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Knowledge for Life.™

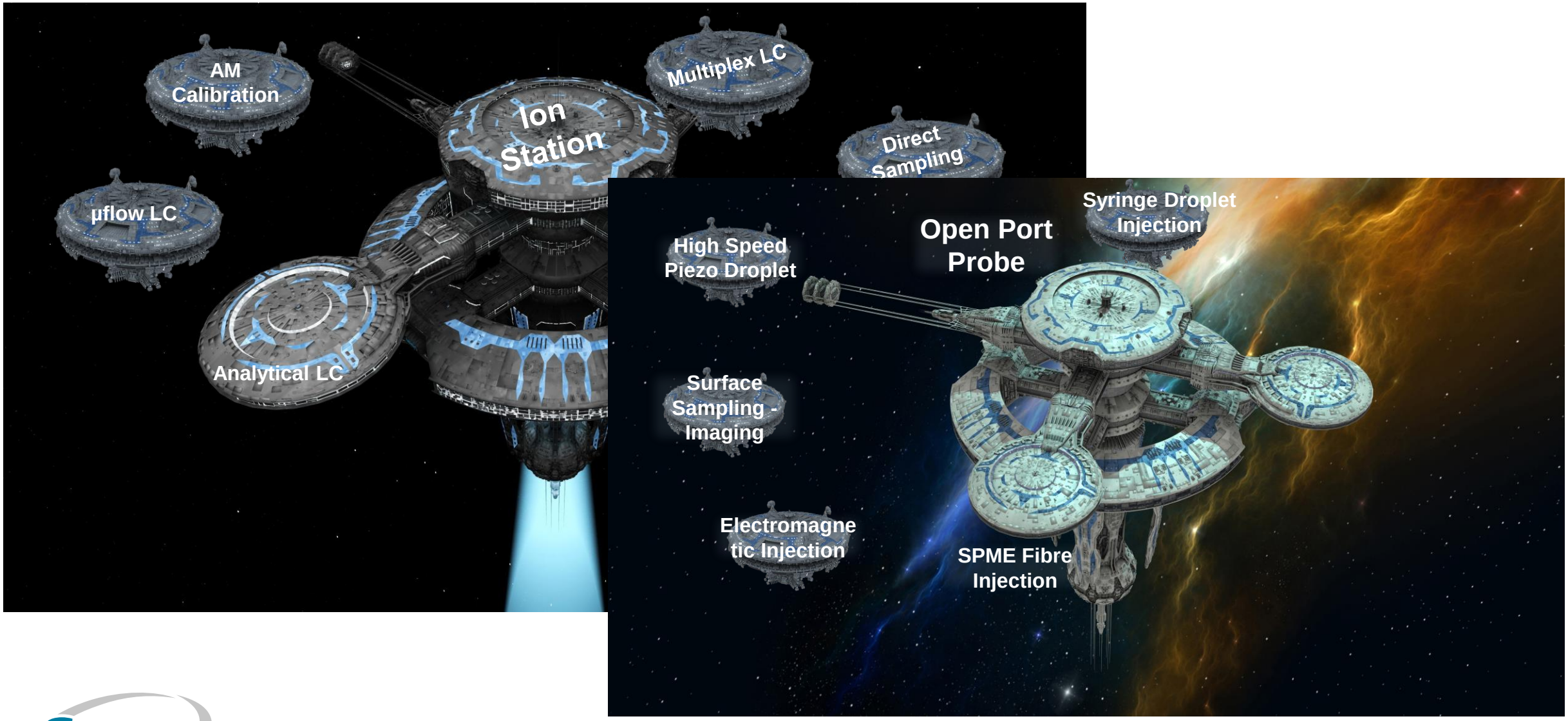
It's Time to
See the Future
Differently

A SWATH Through The Future

Jason Causon,
Senior Application Specialist,
Pharmaceutical & CRO

RUO-MKT-11-6463-A

Ion Station



Sans LC

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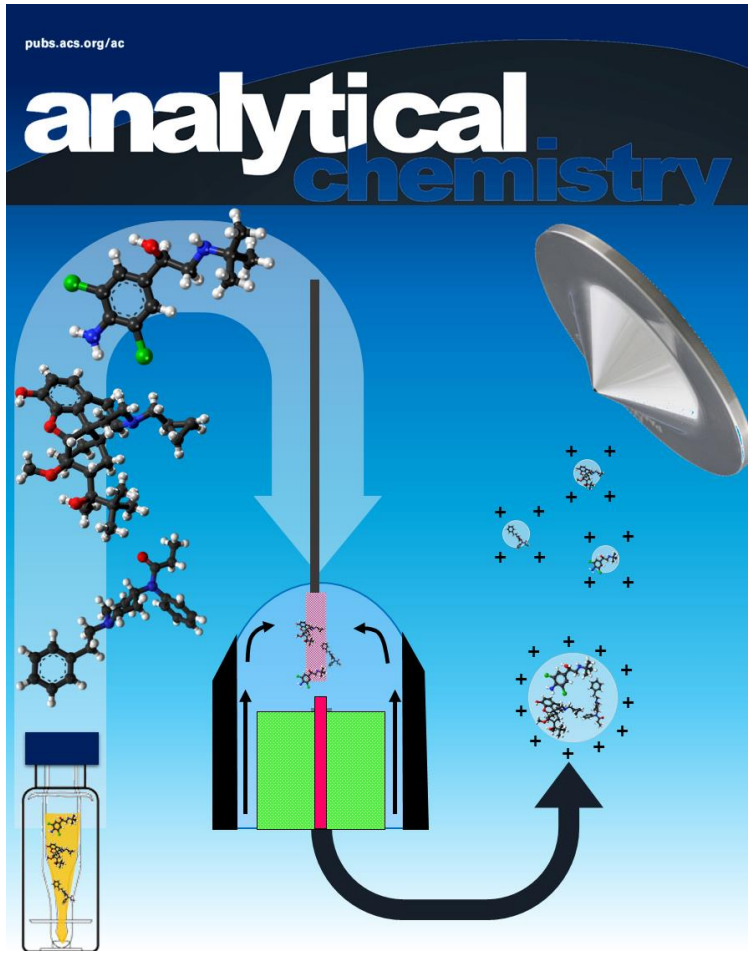
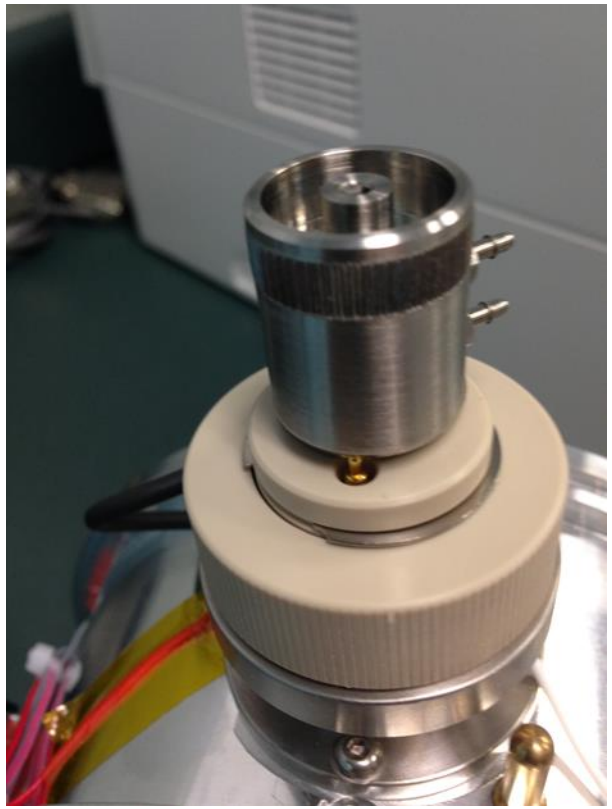
Sans LC – Open-Port Probe (OPP)

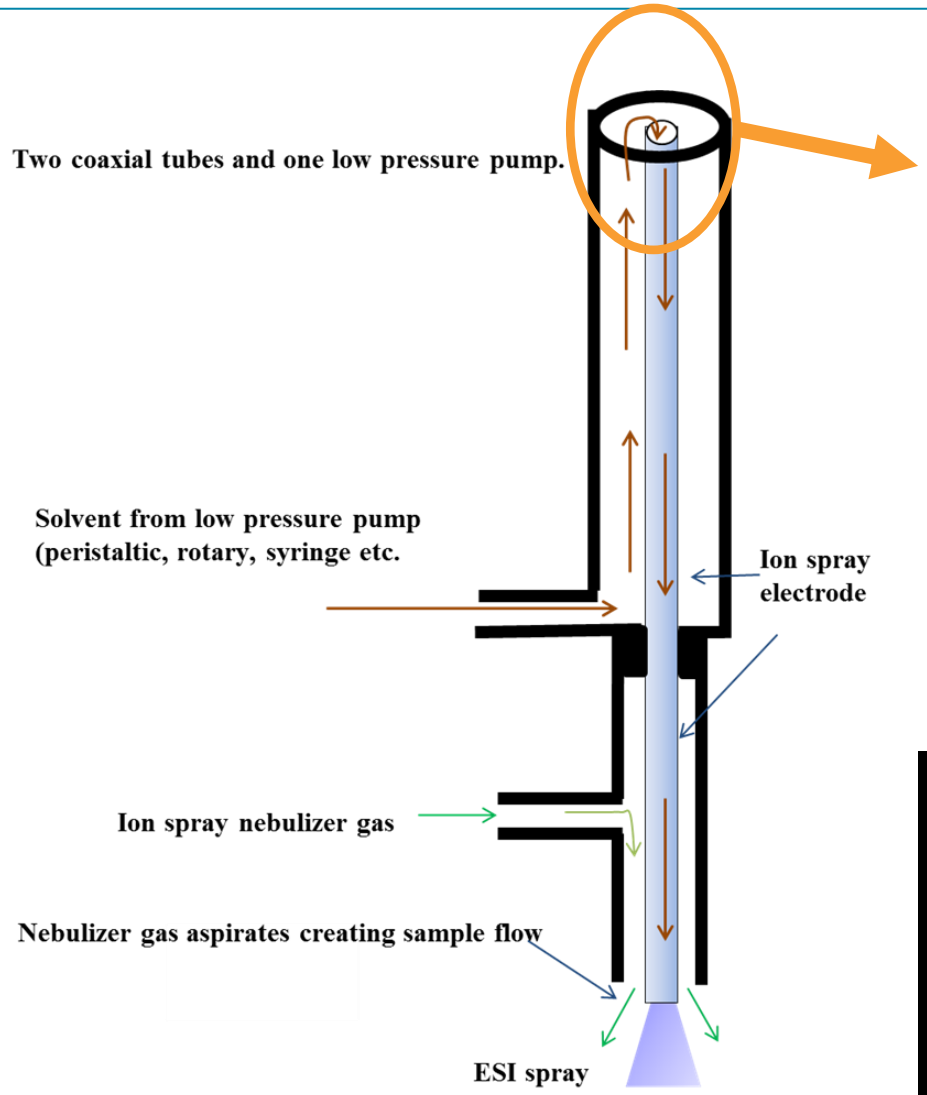


Germán Augusto Gómez-Ríos, Chang Liu, Marcos Tascon, Nathaly Reyes-Garcés, Don W. Arnold, Thomas R. Covey, and Janusz Pawliszyn,
Anal. Chem. 2017, 89, 7, 3805-3089



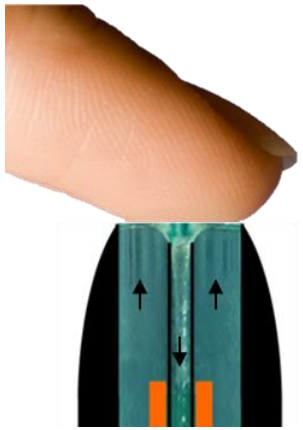
Van Berkel & Kertesz, *Rapid Commum. Mass Spectrom.* 2015, 29, 1749-1756

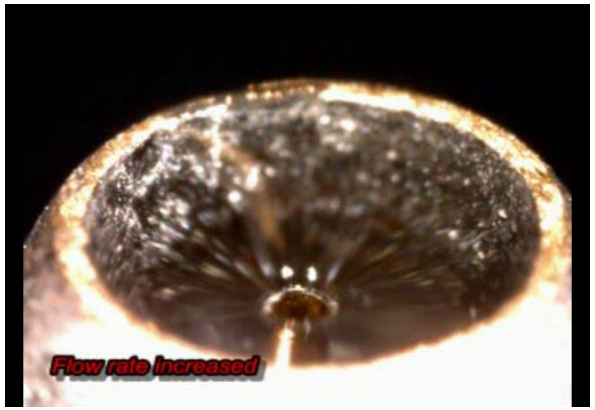
Sans LC – Open-Port Probe (OPP)



Touch Quan

Dome Mode for qualitative surface sampling

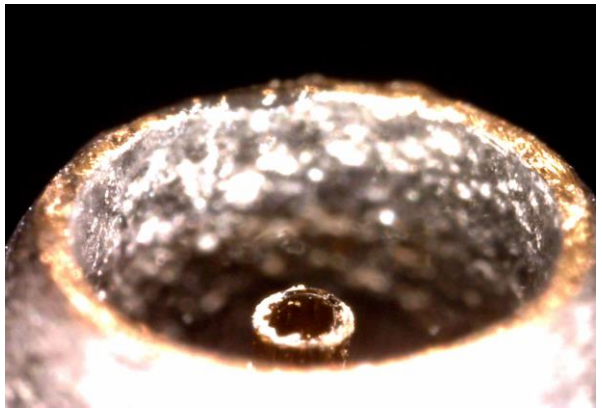




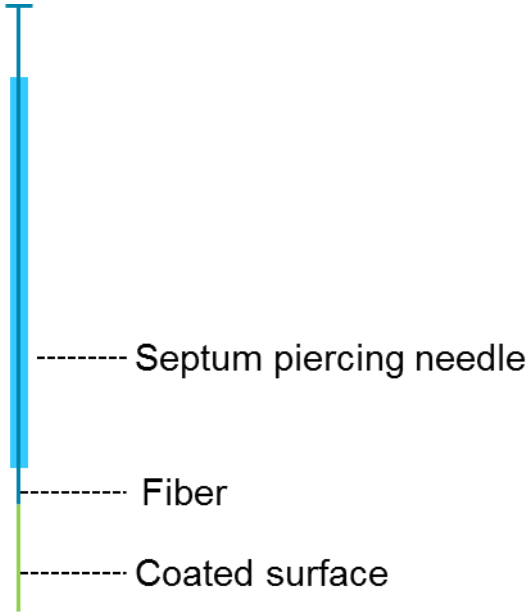
Flush Quan

Vortex mode for quantitative liquid sampling

- SPME fiber extraction & Injection
- Magnetic particle extraction/injection
- Laser particle injection
- Fast droplet injection
- Conventional syringe injection

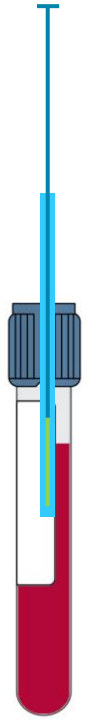


OPP – Flush Quan

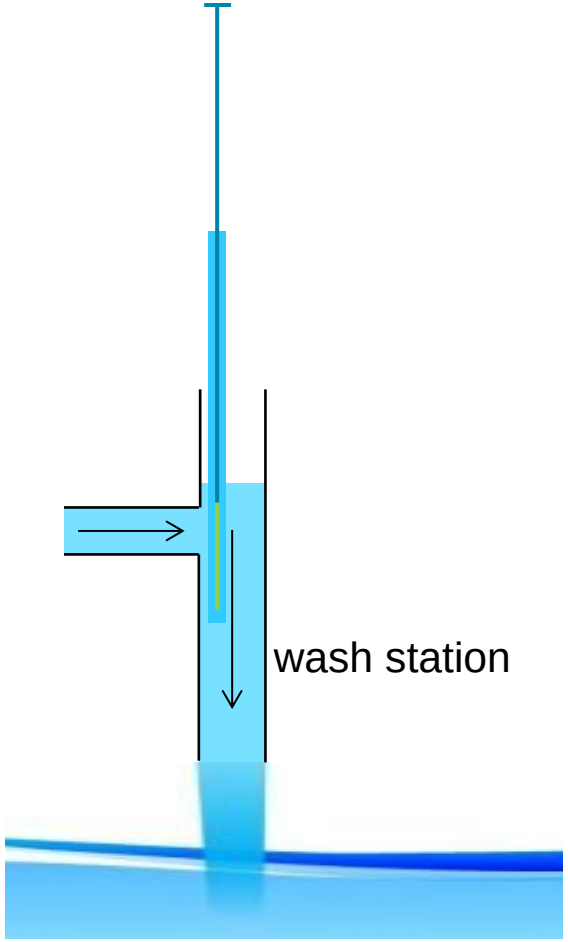


SPME fibers coated with C18 or antibodies

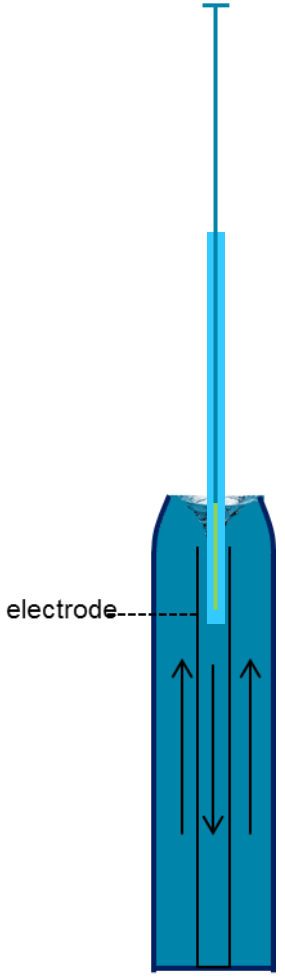
Extraction



Rinse With Water



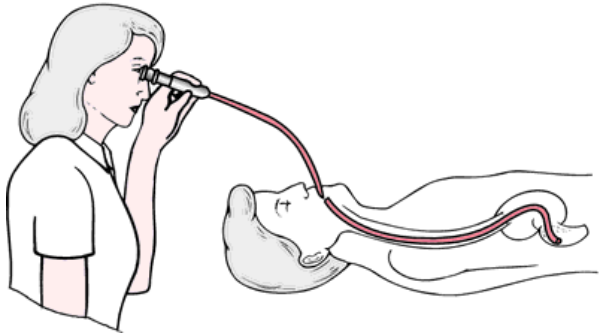
Fiber extracted in vortex. 5 second transfer time for ESI



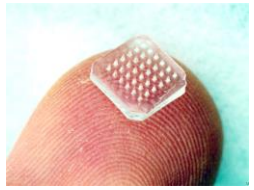
OPP – *In Vivo* SPME Sampling

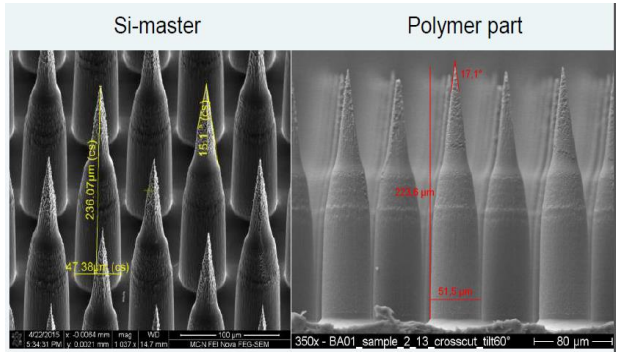
Semi-invasive in-vivo sampling

Blood sampling without bleeding



Optical guided in-vivo sampling





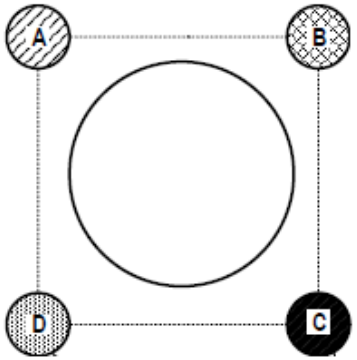
Transdermal blood sampling

OPP – *Electromagnetic Injection*

Moving beads relative to the stationary bulk solution – “dynamic cloud”

- Compatible with microtiter plate
- Low volume version (<0.5 mL) and high volume version (~2 mL)
- Temperature control

~300-350 Hz

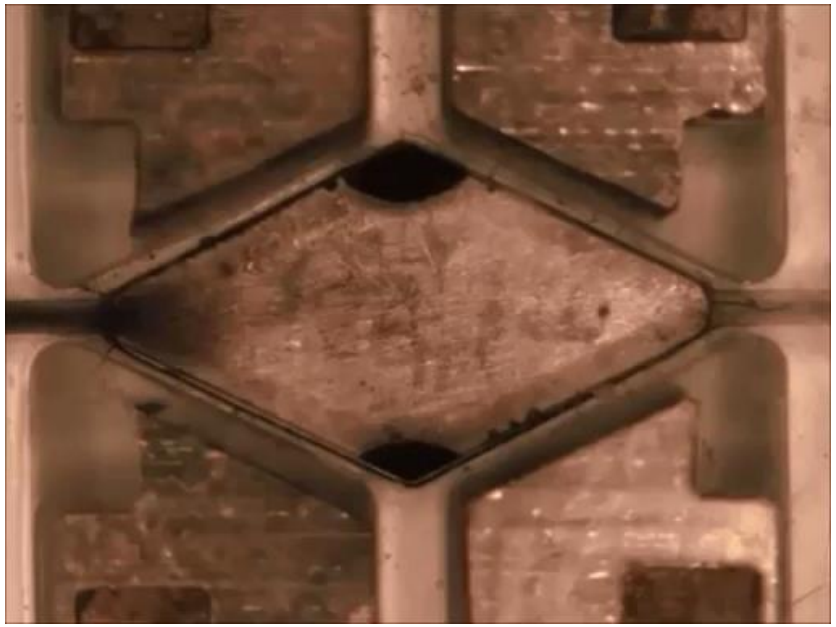


(1) $I_A = I_0 \sin(ft)$

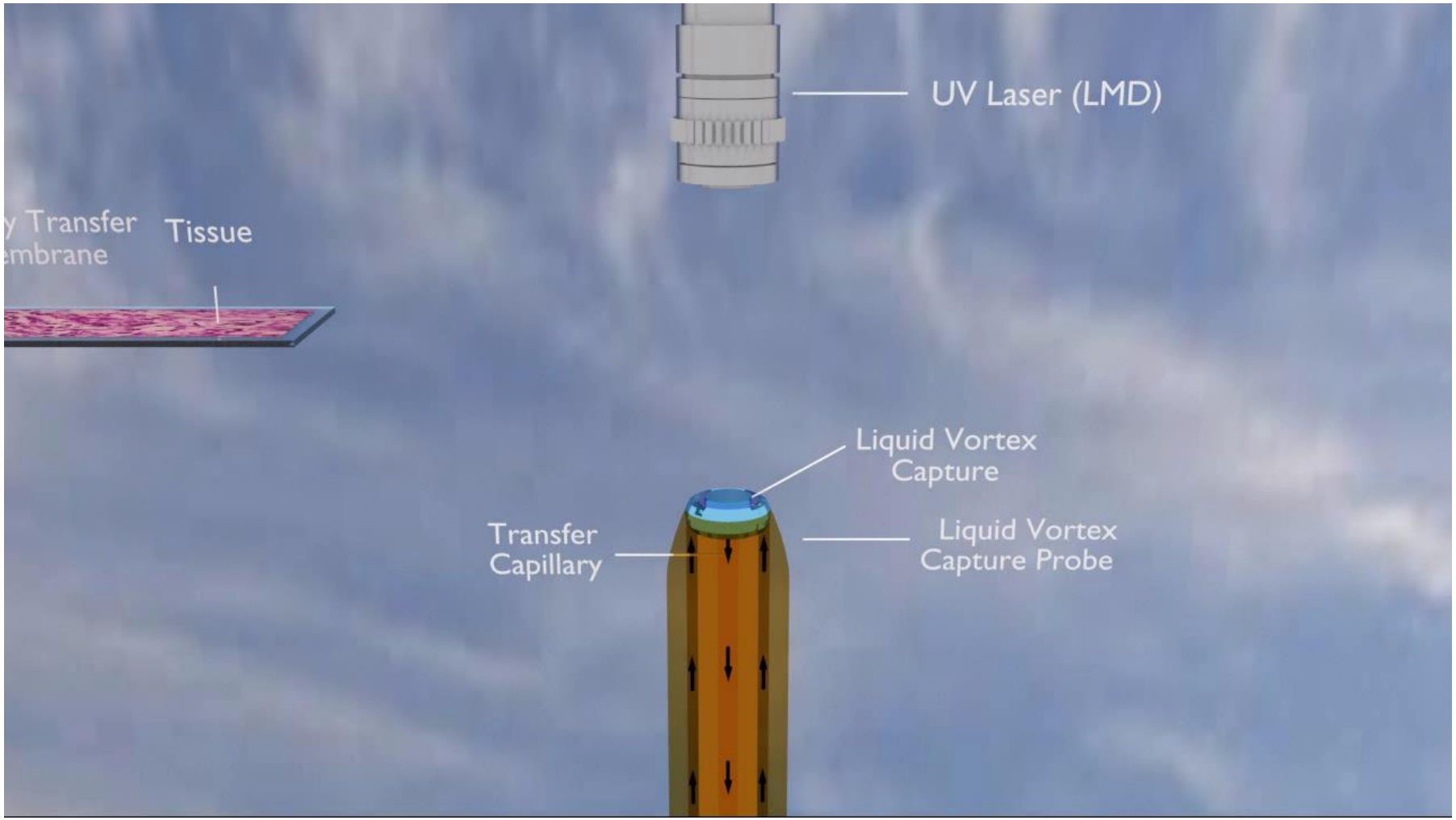
(2) $I_B = I_0 \sin(ft + \frac{\pi}{2})$

(3) $I_C = I_0 \sin(ft + \pi)$

(4) $I_D = I_0 \sin(ft + \frac{3\pi}{2})$



OPP – *Laser Microdissection Surface Imaging*



OPP – *Laser Microdissection Surface Imaging*

analytical chemistry

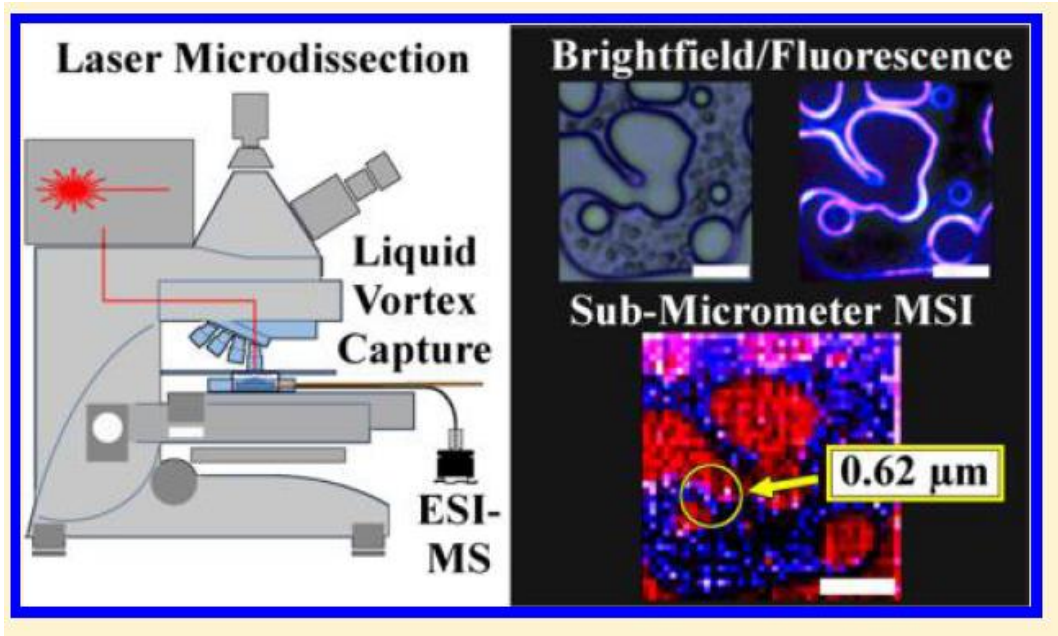
Article

pubs.acs.org/ac

Characterization and Application of a Hybrid Optical Microscopy/ Laser Ablation Liquid Vortex Capture/Electrospray Ionization System for Mass Spectrometry Imaging with Sub-micrometer Spatial Resolution

John F. Cahill, Vilmos Kertesz, and Gary J. Van Berkel*

Analytical Chemistry, 2015, 87(21), 11113-11121

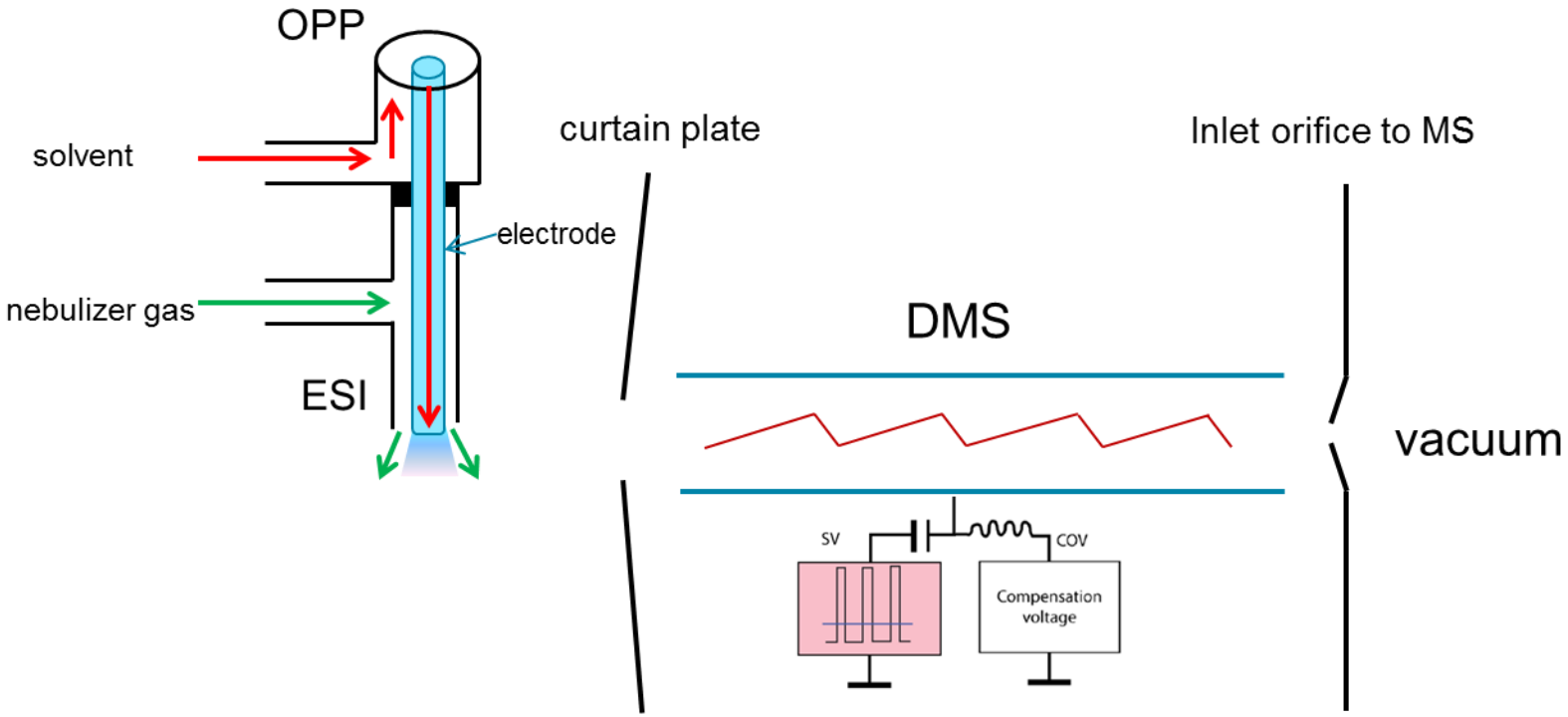


Online, Absolute Quantitation of Propranolol from Spatially Distinct 20- and 40-µm Dissections of Brain, Liver, and Kidney Thin Tissue Sections by Laser Microdissection–Liquid Vortex Capture–Mass Spectrometry

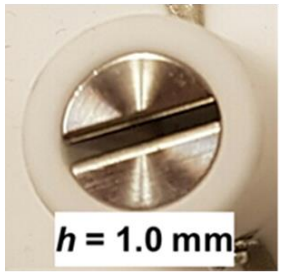
John F. Cahill†, Vilmos Kertesz†, Taylor M. Weiskittel‡, Marissa Vavrek§, Carol Freddo§, and Gary J. Van Berkel*†

Analytical Chemistry, 2016, 88(11), 6026-6034

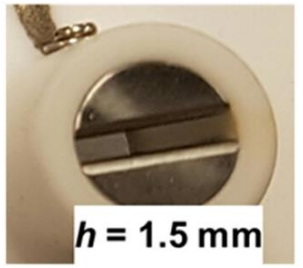
OPP – High-Res DMS for Isomeric Separation



SelexION

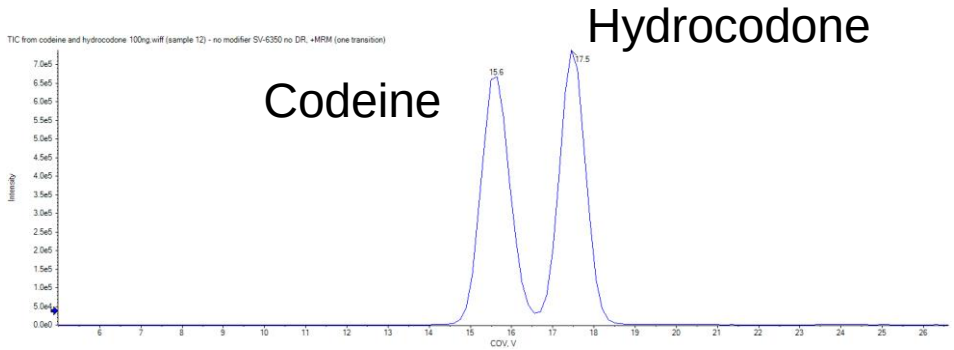


High-Res DMS



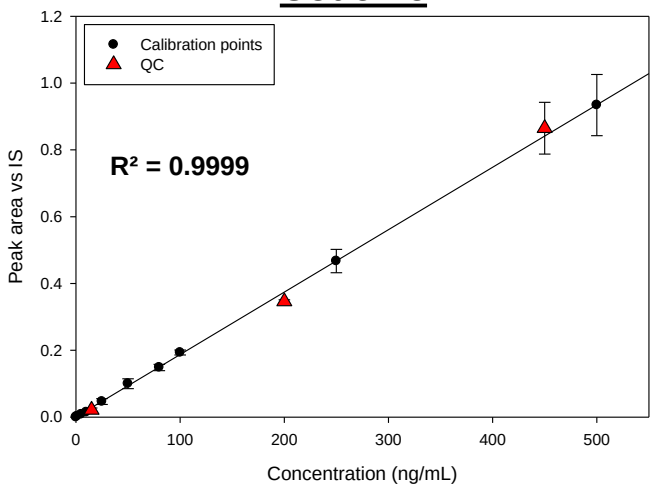
OPP – High-res DMS for isomeric Separation

Real-time Baseline separation with high-res DMS, without the use of modifier or resolving gas

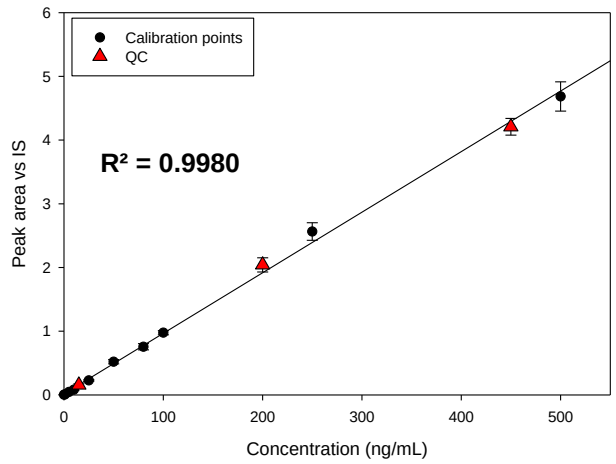


SPME-OPP-DMS analysis (1-500 ng/mL from plasma): ~15 sec per sample

Codeine



Hydrocodone



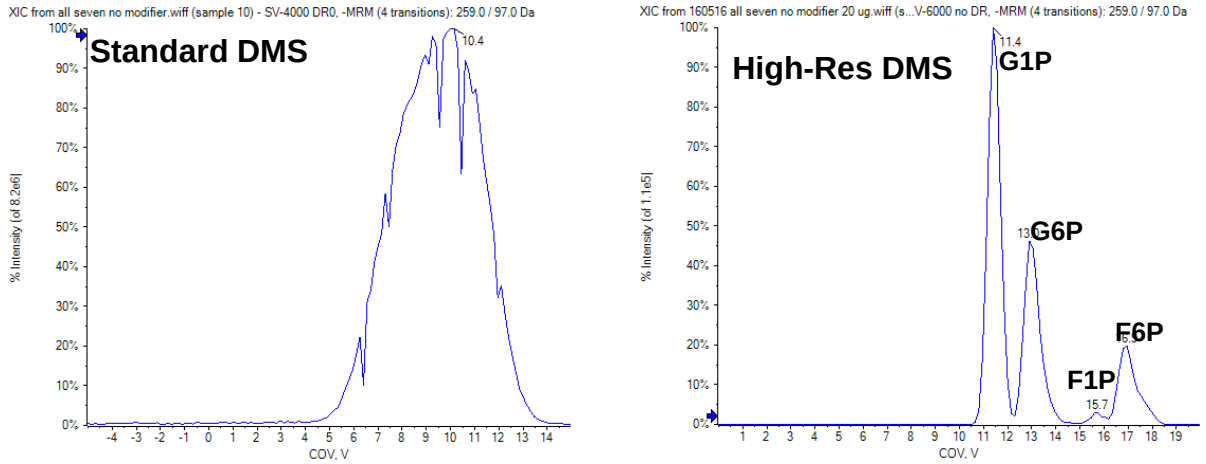
MP352 (ASMS 2016): LeBlanc, Liu, Campbell, Schneider,
Increasing the resolving power of differential mobility…

OPP – High-res DMS for isomeric Separation

Real-time Isomeric Separation

Sugar phosphates: key isobaric intermediates for fluxomics that are difficult to separate chromatographically.

- **glucose-1-phospate (G1P)**
- **glucose-6-phospate (G6P)**
- **fructose-1-phospate (F1P)**
- **fructose-6-phospate (F6P)**



Piotrowski, Durnlao, Keefer, Janiszewski, Kibbey, Liu, IMSC 2016

Lets Take A SWATH Through HRAMS

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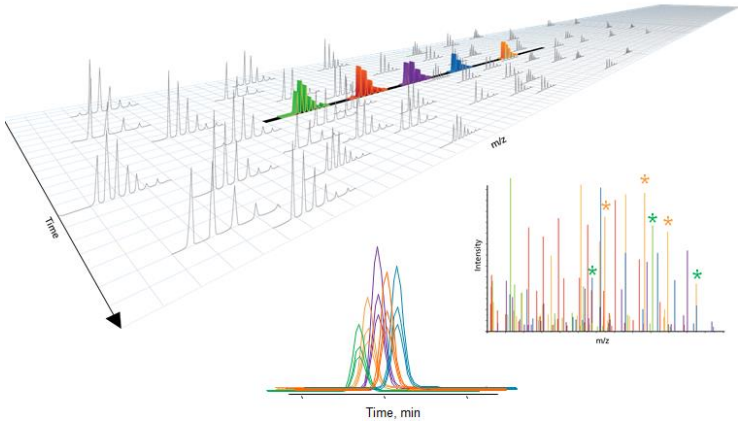
Moving To Scanning SWATH?

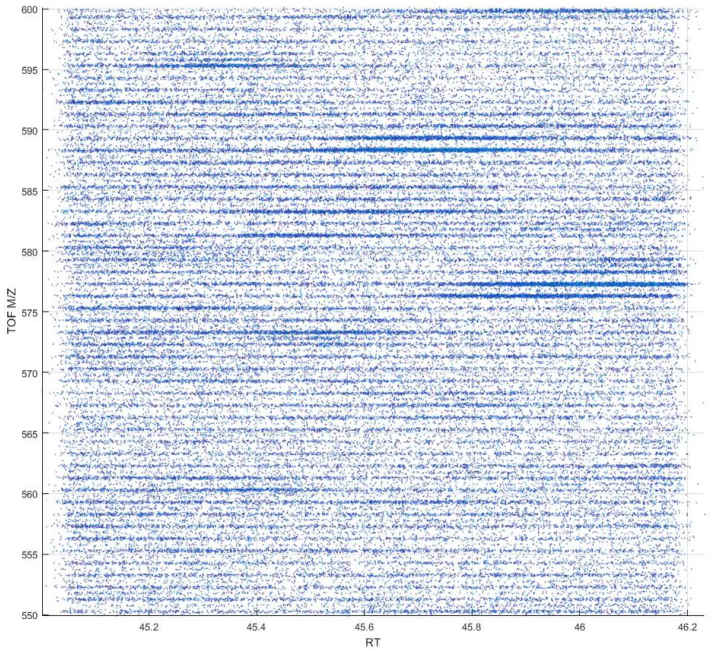
What is it?

- **MS/MS^{ALL}**
  - A ***data-independent*** workflow enabled by TripleTOF® system that acquires high resolution quantifiable MS/MS data for all detectable analytes in a complex sample, in a single run



How does it work?

- **SWATH™ Acquisition**
  - Uses wide isolation windows stepped across a mass range, collecting high resolution composite MS/MS spectra in a chromatographic time scale



What does this enable?

- Data processing post-acquisition: generate fragment ion XICs at high resolution for quantitation **with** confirmation of identity
- Quantitation and confirmation of everything in the sample
- Digital record of everything in your sample
- Single method for acquiring all your data

ASMS 2016 Poster: Using Scanning SWATH Windows to Improve Both Quant/Qual…. Bloomfield et al.

You May Ask

What About Sensitivity?

We Are Talking About Mass Spec After All

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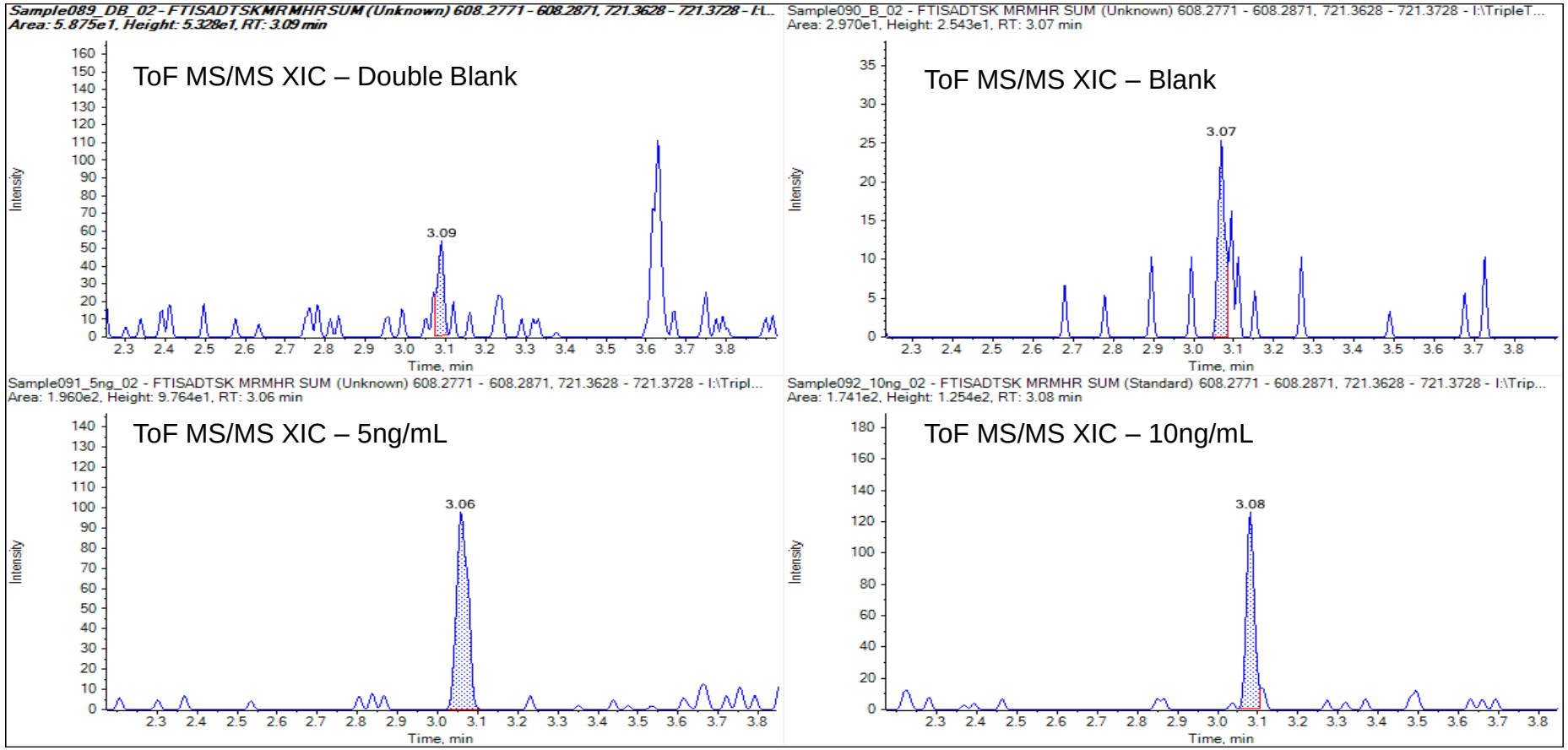
HRAMS – Bioanalytical Quantification



Trastuzumab shows linear response across the concentration range analysed (10ng/mL to 50000ng/mL). The LOD is at **5ng/mL** and a LLOQ of **10ng/mL** (LLOQ accuracy and precision within +/- 25% and less than 10% respectively)

But…

What About Small Molecules???

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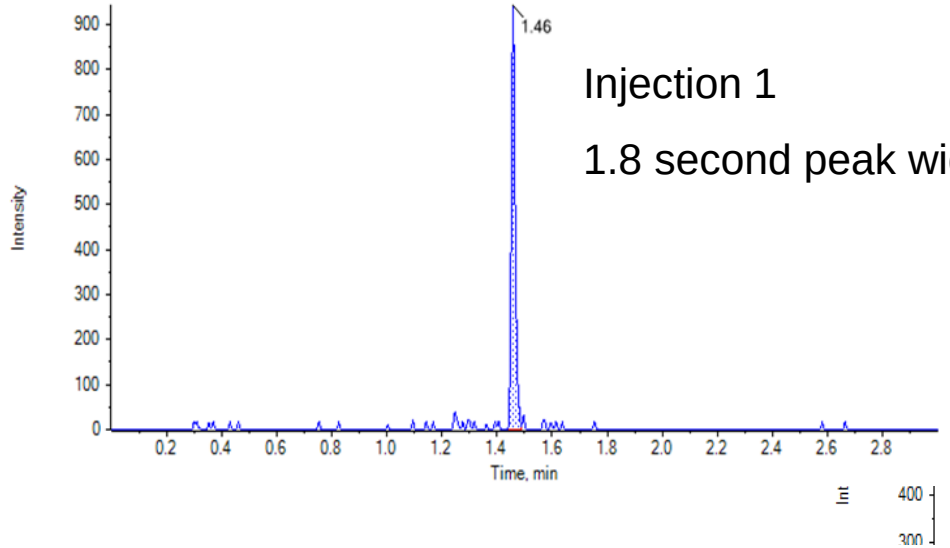
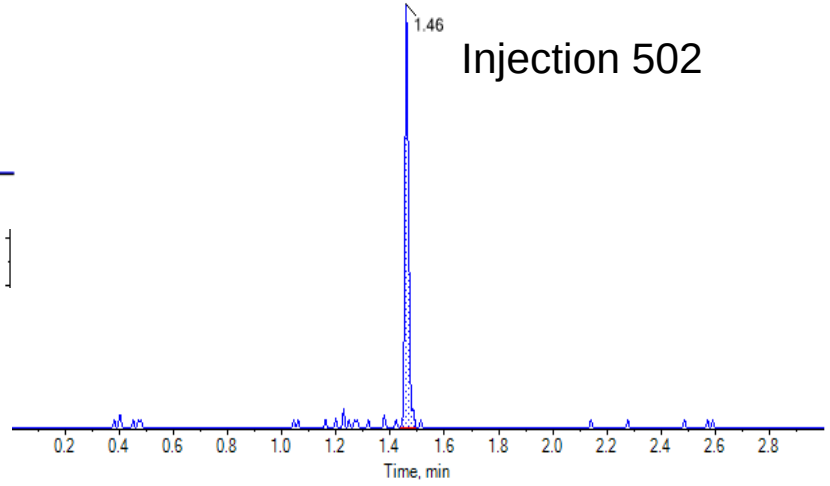
HRAMS – Bioanalytical Quantification

Voriconazole - No Internal Standard Correction

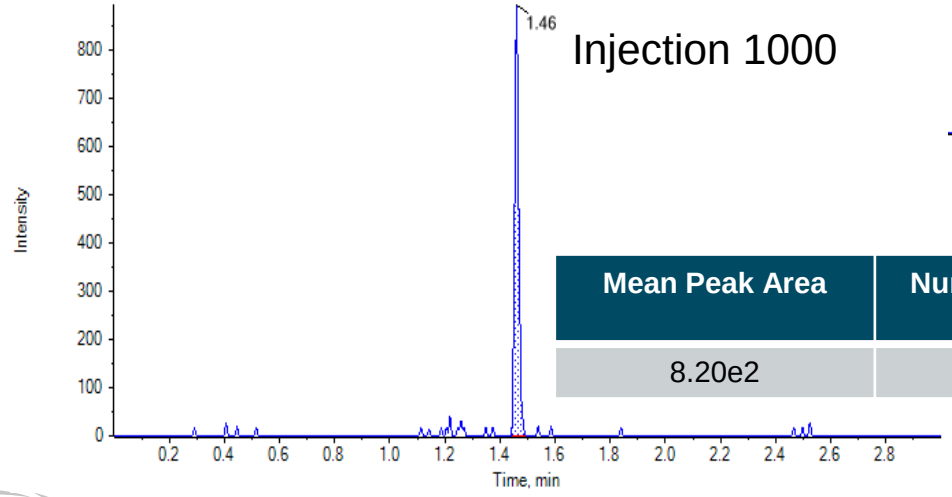


Injection 1

1.8 second peak width – with 5 multiplexed MRM^{HR} experiments



Injection 502



Injection 1000

Mean Peak Area	Number of Values (n=)	Percent CV	Accuracy
8.20e2	540	9.58%	103%

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Thank You For Your Attention
Questions & Answers

For Research Use Only. Not for use in diagnostic procedures.

AB Sciex is doing business as SCIEX.

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