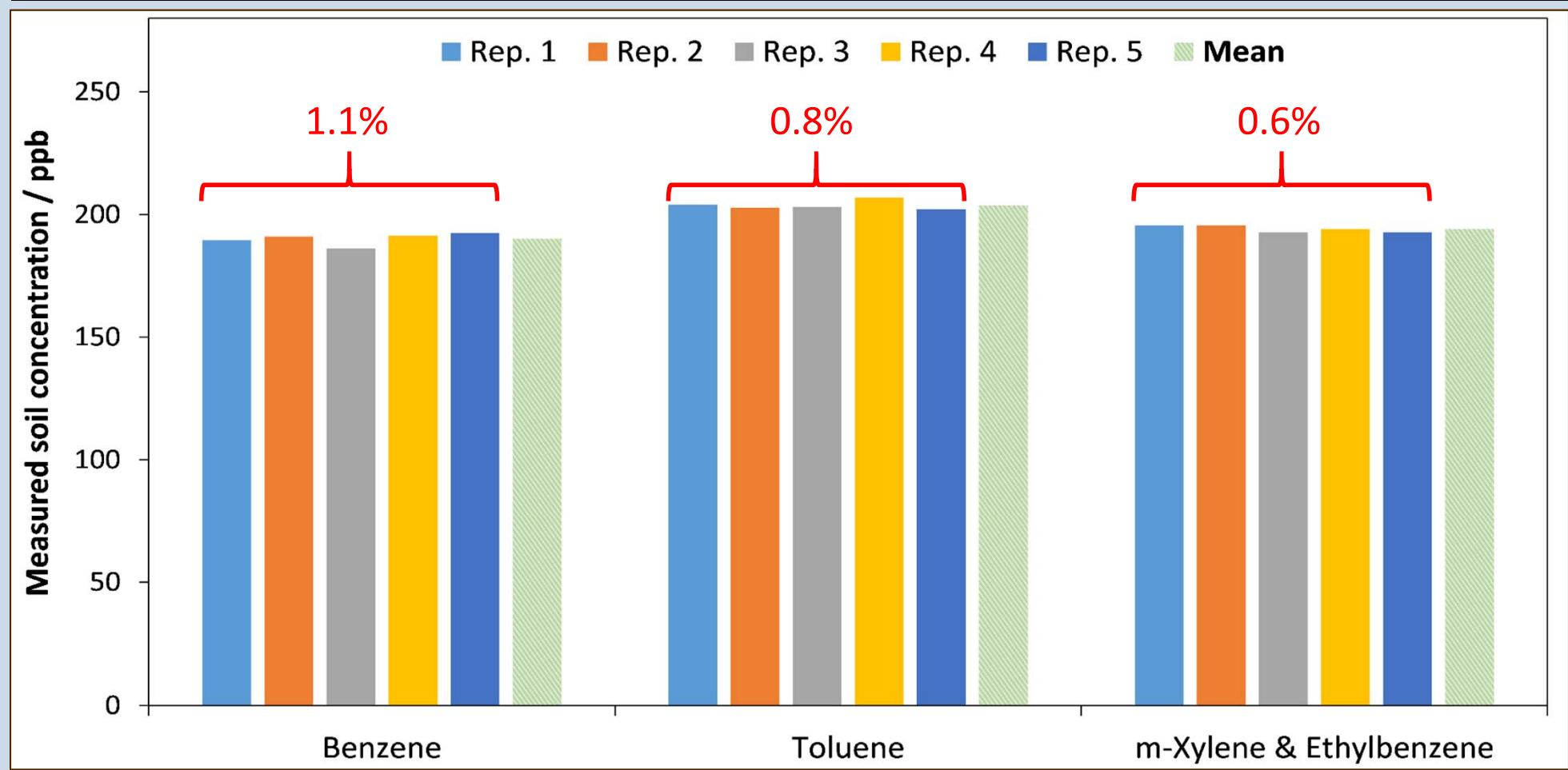
Accuracy and recovery



Accuracy and recovery



Analytical precision





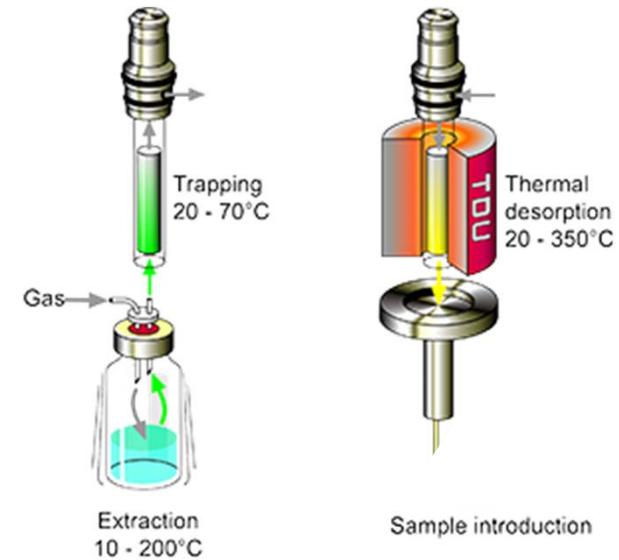
Introducing the DARK TOWER

TD-SIFT-MS configuration

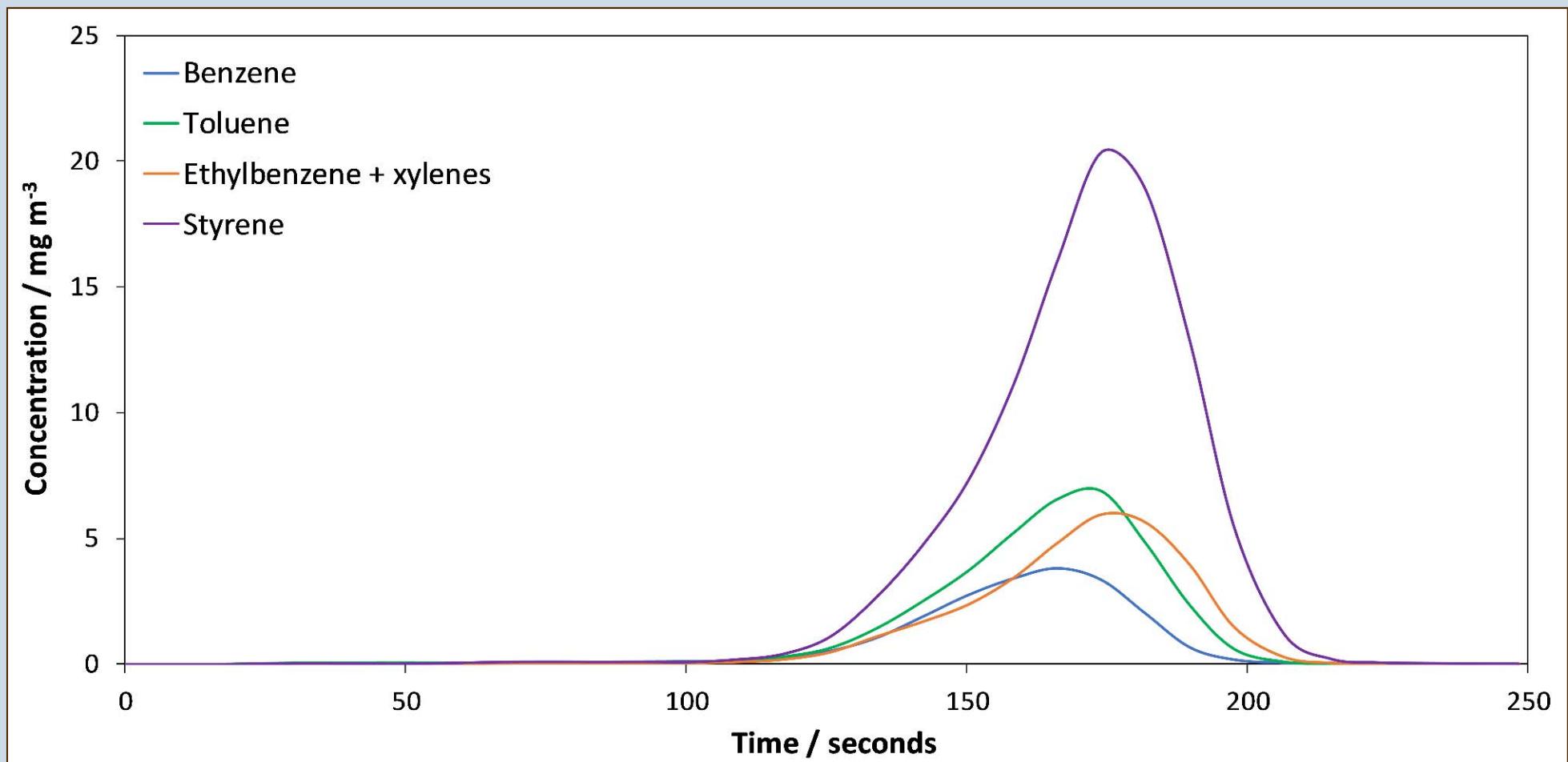


Utilizes GERSTEL TD 3.5⁺ for analysis of standard 3.5" tubes

direct headspace OR purge and trap



Another dimension – real-time desorption profiles



Summary

SIFT-MS analyzes samples directly and rapidly without pre-concentration or chromatography

Automated SIFT-MS greatly increases sample throughput for headspace techniques and accelerates method development and calibration

Applicable to diverse matrices, including air, water and soil

The GERSTEL TD 3.5+ coupled with SIFT-MS enables real-time and high-throughput thermal desorption and thermal extraction

Actively seeking participation in regulation development through ASTM and collaborations with the EPA



Big thanks to Mark Perkins (Anatune, UK), Vaughan Langford (Syft, NZ) and GERSTEL for bringing this research to life

Thank you for your attention

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