BRUKER

HIGH RESOLUTION QTOF MS

impact II VIP

Higher Performance, More Confidence, More impact

Innovation with Integrity

Built to discover more – impact II VIP

The impact II VIP is designed to provide the most efficient ion transmission from atmospheric pressure to high vacuum, with minimized ion loss and reduced maintenance due to the use of dual ion funnel technology.

Wide dynamic range at LC speed

With its 50 Gbit/s data sampling, the system offers a dynamic range of >5 orders of magnitude intra-spectral dynamic range at full sensitivity and enables a detailed insight into your samples - from complex mixtures with different ionizabilities to the detection of trace components in complex matrix samples. Without compromising on sensitivity and resolution, the impact II VIP is a powerful and versatile tool for every workflow.

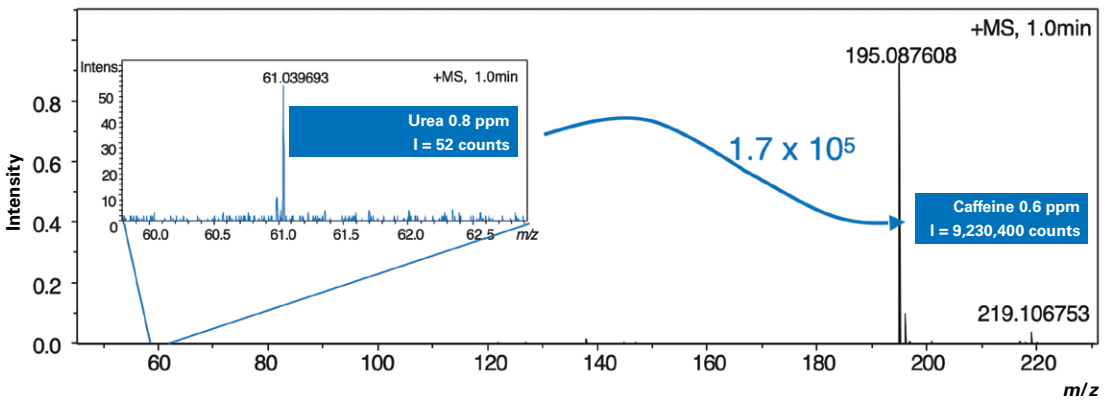


Figure 2 >5 orders of magnitude intra-spectral dynamic range at 1 Hz data acquisition rate. No absence of peaks with low frequency, such as urea in this example.

System robustness and sample protection

Every stage of sample processing is built to provide complete information about your samples, day in and day out. A layer of vacuum between the ESI probe heater and the HPLC eluent dramatically reduces heat transfer from the ceramic heater to the sample. Active exhaust traps effectively capture nebulized gases, preventing their recirculation. This is achieved through a tailored pressure differential between the ionization chamber and the system exhaust, greatly enhancing robustness by reducing system contamination. The long lifetime of the MCP detector further contributes to the impact II VIP QTOF's reliability. With no scintillator required, the lifetime of the detector is far longer, reducing operational downtime and maintenance expenses.

VIP-HESI – Unmatched sensitivity for advanced analytical precision

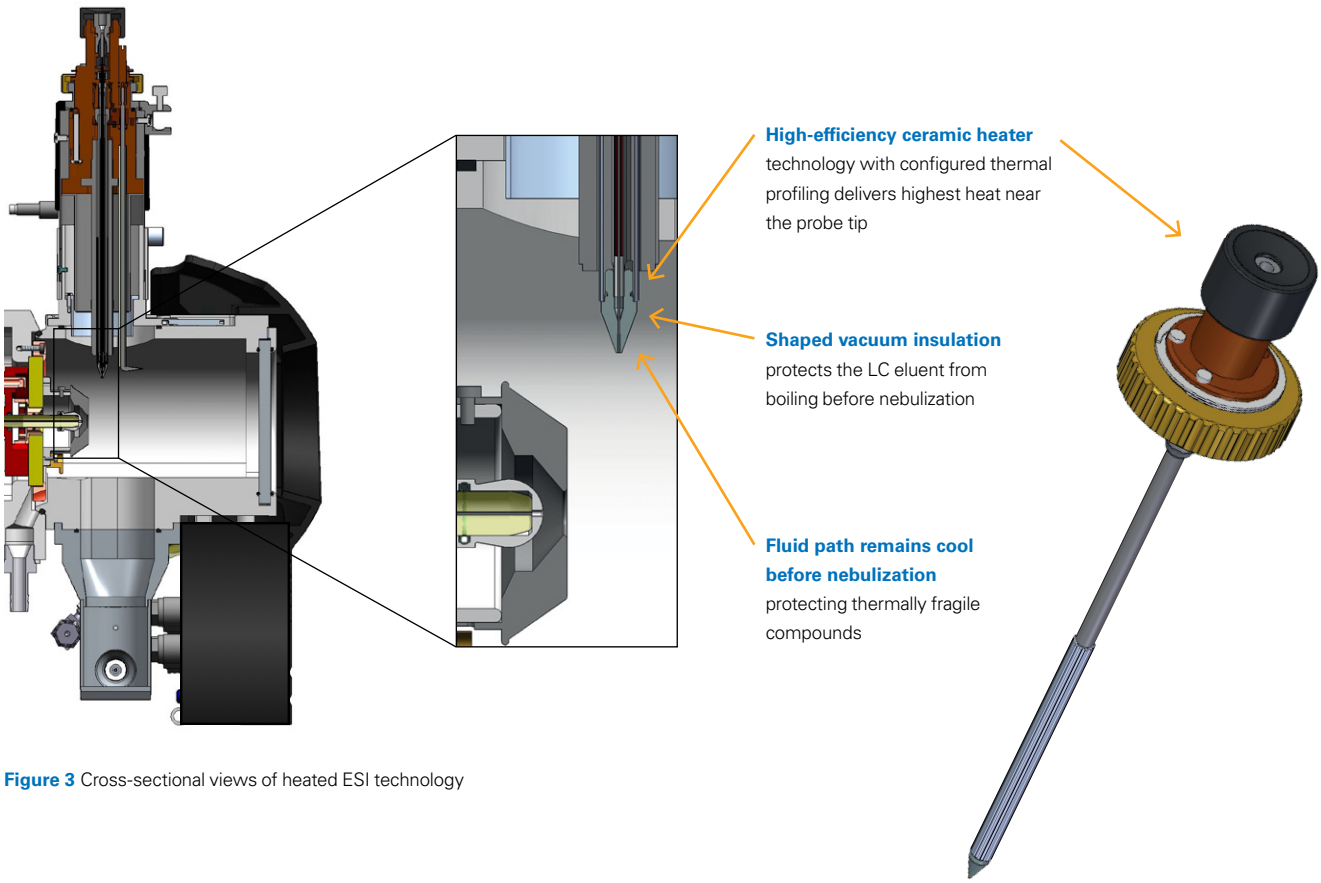


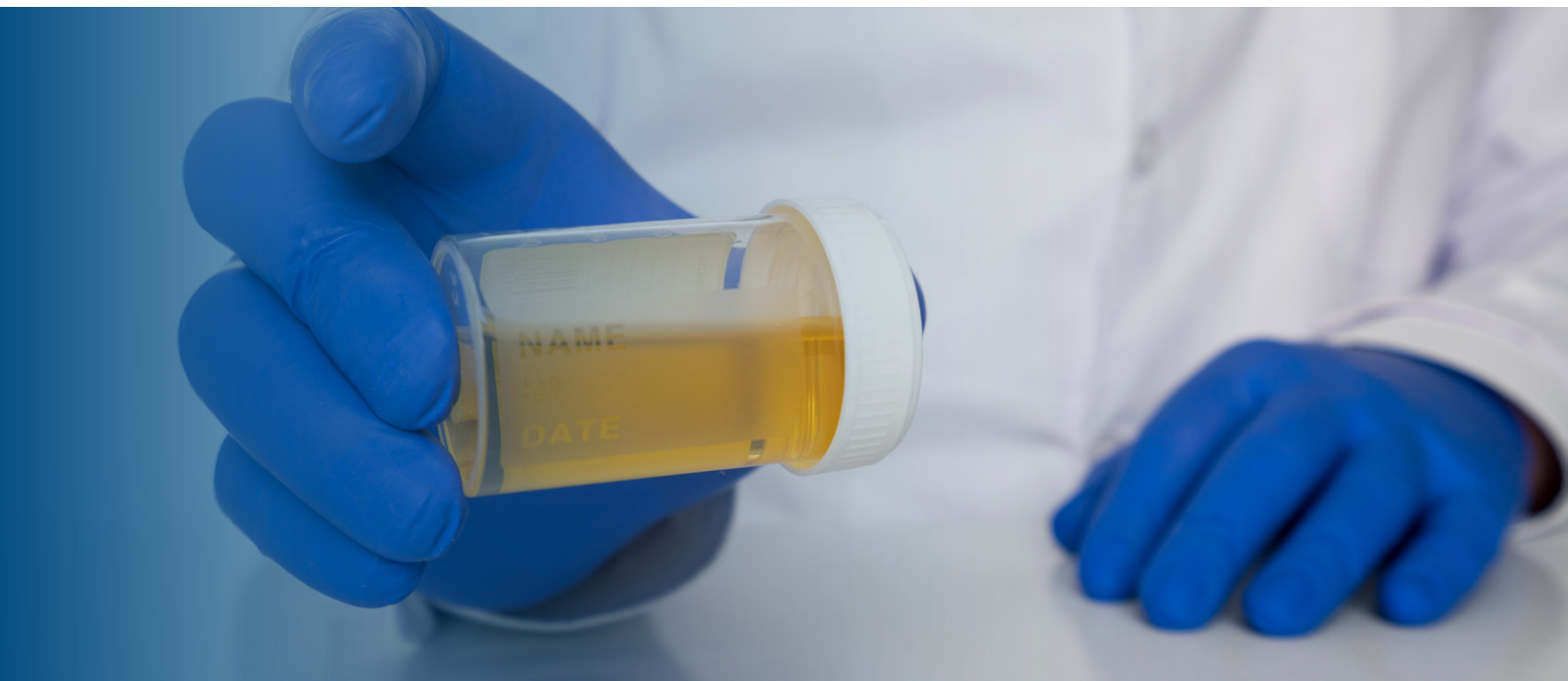
Figure 3 Cross-sectional views of heated ESI technology

Sensitivity, speed, and precision: The metabolomics workhorse

Metabolomics applications demand high precision measurement for the accurate comparison of metabolic profiles across samples. Changes in instrument performance - including signal loss over time - directly compromise the quality of metabolomics data where it matters the most. The impact II VIP is designed to provide high precision measurements that you can count on, with proven stability to maintain high data quality to meet the needs of today's large-scale metabolic research.
Enhancing QC monitoring through RealTimeQC, integrated within TASQ® and MetaboScape® software, involves an initial step of carefully choosing QC analytes that are either naturally occurring in the samples or intentionally introduced (e.g., internal standards). These selected analytes serve as indicative markers for the broader metabolic profile and are subsequently fully monitored throughout the analysis.
Table 1 shows the summary of measurement quality [1] over 300 injections of human urine (NIST SRM 3672) for a series of analytes selected to represent the total metabolic profile. The median %RSD of all feature peak areas determined by TASQ software across all 300 injections was 9.56% without adjustment (e.g., within-batch correction or normalization).

Table 1 Summary of measurement quality over 300 injections of human urine.

	Peak Area [% RSD]	StdDev mass error [ppm]	mSigma (median value of max 1000)
Butyryl-L-carnitine	7.63	0.483	5.12
Glutamine	3.38	0.625	3.04
Isoleucine	3.50	0.470	1.17
Isovalerylcarnintine	9.86	0.486	2.75
Leucine	2.96	0.496	1.23
O-Desmethyl-cis-tramadol	7.69	0.490	3.05
Phenylalanine	4.39	0.442	2.90
Uric acid	3.67	0.440	8.33



Measurement quality over time: RealTimeQC visualization

While the raw data maintained consistent high quality, real-time monitoring proved crucial for evaluating potential deviations. RealTimeQC offers an intuitive visualization tool to inspect both random and systematic variations, unveiling potential trends in data over time and emphasizing measurement outliers.

Figure 5 Development of peak area (Top), mass accuracy (middle) and isotopic fidelity (bottom) over 300 injections.

Click on the image for more information

A complete system, ready to meet critical application needs

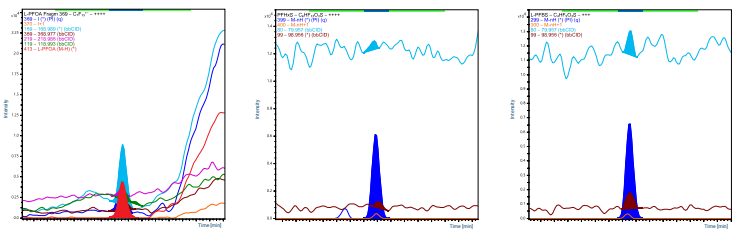
- Ultimate sensitivity with VIP-HESI
- Unmatched stability in measurement performance
- No compromise in full sensitivity resolution (FSR)
- Isotopic pattern fidelity, facilitating molecular formula generation
- Bruker's proven reliability for consistent, worry-free operation

[1] Data was acquired using a method adapted from the open platform standard operating procedure: Lewis M, Chekmeneva E, Camuzeaux S, Sands C, Yuen A, David M, et al. An Open Platform for Large Scale LC-MS-Based Metabolomics. ChemRxiv. Cambridge: Cambridge Open Engage; 2022; https://chemrxiv.org/engage/chemrxiv/article-details/61ebd6fa0716a8529e3823dc.

Providing exceptional sensitivity for targeted quantitation and routine testing

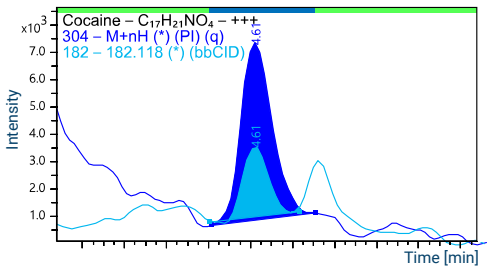
The new impact II VIP QTOF was designed for ultimate performance and provides the highest sensitivity due to the unique dual VIP-HESI ion source. The improved source design, based on a new Vacuum Insulated Probe (VIP) and a Heated ElectroSpray Ionisation (HESI), also offers improved ionization efficiency and reduced fragmentation, increasing sensitivity relative to conventional ion sources. The powerful dual-source system of an Atmospheric Pressure Chemical Ionization (APCI) probe with VIP-HESI dramatically extends analytical power for the most demanding applications.

Quantitation of PFAS compounds with highest sensitivity



PFOA, PFHxS and PFBS at 1 ng/L concentration in drinking water, RSD <5%. The sensitivity meets all current EU and proposed US EPA regulatory requirements.

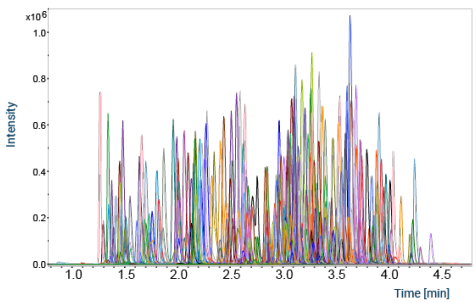
Quantitation of Cocaine



Cocaine in a hair sample at a final concentration of 0.03 ng Cocaine/mg hair.

https://doi.org/10.1016/j.jchromb.2020.122263)

294 Pesticides in just 5 min run time

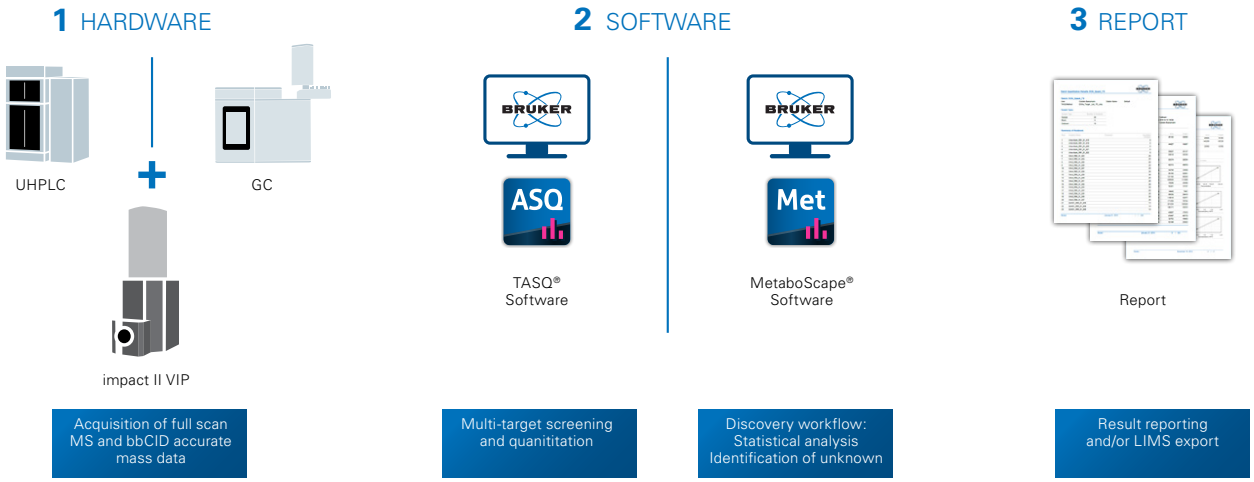


Quantitation of 294 pesticides in wheat matrix at 5 min run time. Zoom: EIC overlays of Methamidophos at concentration levels of 1.25, 2.5 and 5 ng/mL.

Click on the image for more information

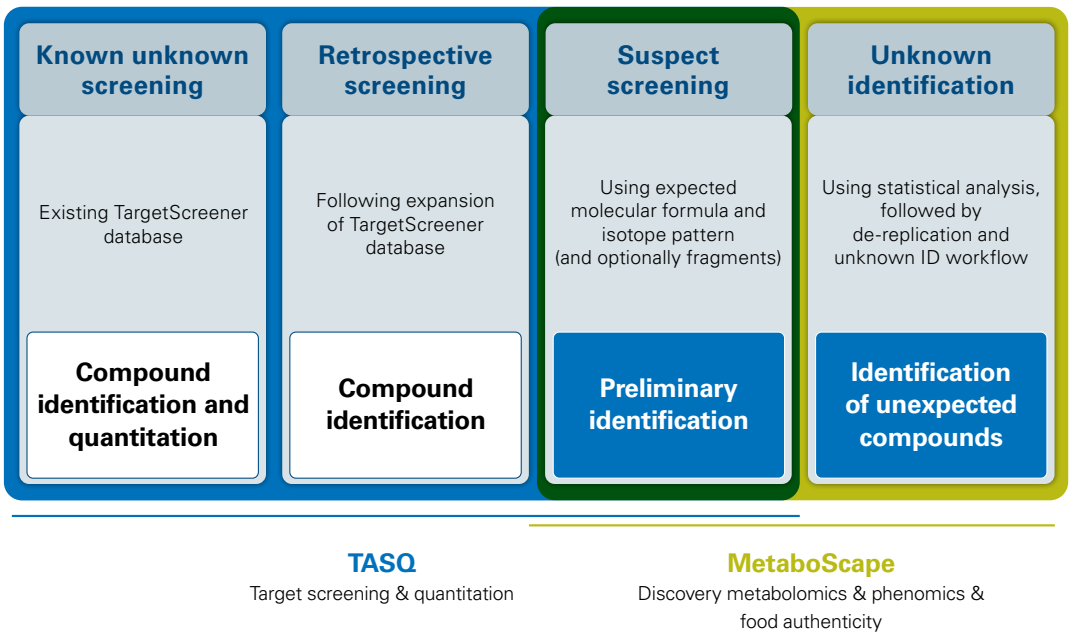
TargetScreener HR: One workflow – all the answers

TargetScreener is the combination of reliable data, powerful software and hardware, and a robust database for truly meaningful results. TargetScreener HR – driven by TASQ – allows data generation from 'vial to report' in seven clicks. Achieving comprehensive screening, both targeted and non-targeted, is essential for comprehensive results. This approach minimizes the occurrence of false positives and false negatives, ensuring maximum quality. Additionally, accurate and precise quantitation adheres to strict regulatory guidelines, underlines the robustness of the methodology.



Full array of identification workflows

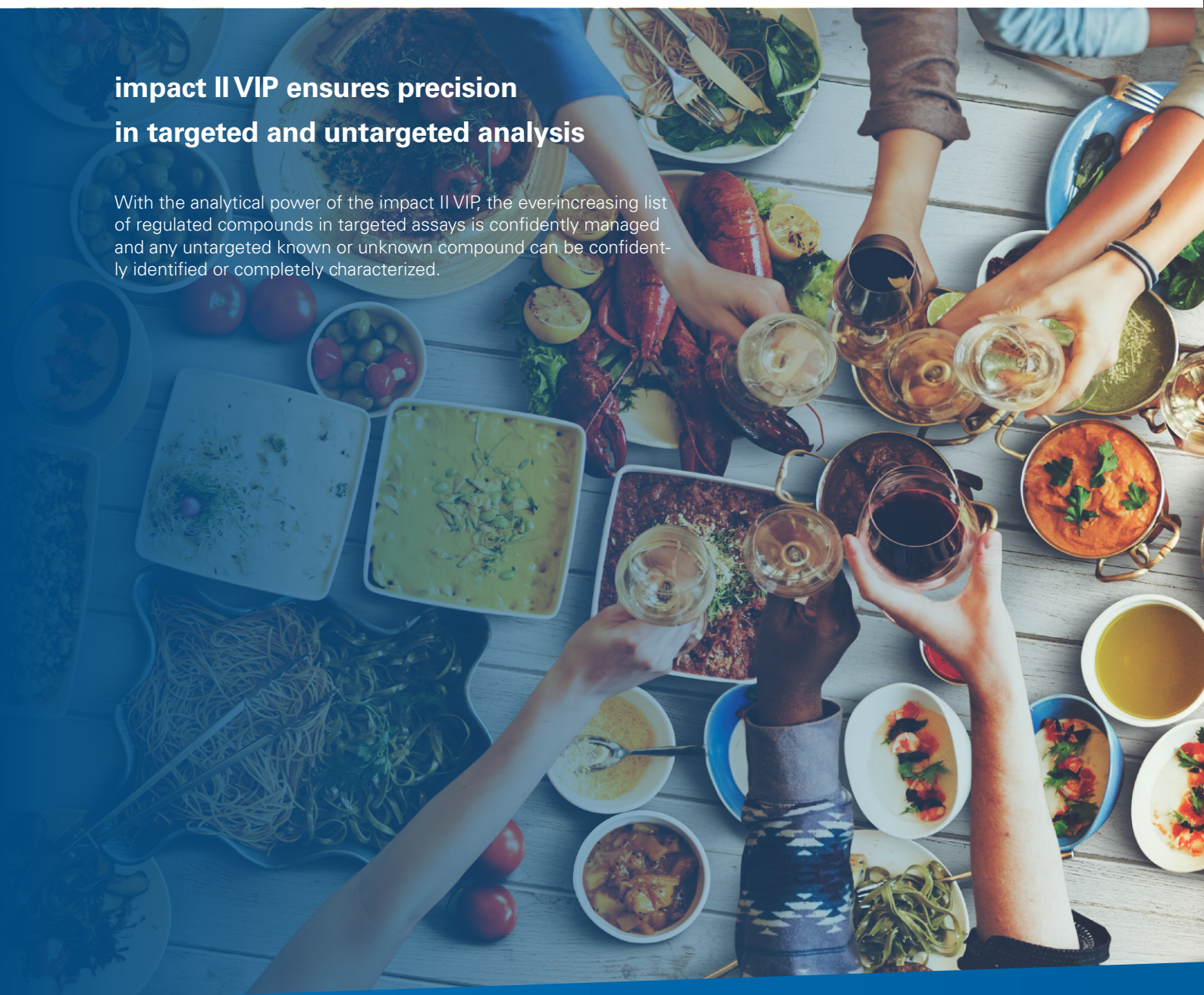
Bruker's TASQ and MetaboScape software packages facilitate the processing of both targeted and non-targeted workflows. TASQ supports various screening methods and offers precise quantitation through available calibration curves that were generated after calibration. MetaboScape employs statistical analysis to uncover unexpected compounds and identifies 'known unknowns' by utilizing public databases and spectral library searches, such as the MetaboBASE® library and NIST 2023.



Resolving food quality and food safety analysis challenges

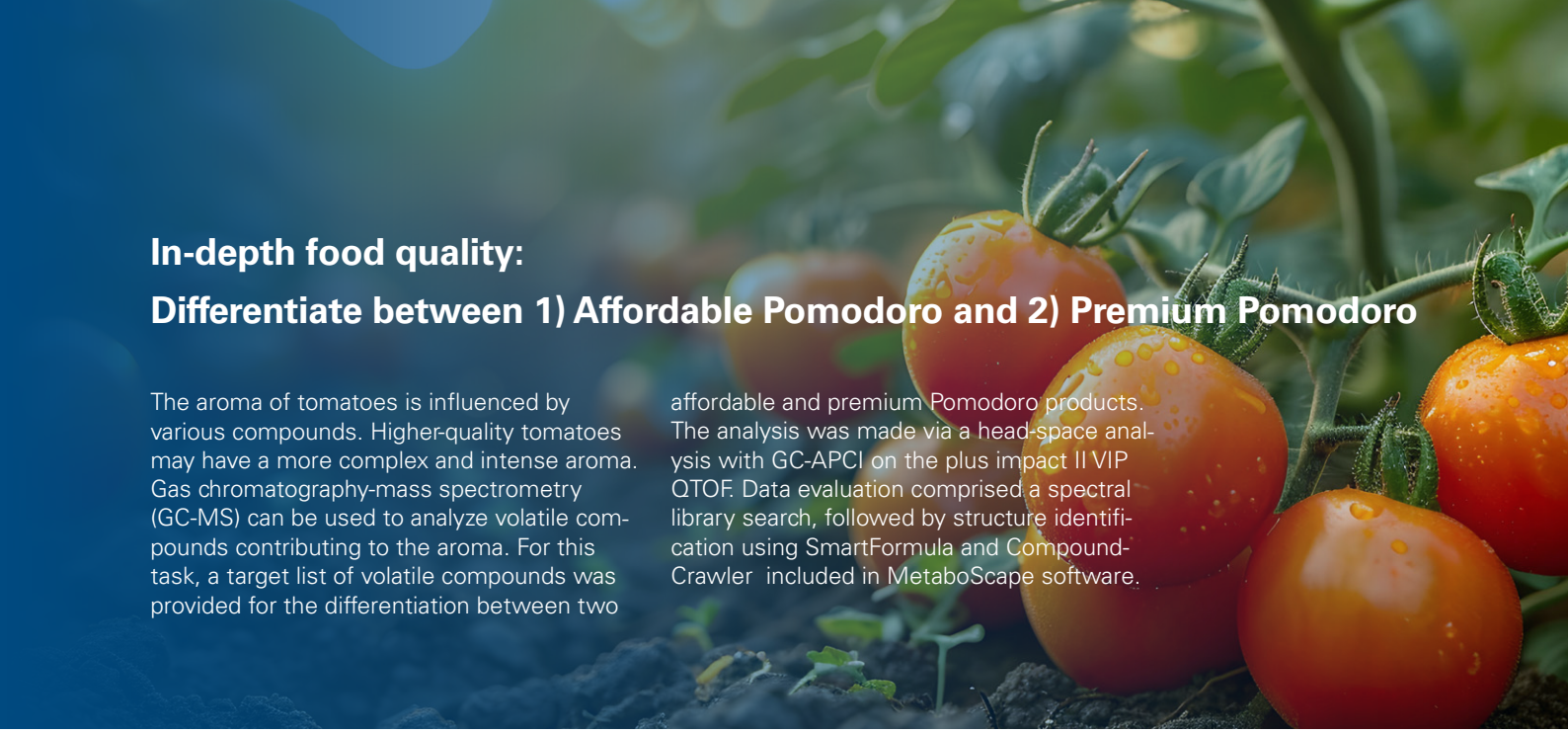
Empowering food quality & safety

Whether rapid screening raw materials and finished products for food quality or solving food safety contaminant screening challenges, the impact II VIP QTOF delivers, high sensitivity, high data acquisition speeds, and high data quality for absolute confidence in targeted and untargeted method workflows.



impact II VIP ensures precision in targeted and untargeted analysis

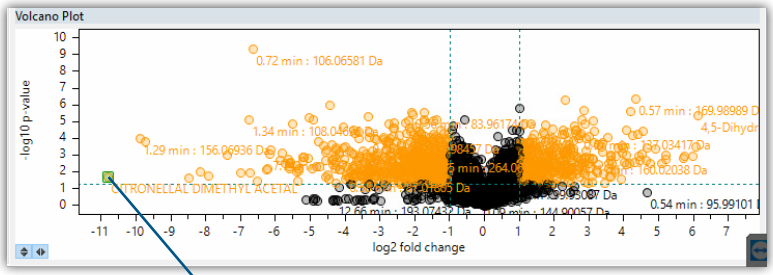
With the analytical power of the impact II VIP, the ever-increasing list of regulated compounds in targeted assays is confidently managed and any untargeted known or unknown compound can be confidently identified or completely characterized.



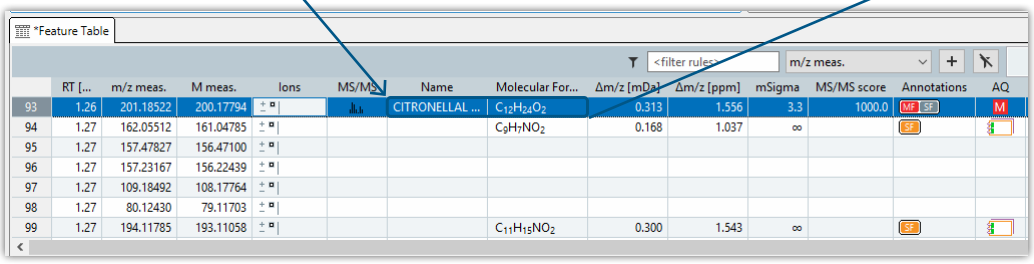
In-depth food quality:
Differentiate between 1) Affordable Pomodoro and 2) Premium Pomodoro

The aroma of tomatoes is influenced by various compounds. Higher-quality tomatoes may have a more complex and intense aroma. Gas chromatography-mass spectrometry (GC-MS) can be used to analyze volatile compounds contributing to the aroma. For this task, a target list of volatile compounds was provided for the differentiation between two affordable and premium Pomodoro products. The analysis was made via a head-space analysis with GC-APCI on the plus impact II VIP QTOF. Data evaluation comprised a spectral library search, followed by structure identification using SmartFormula and CompoundCrawler included in MetaboScape software.

1. t-Test/ANOVA Result Table and Volcano Plot

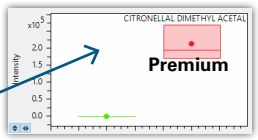


2. Selection of the interested feature in the Volcano Plot



	RT [...	m/z meas.	M meas.	Ions	MS/MS	Name	Molecular For...	Δm/z [mDa]	Δm/z [ppm]	mSigma	MS/MS score	Annotations	AQ
93	1.26	201.18522	200.17794			CITRONELLAL ...	$C_{12}H_{24}O_2$	0.313	1.556	3.3	1000.0	MF SF	M
94	1.27	162.05512	161.04785				$C_9H_7NO_2$	0.168	1.037	∞		SF	
95	1.27	157.47827	156.47100										
96	1.27	157.23167	156.22439										
97	1.27	109.18492	108.17764										
98	1.27	80.12430	79.11703										
99	1.27	194.11785	193.11058				$C_{11}H_{15}NO_2$	0.300	1.543	∞		SF	

Intensity of the the selected feature in the Intensity Plot



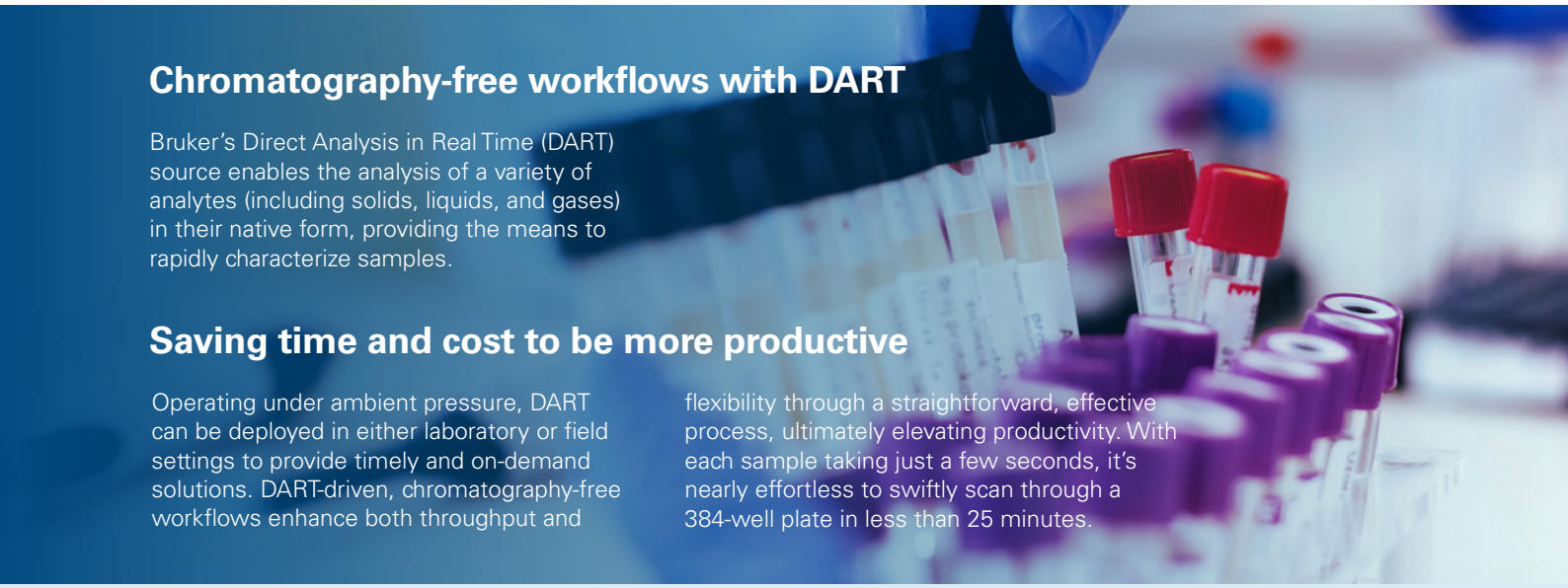
Affordable

3. Unknown ID workflow: SmartFormula -> CompoundCrawler -> MetFrag -> ID

Figure 6 View from the MetaboScape software. Initially, a t-Test/ANOVA Result Table and Volcano Plot were created (Step 1). Upon closer examination of the Volcano Plot (Step 2), a compound was identified that is not included in the target list (TL). This discrepancy became more evident in the Intensity Plot. After completing the unknown ID workflow (Step 3), Citronellal dimethyl acetal was identified. This aroma compound was absent in the Affordable Pomodoro sample.

Comprehensive forensic toxicology and seized drug analysis

Thorough forensic toxicology analysis with maximum confidence is routine with the impact II VIP QTOF. Accurate mass measurement of diagnostic ions, including the molecular ion, adducts, isotopes as well as broadband CID (bbCID) fragment ions provides full characterization of knowns and unknown toxins and significantly reduces drug screening false-positive findings, even in complex matrices such as post-mortem samples.

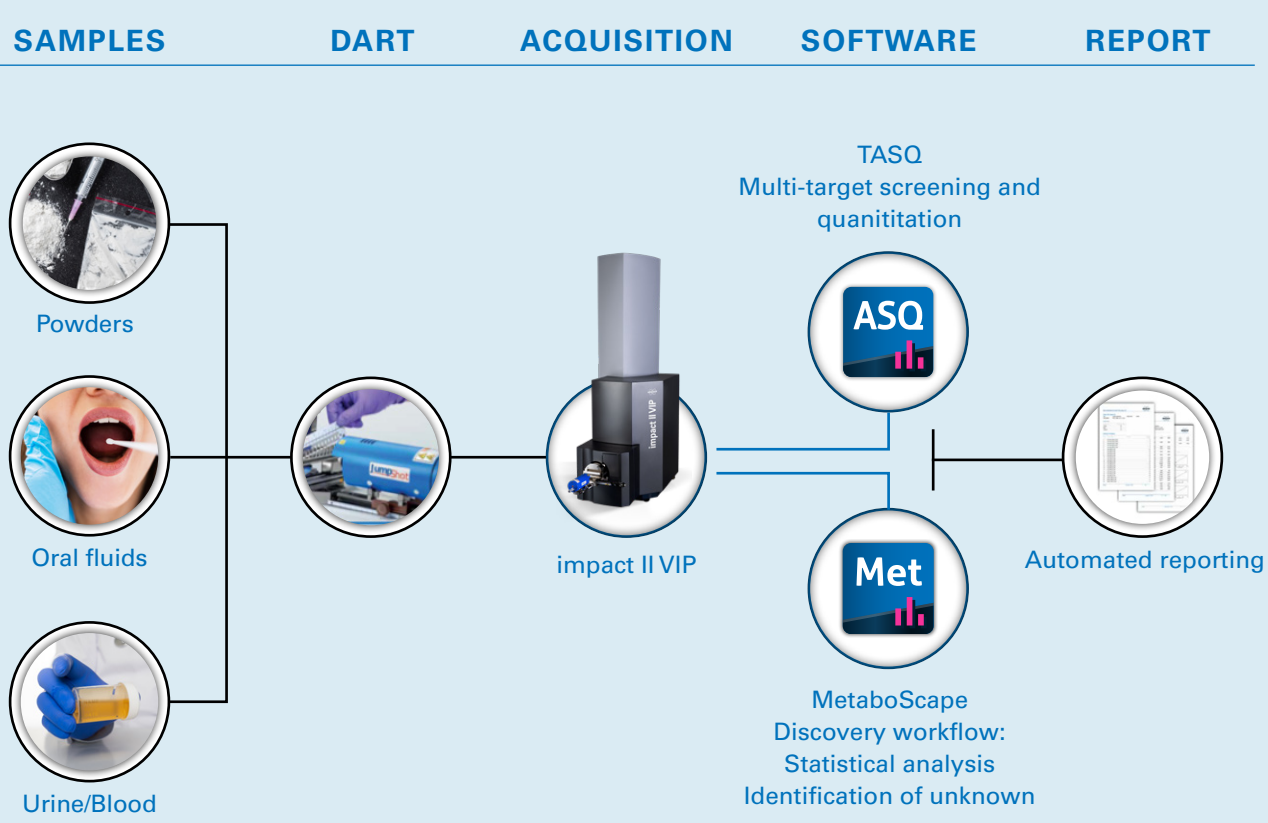


Chromatography-free workflows with DART

Bruker's Direct Analysis in Real Time (DART) source enables the analysis of a variety of analytes (including solids, liquids, and gases) in their native form, providing the means to rapidly characterize samples.

Saving time and cost to be more productive

Operating under ambient pressure, DART can be deployed in either laboratory or field settings to provide timely and on-demand solutions. DART-driven, chromatography-free workflows enhance both throughput and flexibility through a straightforward, effective process, ultimately elevating productivity. With each sample taking just a few seconds, it's nearly effortless to swiftly scan through a 384-well plate in less than 25 minutes.



Analysis of forensic paper samples using DART-HRMS

DART-HRMS is a profiling solution including plastics, seized drugs as well as for QC of raw ingredients and materials. In this example paper samples [2] found at routine controls in prisons are screened for synthetic cannabinoids and other drugs of abuse with DART-HRMS. Substances are usually either sprayed onto the paper or it was completely soaked with drug solution and dried.

The analysis time per sample is low, which enables a high sample throughput.

Samples were analyzed with DDA MS/MS and compounds were identified using library search.

- NIST DART-MS Forensics Database (2021)
- Maurer, Meyer, Helfer, Weber: LC-HR-MS/MS Library of Drugs, Poisons, and Their Metabolites
- NIST/EPA/NIH Mass Spectral Library 2023
- other libraries in different standard formats

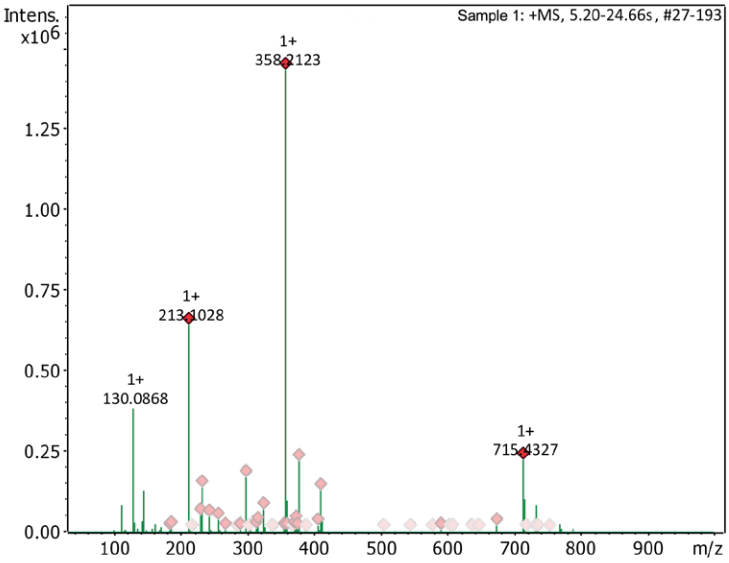


Figure 7. MS chromatogram of paper sample extracted with Methanol.

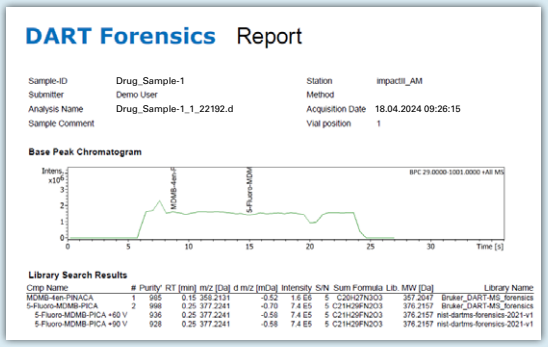
[2] Samples kindly provided by the Institute of Forensic Medicine of the University of Freiburg, Germany

Identification of MDMB-4en-PINACA and 5-Fluoro-MDMB-PICA

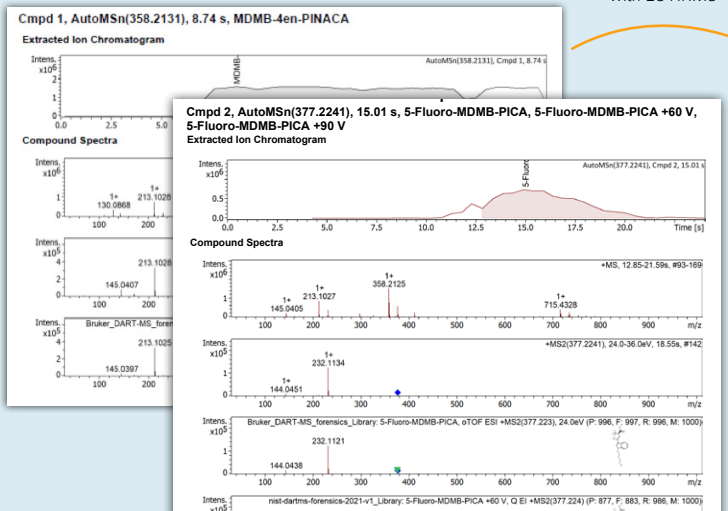
MDMB-4en-PINACA and 5-Fluoro-MDMB-PICA are indazole-based synthetic cannabinoids that have been sold as a designer drugs.

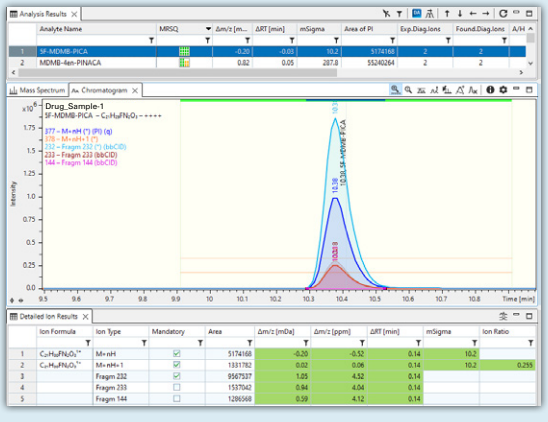
20 s/sample

Up to 200 MS/MS spectra



Confirmation with LC-HRMS





TargetScreener method was used for confirmation.

Cover the full spectrum of analytes

GC-APCI II

GC-APCI II source with unique flexible, heated transfer line and calibrant delivery enables GC coupling to any Bruker timsTOF or QTOF, or FTMS system.

APPI II

Atmospheric Pressure Photo Ionization is used for less polar or non-polar molecules that can not be ionized in either ESI or APCI.

CaptiveSpray 2

The CaptiveSpray 2 is the proteomics ion source that brings your MS to the next performance level, with operation as easy as performing electrospray but at nano-flow ranges.

Further reading

- AppNote LCMS 207: Quantitation of PFAS in water by LC-HR-QTOF MS/MS
- AppNote TN 56: A new paradigm in forensic analysis
- AppNote AMS 009: Microplastic analysis and additive screening using thermal desorption/pyrolysis DART-MS
- AppNote LCMS 211: Real-time and post-acquisition quality control (QC) in MetaboScape
- AppNote AMS 007: Fast food fraud testing of truffle
- Brochure: TargetScreener: One workflow – all the answers
- Read about Bruker's commitment to a sustainable future

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