Applied Mass Spectrometry

TargetScreener HR

One workflow – all the answers

Innovation with Integrity

Answers today, tomorrow, every day

Always Accurate Results

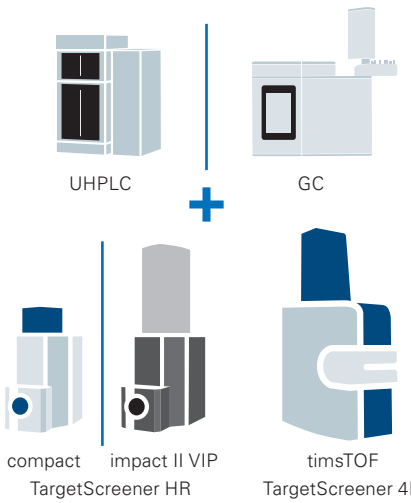
Food Safety **Forensics** **Toxicology** **Environment**

Environmental, food safety, toxicology and forensic laboratories need tools to rapidly screen for target compounds with accuracy and certainty. Bruker's workflow offers several benefits including providing data-independent acquisition and all ion fragmentation data, enabling the analysis of an unlimited number of compounds, and allowing retrospective analysis. TargetScreener HR encompasses all these features.
TargetScreener HR represents the modern way of monitoring: beyond obligatory testing, towards a complete picture to avoid surprises and headaches.

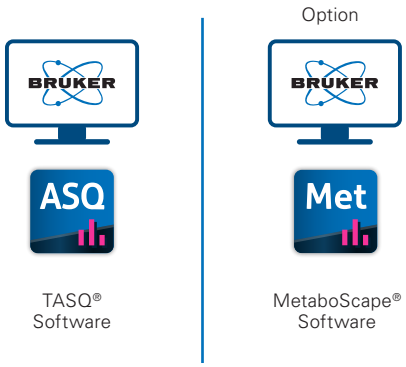
Comprehensive screening workflow

Combination of reliable data, powerful software, and robust database for sophisticated results

1 HARDWARE



2 SOFTWARE



3 REPORT

Report

Acquisition of full scan MS and bbCID accurate mass data

Target and untargeted analysis: Screening and quantitation

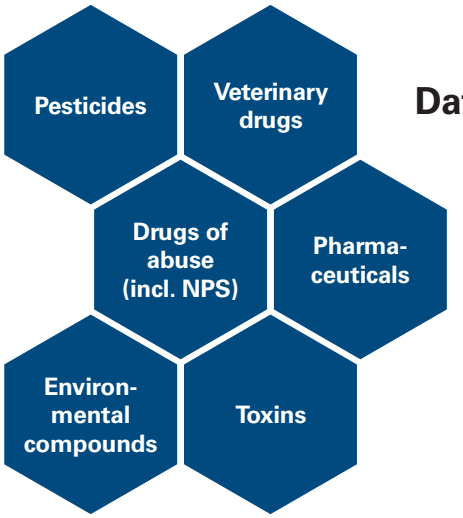
Discovery workflow: Statistical analysis Identification of unknown

Result reporting and/or LIMS export

- **TargetScreener HR**
  - Comprehensive screening – targeted and non-targeted
  - Minimizes false positive and false negative reporting
  - Accurate and precise quantitation meets stringent regulatory guidelines
- **TargetScreener 4D**
  - Plus Trapped Ion Mobility Spectrometry (TIMS) resulting in Collision Cross Section (CCS) values - a new 4th dimension of orthogonal selectivity for absolute confidence

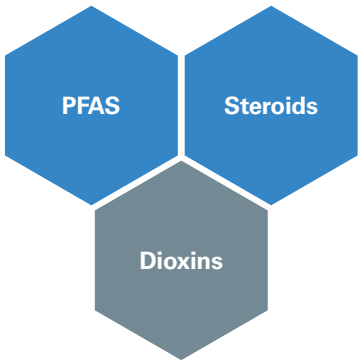
Extended compound database: Drugs, pesticides, and environmental pollutants

One solution for GC and LC workflows



Database of > 3000 entries

Inclusive



The core of the TargetScreener HR workflow lies in its precise database. This comprehensive database includes high-resolution monoisotopic precursor ion masses, retention time data, and up to ten detailed qualifier ions. The qualifier ion data encompasses accurate mass bbCID fragments, 'in source' fragment ions, adduct information, and isomer details. Additionally, CCS values are included to enhance the confidence in identification.
A perfect match to the TargetScreener HR database is indicated by the green color of the MRSQ or MRSQC score.

Color-coded screening results
Straightforward reviewing of either a sample or an analyte as desired by the analyst. Once reviewed, qualitative and quantitative sample reports are then easily generated.

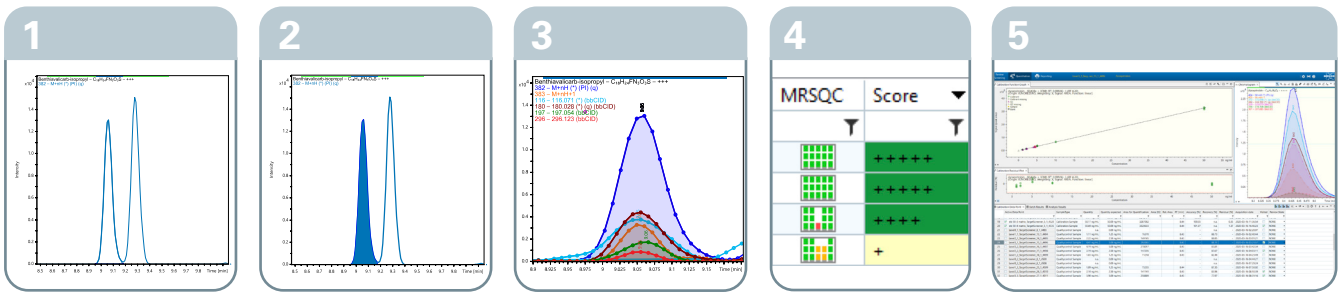
Mass accuracy
Retention time
m**S**igma value (Isotopic pattern)
Qualifier ions (Diagnostic ions)
CCS value

Parameter within narrow window
Value between narrow and wide limits
Parameter outside the wide tolerance window
No score available

5 Steps from sample to report

Powerful for in-depth investigative screening and quantitation as well as retrospective data mining

Ready-to-use LC/GC-, MS- and software methods reduce lab time. Reaching confident results in just 5 steps with the TASQ software:



Screening

Generation of EIC traces for Principal Ions

Peak detection

Automatic Retention Time check

Verification

Check diagnostic ions: in-source and bbCID fragments, isotopes and adducts

Scoring

Scoring by mass accuracy (M), Retention Time (R), Isotope pattern (S), diagnostic Qualifier ions (Q) and CCS values (C)

Quantitation

Instant calculation of concentration of confirmed compounds

TargetScreener HR searches all ions all of the time by full scan MS and MS/MS without compromising sensitivity, resolution or mass accuracy. Datasets are complete and unrestricted. The diagnostic qualifier ions are used as an enhanced confirmation criterion to eliminate false positives as well as deliver unambiguous identification for co-eluting isobaric drugs.

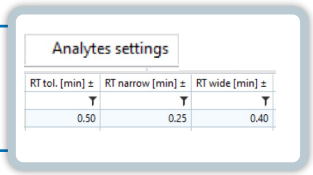
Compliant with international guidelines

Start with ready-to-use methods

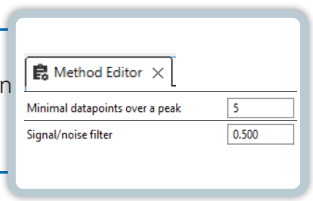
With Bruker's innovative technologies and default software methods, your lab will pass the method validation and analytical quality control requirements that are necessary to support the validity of data.

Summary of SANTE 11312/2021 guideline criteria

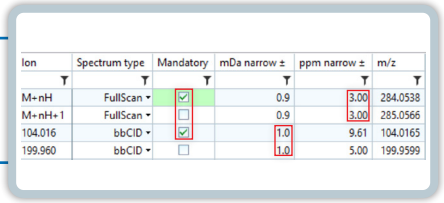
1 RT tolerance (standard sample): ±0.1 min



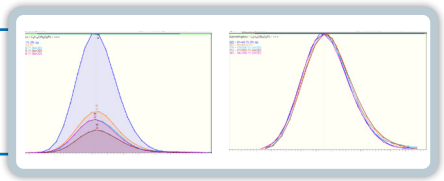
2 S/N ≥ 3 or signal should be present in at least in 5 subsequent scans



3 2 Ions with mass accuracy ≤ 5 ppm (or ≤ 1 mDa below 200 m/z)



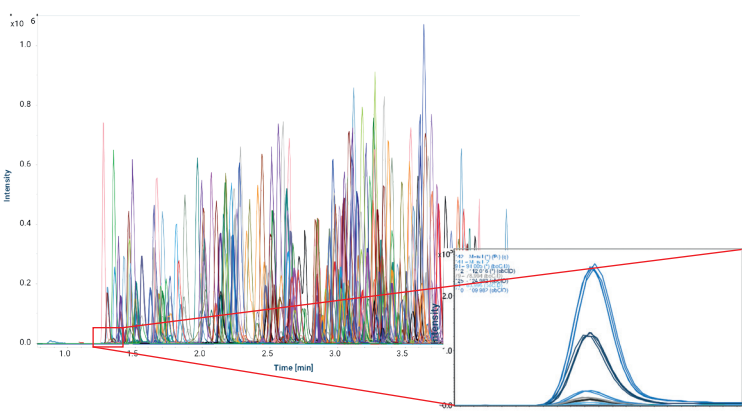
4 Full overlap of precursor and product ion EICs



Accelerate – Pesticides in wheat matrix in just 5 min

Analysis of 294 pesticides in wheat matrix with a 5 min method.

The pesticides were spiked at concentrations of 5, 10 and 20 µg/kg resulting in an analyzed concentration of 1.25, 2.5 and 5 ng/mL. The data was evaluated with the TASQ software.

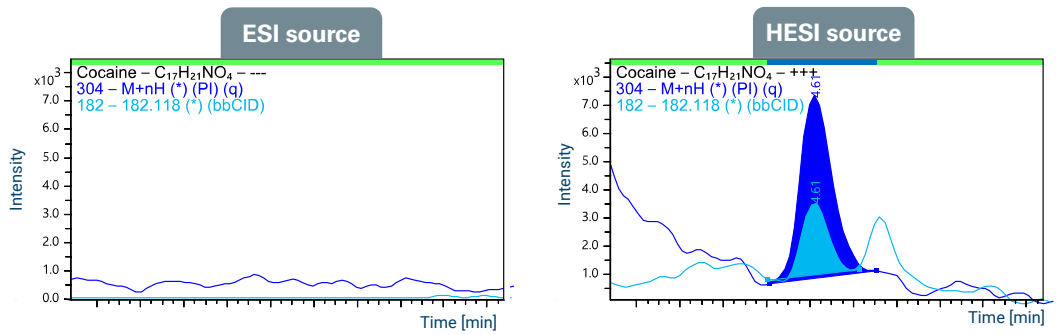


Analytical tools in forensic science

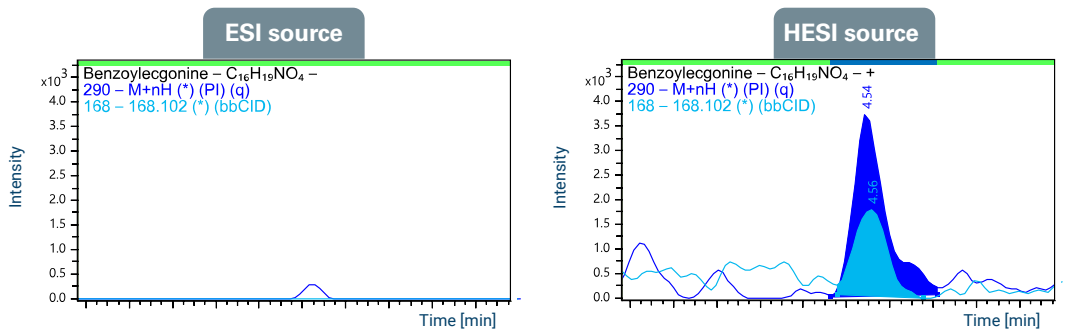
Increased sensitivity for forensic drug investigations

The VIP-HESI source, a novel dual source, is equipped with Heated Electrospray and Atmospheric Pressure Chemical Ionization (APCI) probes. Less thermal degradation and high-efficient ionization leads to a highly improved limit of detection (LOD). The reporting of false positives is minimized due to accurate mass data and the highly curated database.

Cocaine



Benzoylecgonine



Hair samples analyzed with ESI or VIP-HESI. Hair samples were cut into small pieces. After sample preparation a solution was injected into the UHPLC and analyzed with the impact II VIP HR-MS. Shown are the EICs from Cocaine (concentration 0.3 ng/mL) and its metabolite Benzoylecgonine.

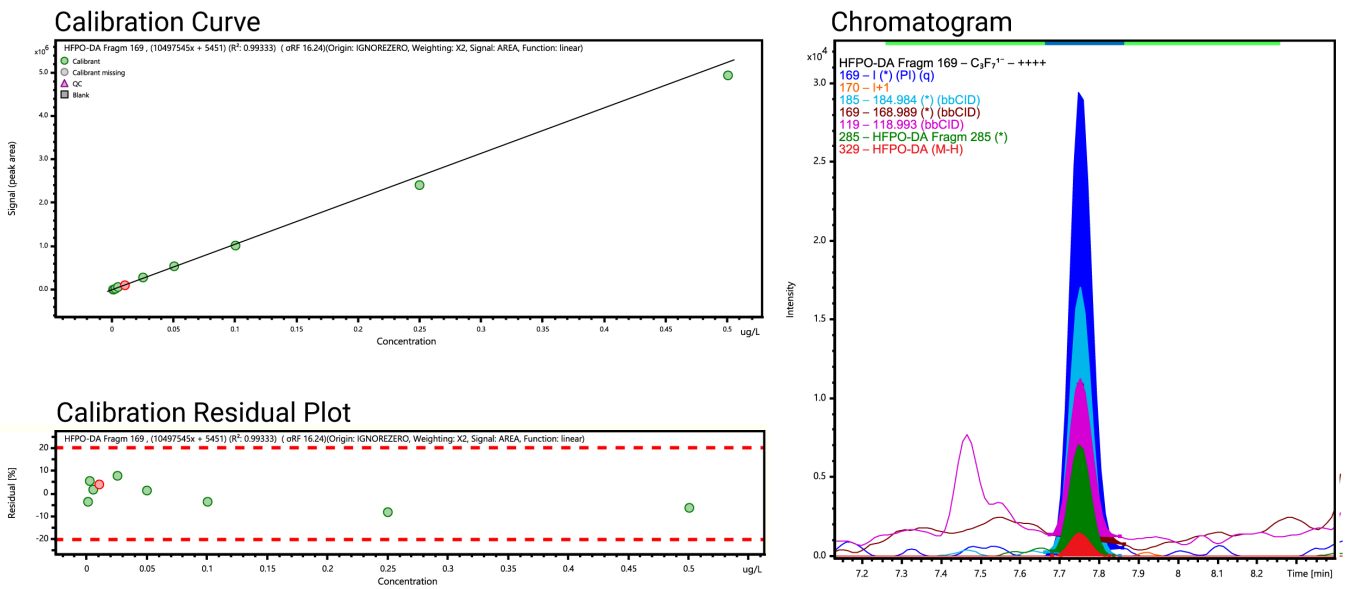
TargetScreener HR workflow allows for an **easy addition of new compounds** to the HR-MS database, which is of extreme importance for the rapid emergence of new drugs. TargetScreener HR collects all data, all of the time, allowing for retrospective analysis of previously screened samples with the addition of new compounds to the database.

Powerful for screening and quantitation

Accurate quantitation of analytes

PFAS, known as per- and polyfluorinated alkyl substances, represent a broad category of industrial chemicals that have been widely utilized. As a result of their potential toxicity, PFAS pose an escalating danger to both humans and wildlife. Consequently, the analysis of these substances has become an increasingly crucial undertaking for analytical chemists. With the TargetScreener HR workflow it is possible to screen and quantitate PFAS.

GenX (HFPO-DA)



Quantitation of GenX – a PFAS compound

Extract from TASQ software. Shown are the calibration curve (concentration range: 0.001-0.5 µg/L), the calibration residual plot and the chromatogram of GenX/HFPO-DA (concentration 0.01 µg/L).

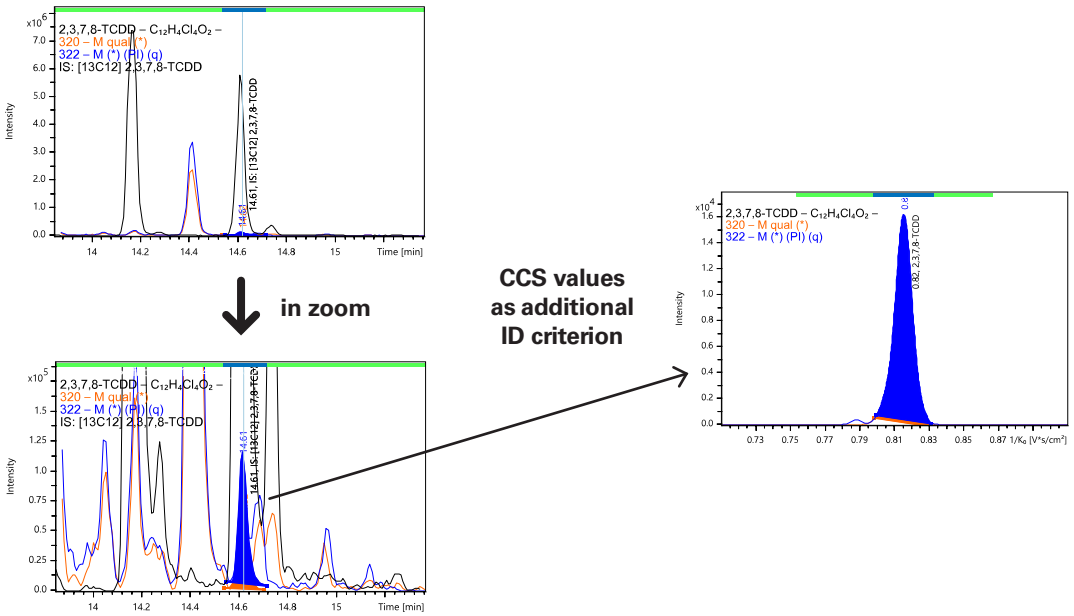
Addressing the crucial challenge of screening and quantitation of analytes in diverse matrices

Bruker's TASQ software, included in the TargetScreener HR workflow package, is specifically designed to the comprehensive requirements of customers. It offers a user-friendly method setup with a menu-driven, quick start wizard, expertly guiding users through qualitative and quantitative workflows. TASQ provides the convenience of preconfigured reports or the option to export data to a Laboratory Information Management System (LIMS) for further customization in processing and reporting.

A new standard in GC-APCI

High-speed TIMS coupled to GC-APCI-HR-MS: The ultimate screening power

TargetScreener 4D provides a ready-to-use method for the analysis of Dioxins, Furans, and PCBs in the same run and matching Regulation (EU) 2017/644. Bruker's solution enables monitoring of the levels of dioxins, dioxin-like PCBs and non-dioxin-like PCBs in certain foods. Save lab time and increase productivity with Bruker's ready-to-use method for 350 contaminants.



Quantitation of 2,3,7,8-TCDD in certified reference material. Sludge extract spiked with a mixture containing several congeners of dioxins and furans (specially several congeners of TCDF and TCDD) and diluted 10 times before injecting.

§ REGULATION (EU) 2017/644 (METHODS OF ANALYSIS FOR THE CONTROL OF LEVELS OF DIOXINS)

- RT tolerance (relative RT in relation to IS or ref. standards): ± 0.25 %
- Repeatability (RSDr) < 20 %
- Intermediate precision (RSDR) < 25 %
- Monitoring of at least two specific ions

TargetScreener 4D
One package – Unlimited solutions!

Add a new dimension for more confidence

1 RT
2 m/z
3 MS/MS
4 Mobility

- Additional ID criterion
- Separation and quantitation of isomers
- Clean-up of chromatograms and spectra

Trapped ion mobility spectrometry (TIMS) provides an additional dimension of separation, unlocking and eliminating all uncertainties of the sample analysis and generates ultimate confidence in compound identification.

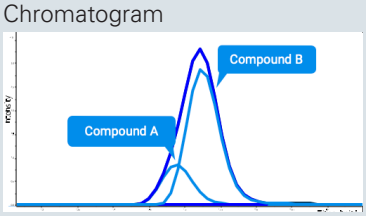
Additional ID criterion

M R S Q C

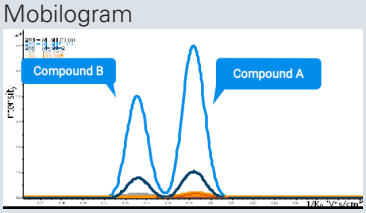
Mass accuracy
Retention time
m**S**igma value (Isotopic pattern)
Qualifier ions (Diagnostic ions)
CCS value

Separation and quantitation of isomers

Chromatogram

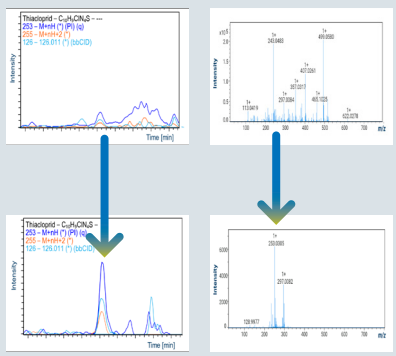


Mobilogram



Clean-up of chromatograms and spectra

Mobility filter OFF

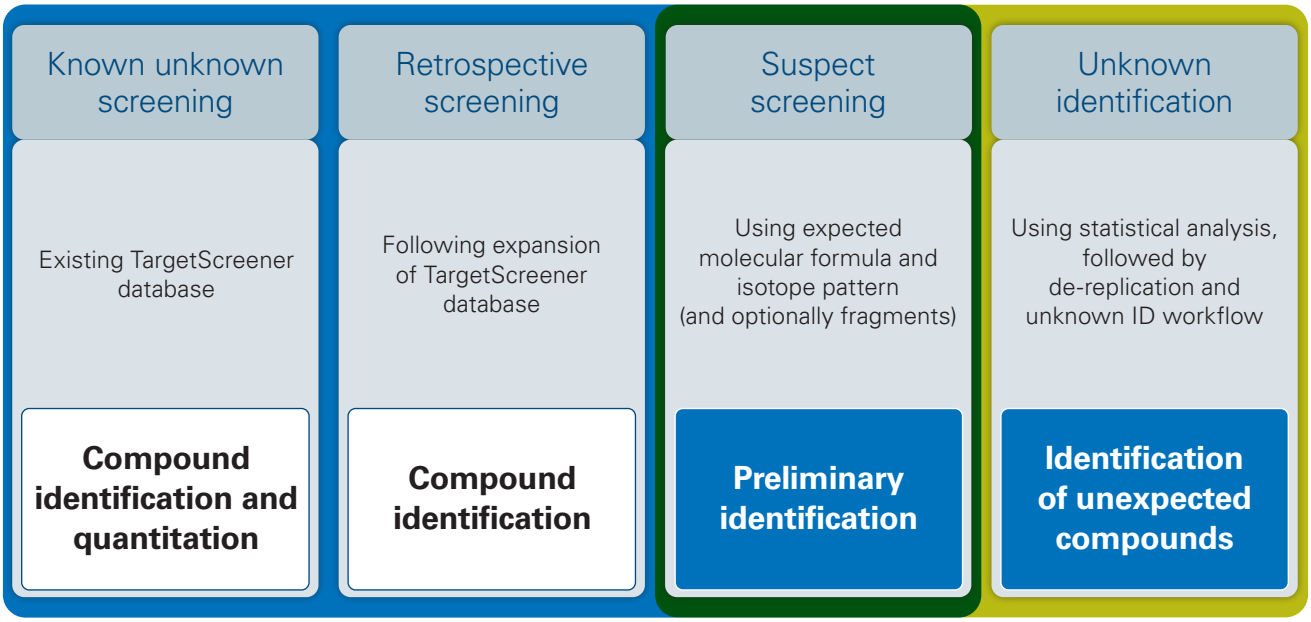


Mobility filter ON

Full array of identification workflows

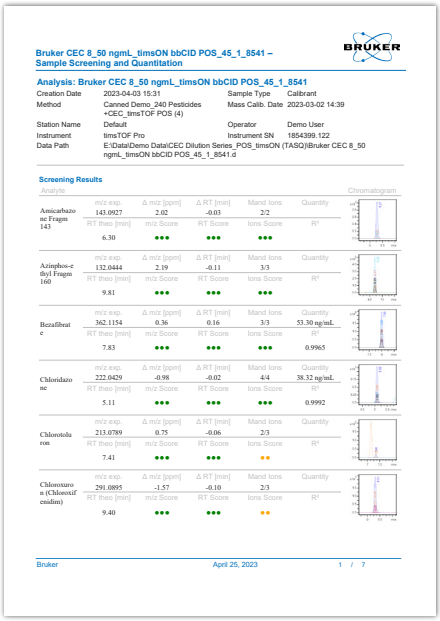
Bruker's software suites **TASQ®** and **MetaboScape® software** process target and non-targeted workflows. TASQ supports various screening methodologies, plus accurate quantification based on an available calibration curve. MetaboScape® uses statistical analysis to detect unexpected compounds and identifies 'known unknowns' using public databases and spectral library searches (e.g. MetaboBase® library, NIST 2023).

Identification workflows



High-resolution mass spectrometry (HR-MS) is made with data-independent acquisition, with unbiased ion fragment generation and detection, enabling analysis of an unlimited number of compounds.
Spectral libraries with high mass accuracy are then utilized for the identification of unknowns. For added flexibility, users can add new compounds to the HR-MS database as they become available. This is future proof for any investment for years to come, enabling retrospective data mining of previously screened samples.

- High sensitivity with the novel VIP-HESI source down to ppt levels.
- Generation of HR accurate mass parent ions, true isotope pattern intensities and fragment qualifier ions in combination with Retention Time.
- Multiple level MRSQ(C) scoring of results provides efficient reduction of false positive and negative results by simple default methods.
- Reliable quantitation and comprehensive screening possible using the same data sets.
- Unique addition of CCS values in the 4D mode.



Bruker CEC 8_50 ngmL_timsON bbCID POS_45_1_8541 – Sample Screening and Quantitation

BRUKER

Analysis: Bruker CEC 8_50 ngmL_timsON bbCID POS_45_1_8541

Creation Date	2023-04-03 15:31	Sample Type	Calibrant
Method	Canned Demo_240 Pesticides +CEC_timsTOF POS (4)	Mass Calib. Date	2023-03-02 14:39
Station Name	Default	Operator	Demo User
Instrument	timsTOF Pro	Instrument SN	1854399.122
Data Path	E:\Data\Demo Data\CEC Dilution Series_POS_timsON (TASQ)\Bruker CEC 8_50 ngmL_timsON bbCID POS_45_1_8541.d		

Screening Results

Analyte	m/z exp.	Δ m/z [ppm]	Δ RT [min]	Mand Ions	Quantity	Chromatogram
	RT theo [min]	m/z Score	RT Score	Ions Score	R²	
Amicarbazone Fragm 143	143.0927	2.02	-0.03	2/2		
	6.30	●●●	●●●	●●●		
Azinphos-ethyl Fragm 160	132.0444	2.19	-0.11	3/3		
	9.81	●●●	●●●	●●●		
Bezafibrate	362.1154	0.36	0.16	3/3	53.30 ng/mL	
	7.83	●●●	●●●	●●●	0.9965	
Chloridazone	222.0429	-0.98	-0.02	4/4	38.32 ng/mL	
	5.11	●●●	●●●	●●●	0.9992	
Chlorotoluron	213.0789	0.75	-0.06	2/3		
	7.41	●●●	●●●	●●		
Chloroxuron (Chloroxifenidim)	291.0895	-1.57	-0.10	2/3		
	9.40	●●●	●●●	●●		

Bruker April 25, 2023 1 / 7

Sample to report just in a few steps

Kristoffer Kilpinen

Development chemist, Eurofins Environment Galten, Denmark

"After using TargetScreener for more than two years, we have found it to be a valuable tool for conducting wide-range suspect screenings of environmental samples."

TargetScreener HR – Meeting the demands

Food safety

Dioxins

Pesticides

Doping

Veterinary drugs

Mycotoxins

PFAS

Drugs of abuse

Homeland security

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

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