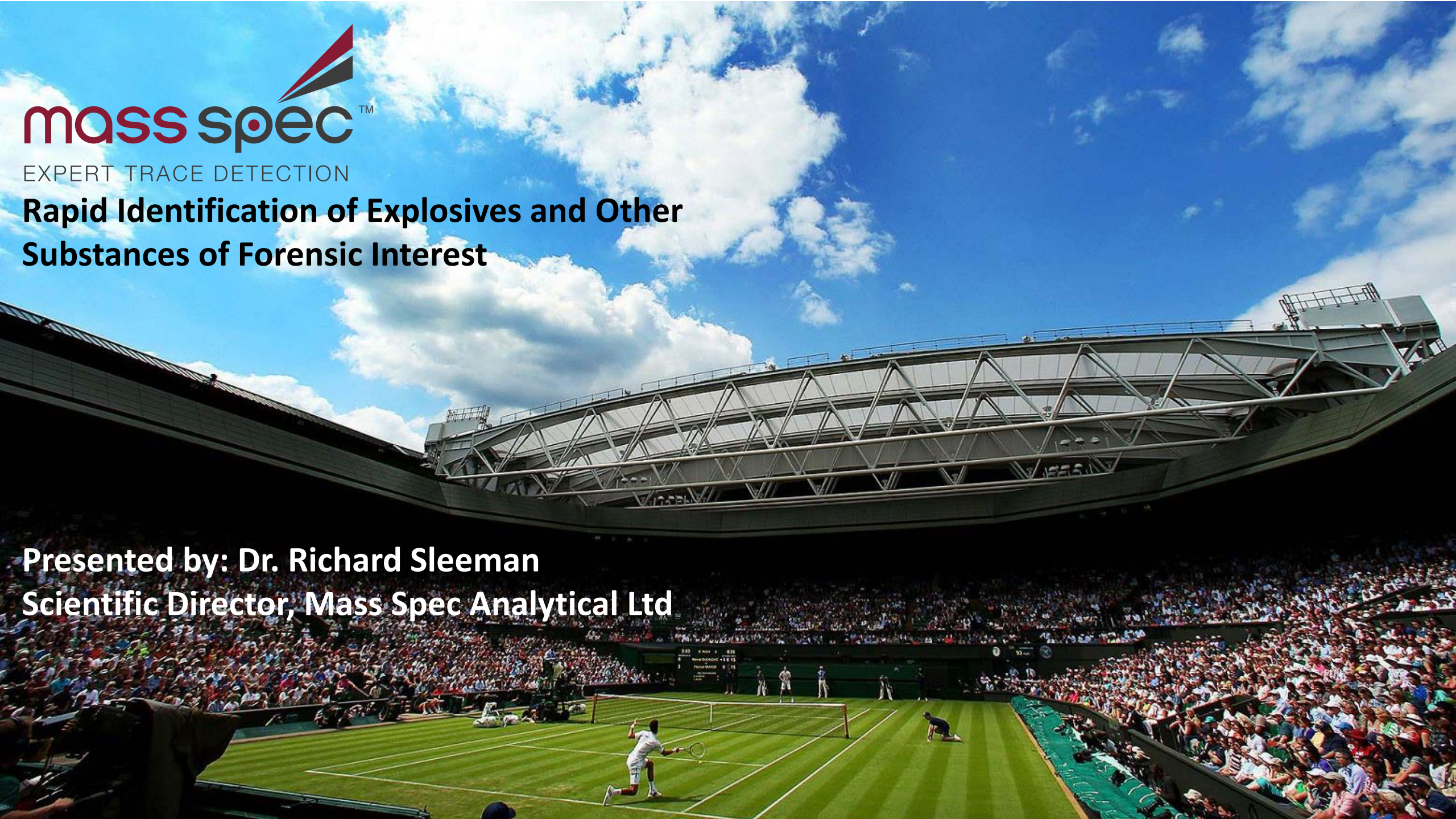

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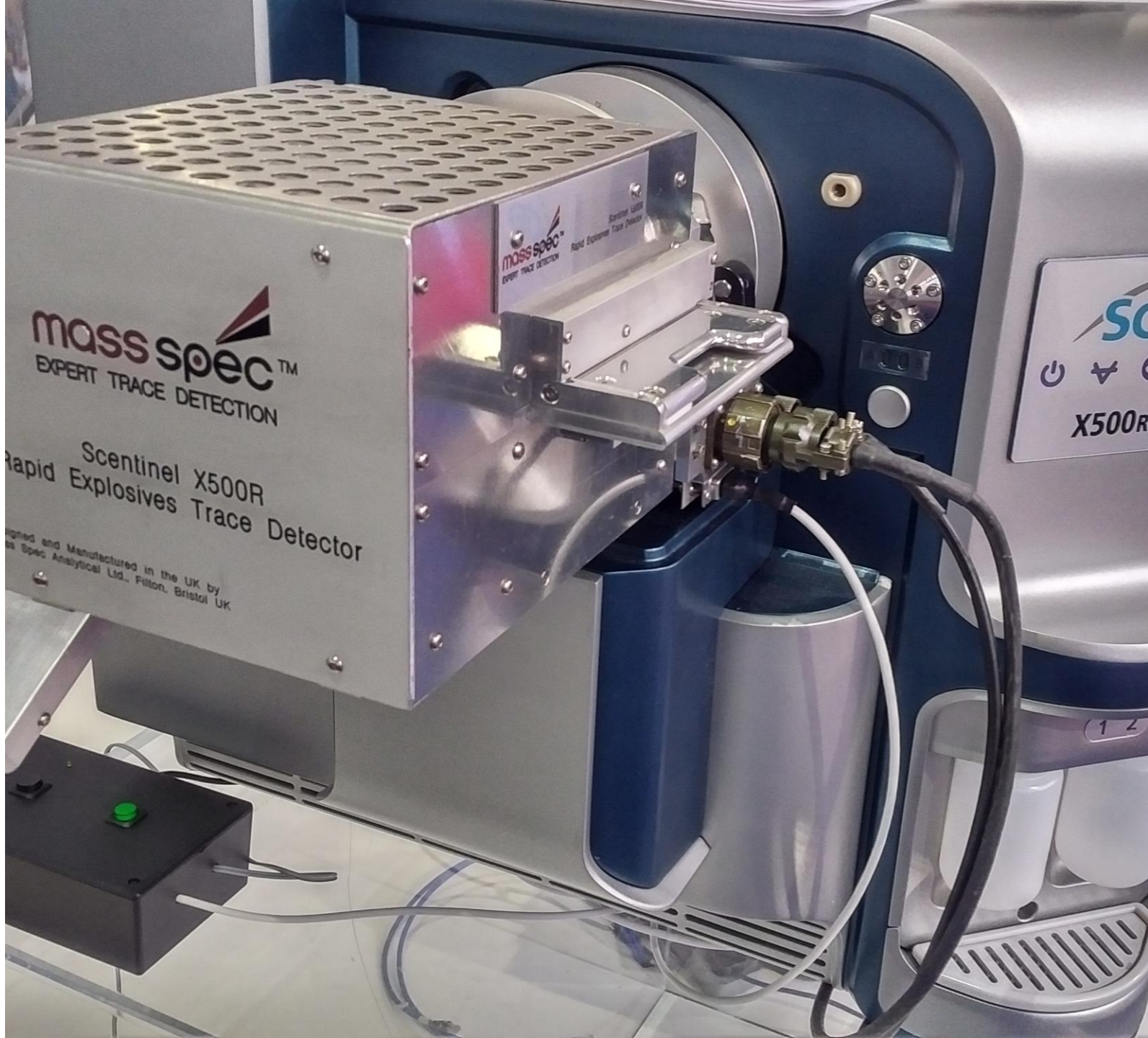
EXPERT TRACE DETECTION

Rapid Identification of Explosives and Other Substances of Forensic Interest

Presented by: Dr. Richard Sleeman
Scientific Director, Mass Spec Analytical Ltd

Who we are

- A spin-out of of British Aerospace, established over 20 years in Bristol
- We design and build in the UK mass spectrometer ion sources and field transportable mass spectrometers
- We are ISO 17025 (UKAS) accredited and provide forensic services to law enforcement organisations and private corporations around the globe
- Our expert evidence involving trace detection has been presented to courts of law for thousands of cases



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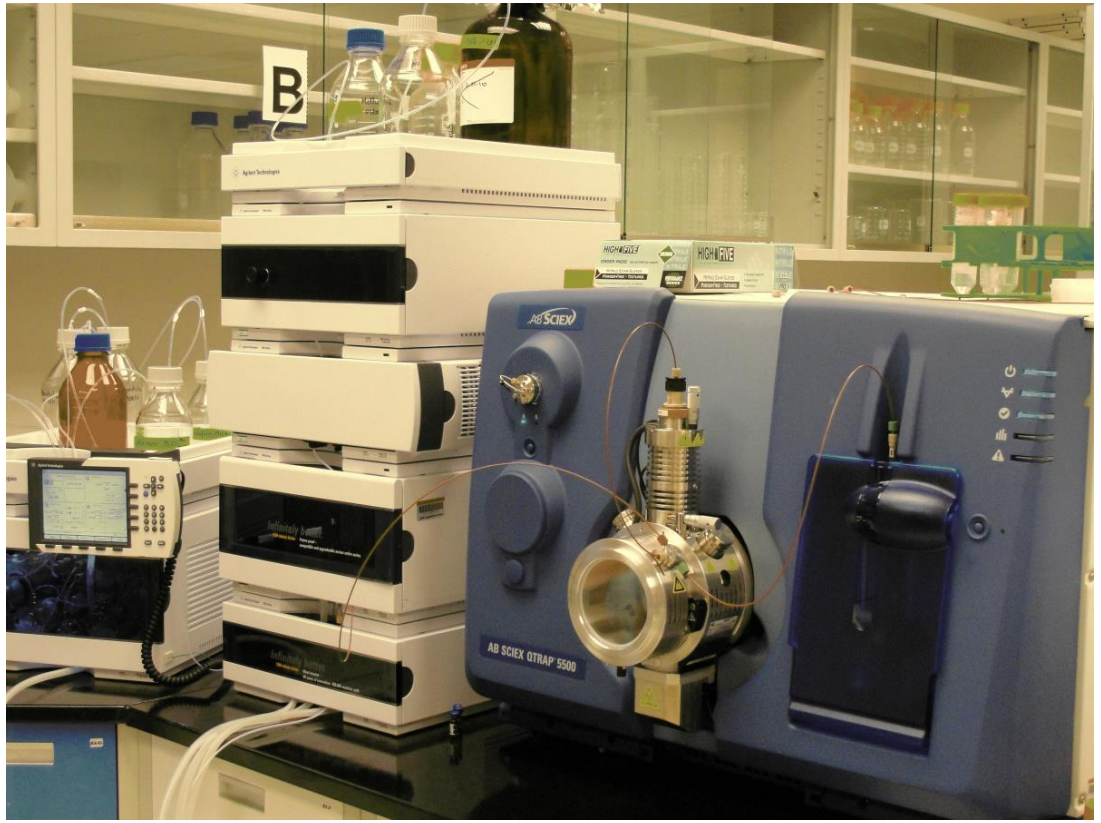
Alternatives to GC and LC

- GC and LC-MS are well established techniques over many years
- Main objective was to separate-out the target substance for analysis
- i.e. only one substance goes into the mass spec at a time – which in turns help eliminate matrix effects
- Needed retention time and mass spec spectrum



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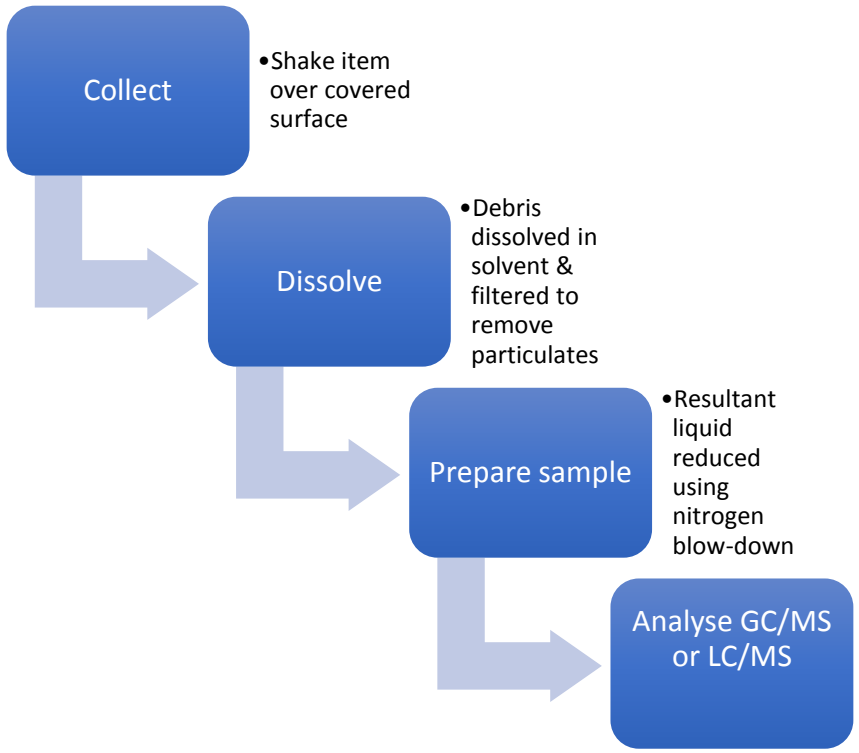
Need for speed

- **Applications that require rapid identification and high selectivity (identification point criteria) need a new approach**
- Nowadays, mass spectrometers can do a lot more
- For many compounds you no longer need to separate out the different constituents
- That being the case, chromatography is no longer a requirement – especially for small molecule applications such as drugs and explosives.

Conventional methods

- **GC and LC – Time, chemicals, gas, glassware**
- Conventional trace substance detection methods are time consuming and expensive
- Location of traces lost
- Evidence may be compromised during testing process



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Intro to Thermal Desorption

- We have developed a range of thermal extraction ion sources (TEIS) for testing particles, liquids and vapour
- We couple the TEIS devices to Sciex triple quad and QTOF mass spectrometers controlled by our bespoke application software
- Fast, no sample preparation, ideal for field deployment and suitable for a wide range of substances.
- The result is a product that can detect illicit drugs, explosives, and many other substances with virtually no false positives
- The system can test hundreds of samples per hour with no loss of performance

TEIS-3200-HB Hot Block Desorber with Sciex API3200 Triple Quad Mass Spectrometer

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The simpler the process, the less that can go wrong….

LCMS

With LCMS, you have to show that every item which may come into contact with an exhibit is clean:

- Gloves
- Tweezers
- Swab (if used)
- Solvent used to extract the trace
- Vials and caps
- Syringes
- Derivatising agents
- etc., etc.

Thermal Desorption

With TEIS, you take a swab and analyse it directly, all you have to prove is that the swab (and by inference, the hands holding it) are free of contamination:

- Swab (if used)
- Hand/glove holding it

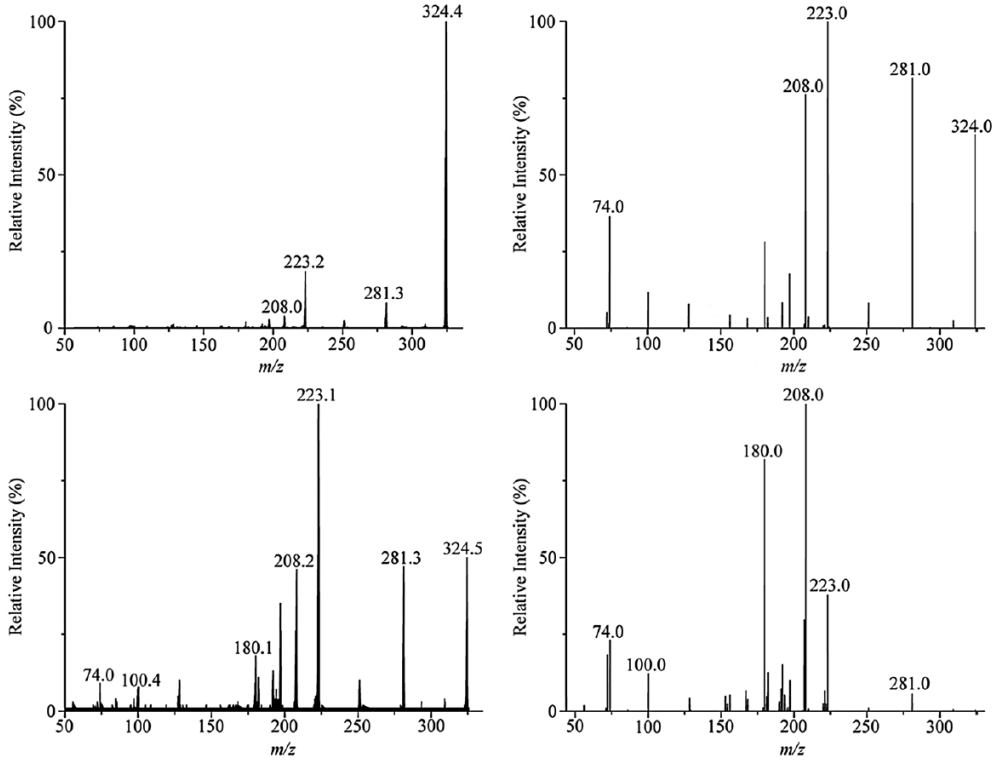
The TEIS is self-purging so there is no clean-up required between tests

Peer-reviewed study validates method

A recently published paper* demonstrates the capability of using thermal tandem mass spectrometry (MS/MS) for the identification of substances of abuse and related compounds without the need for chromatography.

- MS/MS was shown to be capable of the identification of the same drugs within the samples as the conventional method of GC/MS, but with better sensitivity and shorter analysis times.
- The run times of chromatographic techniques can vary from a few minutes to hours per sample. For the analysis of drug samples by GC/MS, a 15-min run time is typical.
- Quasi real-time vs. 9s for autosampler

*The paper, published in Rapid Communications in Mass Spectrometry, 15 April 2016 is authored by CM Fletcher, Department of Physical Sciences, University of Kent at Canterbury, and R Sleeman, Mass Spec Analytical Ltd.



How reliable is MS/MS without chromatographic Separation? MS/MS spectra of a sample suspected of containing LSD at collision energies of 20 eV (top left) and 30 eV (bottom left) compared with a NIST MS/MS library spectrum of LSD at 22 eV (top right) and 32 eV (bottom right).

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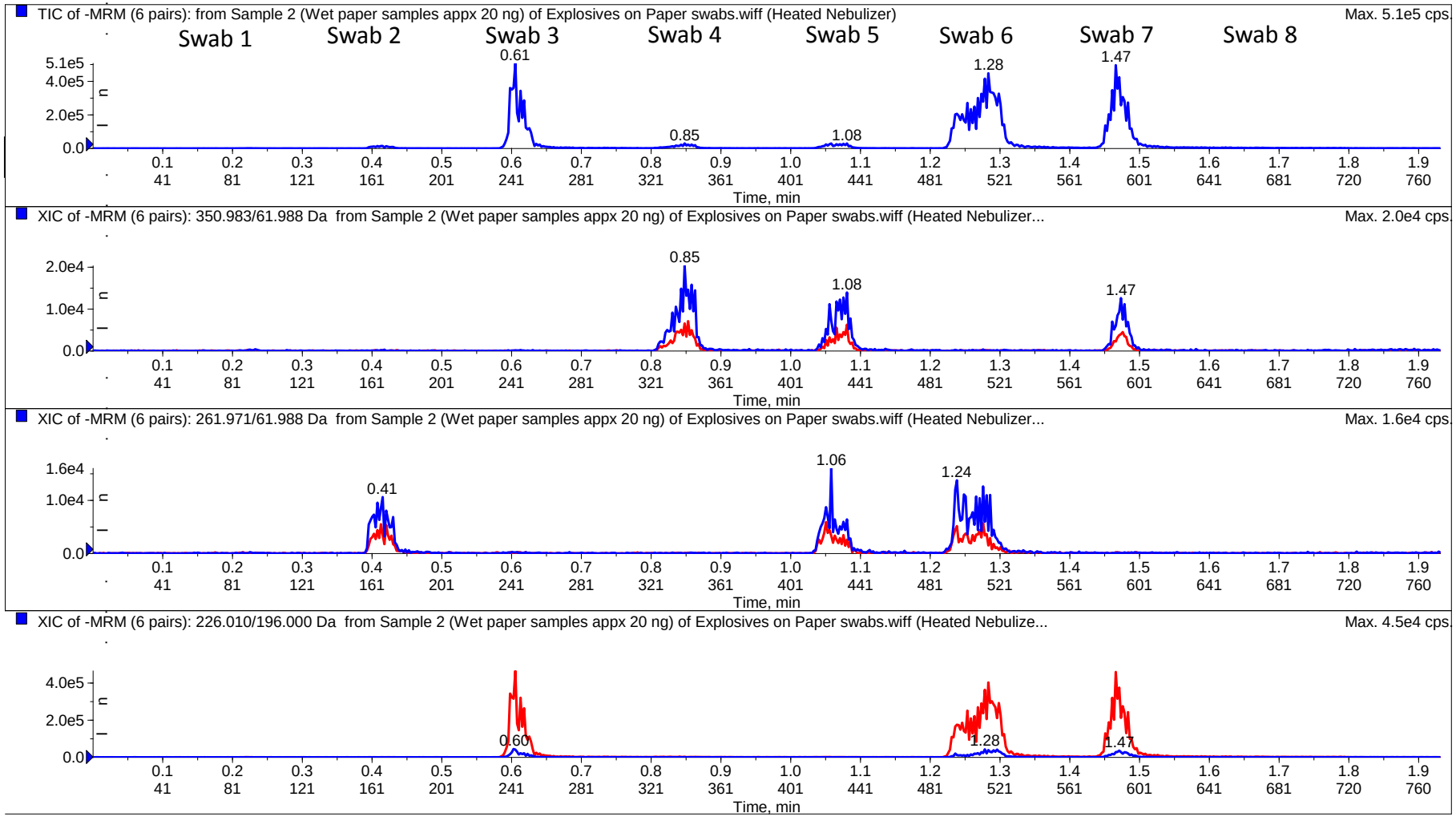
Examination of explosives from swabs



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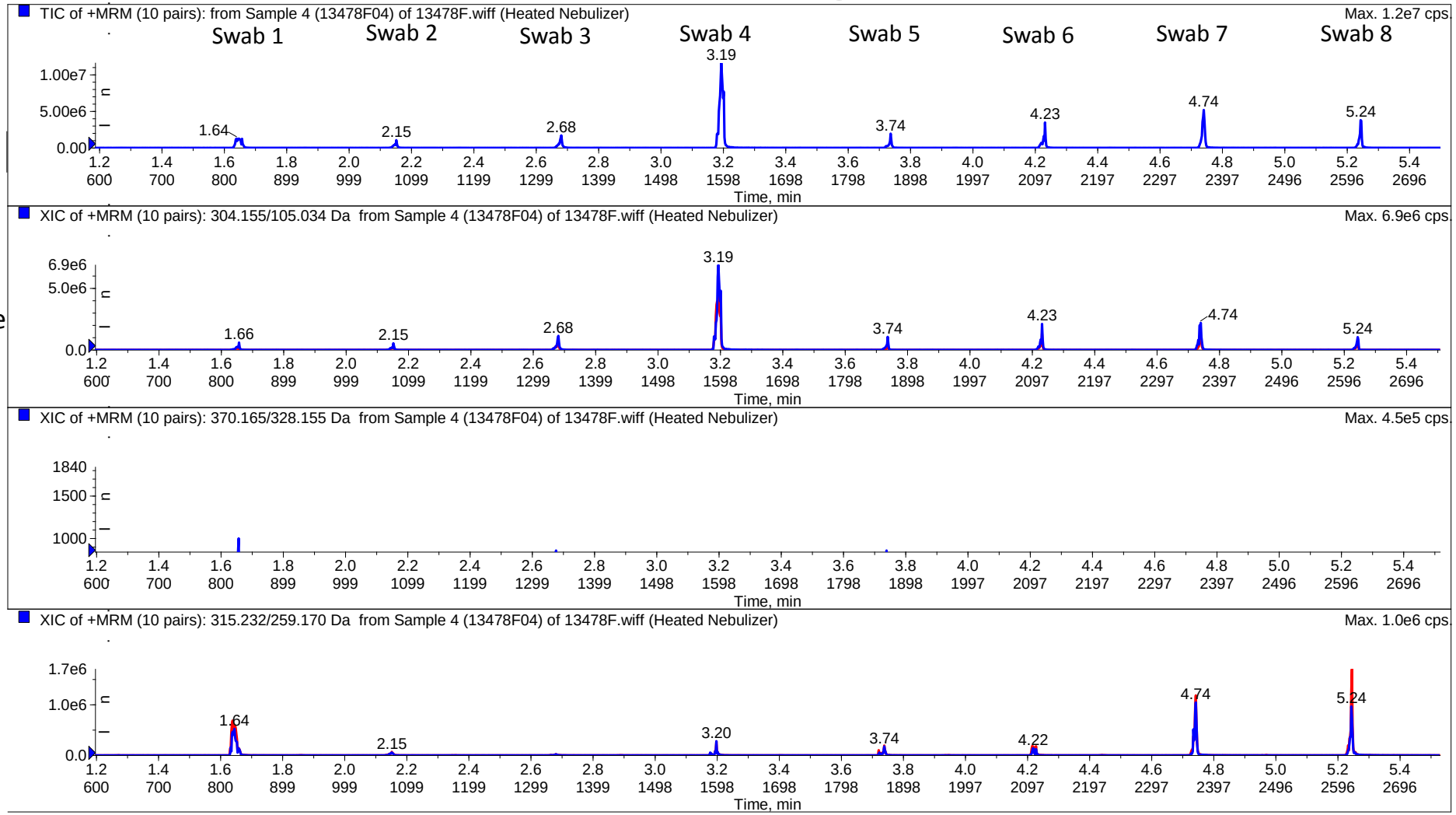
Examination of drugs from swabs



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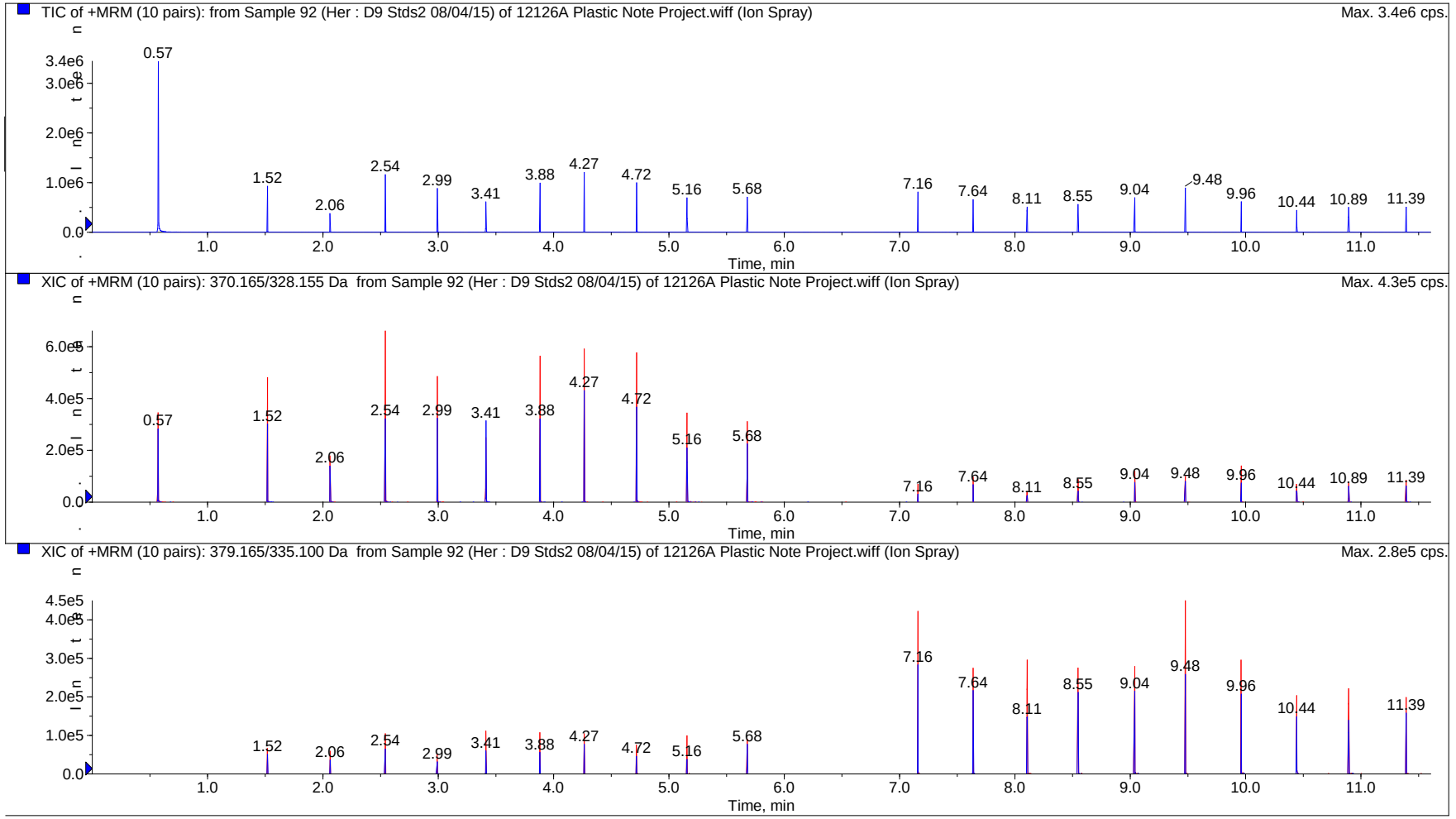
Quantification with deuterated standards



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Analysis of explosives using SWATH

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BMSS* Inter-laboratory Comparison

Participant	Technique	MS Platform	PARA1	TNT1	HMX1	CHOL1	ALD1	PEG1	DIE1	DIE2	DIE3	BEN1	PARA Curve	TNT Curve
AIG01 vapor	DART vapor	ToF												
AIG01 no vapor	DART no vapor	ToF												
AIG03	Nanomate nanospray	Ion Trap												
AIG04	ASAP	QqQ												
AIG06 Glass	DART - Glass Rods	Ion Trap												
AIG06 Mesh	DART - Mesh	Ion Trap												
AIG08 Thermo	ASAP	Orbitrap												
AIG08 Waters	ASAP	ToF												
AIG11	AP MALDI	QToF												
AIG12	ASAP	QqQ												
AIG13	ASAP	ToF												
AIG14	ASAP	QToF												
AIG15	ASAP	Quad												
AIG16	Dart	Orbitrap												
AIG17	**Thermal Desorption CDI**	**QqQ**												
AIG18	ASAP	QqQ												
AIG19	DART	Ion Trap												

- BMSS set out to test five different ambient ion source techniques with 5 different types of mass spec
- Mass Spec Analytical (lab AIG17 in the report) is one of three labs to successfully detect all the target substances in the trial. The other two successful labs used an Atmospheric Solids Analysis Probe method.

* British Mass Spectrometry Society, Ambient Ionisation Special Interest Group Inter-laboratory Study, 1 June 2016

High Security events: case study

- High sensitivity and selectivity of the TEIS-Sciex MS system render it ideal for screening large venues, concert halls or stadia
- High sensitivity delivers a better chance of identifying a threat
- High selectivity reduces the chances of false alarms
- Mobile systems, mounted in vans, are in use by the UK police to screen high-security events

Scentinel deployed as a mobile trace detection system

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Choose your mass spec

API3200 V-Series

- Ideal for targeted detection
- Available now, based on the Sciex API 3200 Triple-Quad and other V-Series Mass Spectrometers
- Combines high-sensitivity and selectivity with a rugged, reliable compact package
- Deployed with North American Border Agencies

X500R QTOF

- Ideal for Unknown Substance Screening
- Available Q2 2018, based on the Sciex X500R QTOF Mass Spectrometer
- First High-Resolution portable QTOF mass spec for accurate mass measurements in the field. Massively increases the substances that can be detected.
- Delivers real-time and retrospective analysis in a single package

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Further reading and References

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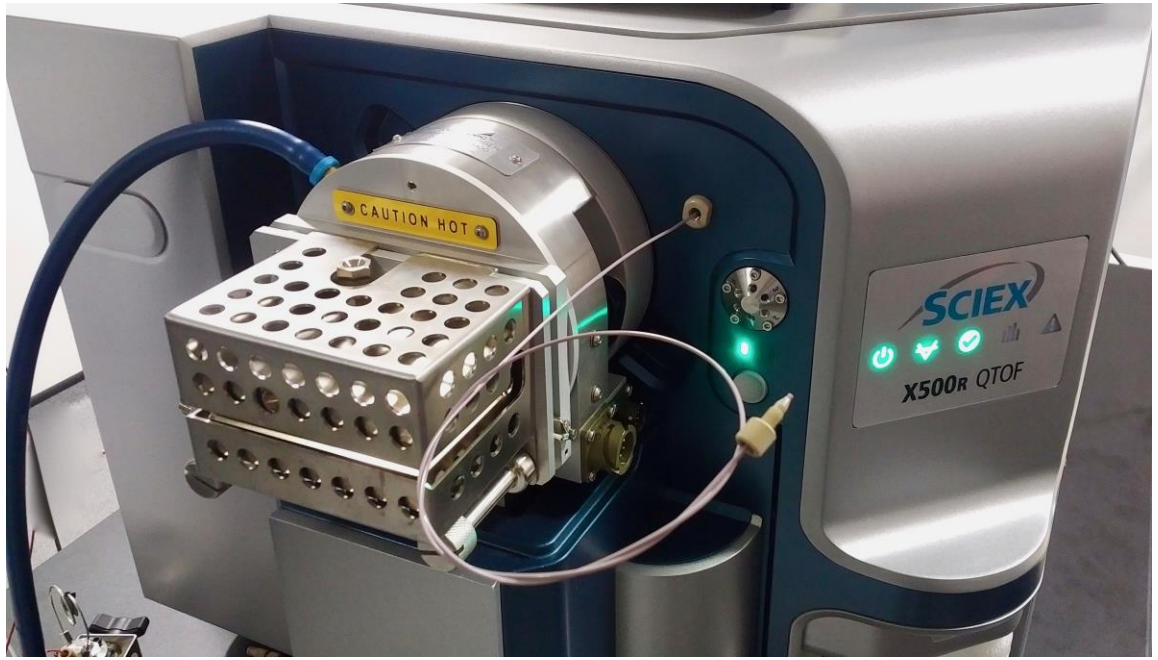

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Thank you!

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