
# TargetScreener

- A Comprehensive Solution for Screening and Multi-target Quantitation

UHR-TOF MS

Innovation with Integrity

# Target Screening and Quantitation Demands

*For a variety of applications, including toxicology, forensics, food safety, environmental protection, and doping control, many laboratories need tools to rapidly screen for target compounds with a high degree of accuracy. These targets are often sought from diverse matrices and may be present across a broad dynamic range. In addition to qualitative screening information, there is often a need for multi-target quantitation.*

Bruker's TargetScreener is designed for both targeted and non-targeted workflows in routine and research laboratory environments. With high resolution and sensitive instrumentation, an accurate and highly curated database, and powerful software for data analysis, TargetScreener provides unique capabilities for reliable, simultaneous detection and quantitation of multiple targets in a large variety of different matrices.

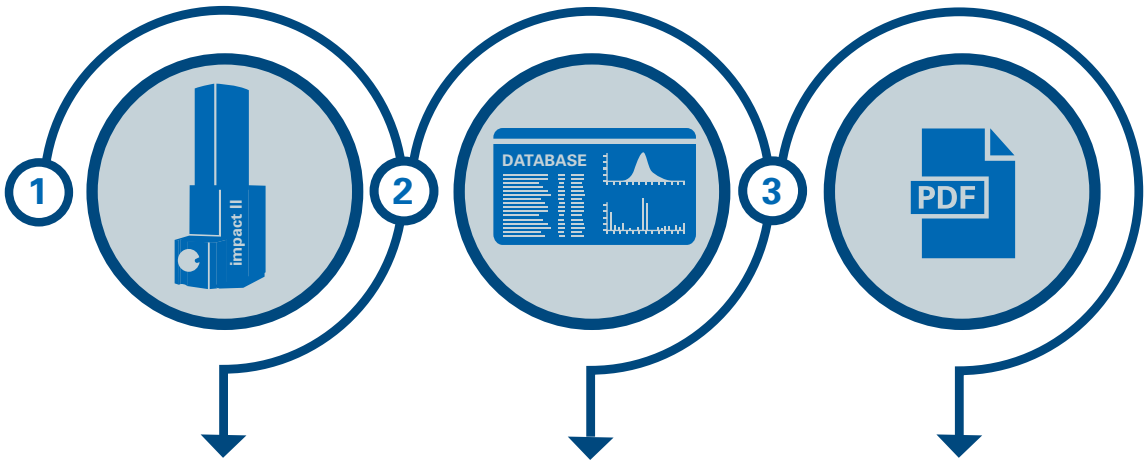
Additionally, the methodology for data collection generates a unique depth and breadth of data, supporting routine retrospective analyses and non-targeted discovery screening to help deliver the critical answers you need - both today and tomorrow.

## Toxicology · Forensics · Food Safety · Environmental Protection

# Bruker's TargetScreener Solution

Bringing the full power of exact mass analyses to multiplexed laboratory screening and quantitation demands, this comprehensive UHPLC-QTOF analytical solution is ready to work directly "out of the box" and includes:

- UHR QTOF mass spectrometer with Full Scan MS and broadband CID (bbCID) MS/MS methods
- An Elute UHPLC system, with Bruker columns, mobile phases, and QC standard
- TASQ screening and quantitation software for rapid data processing, including ready methods for multi-target screening
- The high quality and robust TargetScreener database including more than 3000 entries relevant for food safety, environmental protection, and toxicology research screening.




**UHPLC-QTOF analysis: Acquisition of full scan MS and bbCID accurate mass data**

**Compound identification and quantitation in TASQ using accurate mass, retention time and diagnostic fragment ions from the TargetScreener database**

**Result reporting and/or LIMS export**

The combination of high quality MS and MS/MS data, a highly curated database, and powerful data processing software enables both routine screening and in-depth retrospective analyses to detect criminal activity or industrial negligence, support better patient care, and promote better human, animal, and environmental protection.

# A Highly Curated Database of >3000 Compounds

- ✔ *Pesticides*
- ✔ *Veterinary drugs*
- ✔ *Drugs of abuse incl. NPS*
- ✔ *Pharmaceuticals*
- ✔ *Environmental compounds*
- ✔ *Toxins*

*Encompassing a broad array of target compounds relevant to current regulatory screening requirements, the TargetScreener database has been created with multiple analytical elements for confident identification using full scan MS and bbCID MS/MS accurate mass data acquired on UHR QTOF instruments with up to 10 annotated qualifier ions per target, supported by the use of the 'True Isotopic Pattern' (TIP™) and retention times.*

The database is consistently updated in collaboration with customers around the world with an eye to increasingly stringent governmental detection and reporting demands. Individual laboratories may add their own targets to support supplemental screening and research interests.

Target analytes are confidently differentiated based on four key components: mass accuracy, retention time, detection of diagnostic ions, and observed isotopic patterns, with color-coded scoring for easy visualization of results. Coupled with the high quality of the curated TargetScreener database, this approach significantly reduces false positives.

# Fully Compliant with SANTE/ 11813/2017 International Guidelines

The criteria for SANTE guidelines have been met in validation studies, including for difficult matrices (such as leek and orange), using the TargetScreener. TASQ software further supports criteria fulfillment and result reporting.

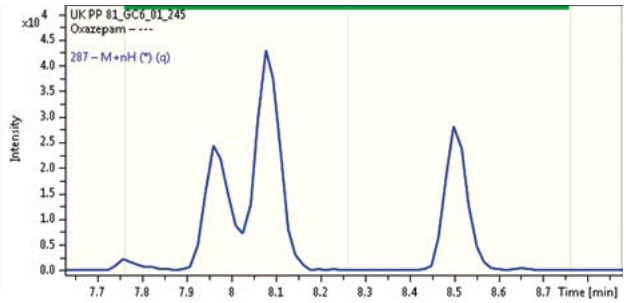
- **RT difference** (peak in chromatogram of sample versus standard): **≤0.1 min**
- **2 MS ions present,** preferably molecular ion plus fragment ion using **QTOF:**
  1 ion from **full scan MS and** ≥1 ion from **bbCID MS/MS**
- **Mass error:**
  **For m/z <200 Da: < 1 mDa**
  **For m/z ≥200 Da: ≤ 5 ppm**

*"Analytical Quality Control and Method Validation Procedures for Pesticide Residues Analysis in Food and Feed" SANTE-11813-2017*

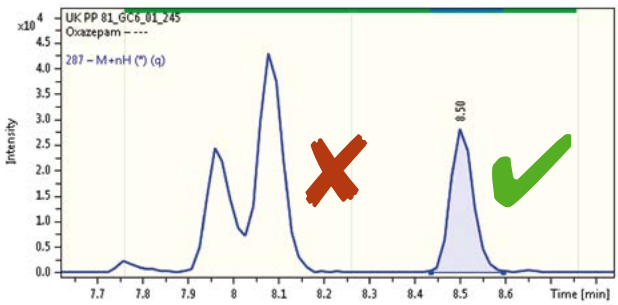
# TargetScreener Workflow

1. Generation of EIC traces for Principal Ions

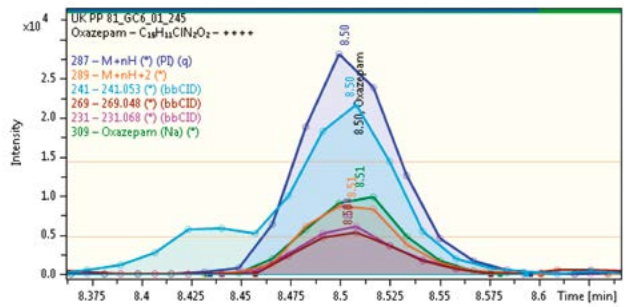
➔ Oxazepam: $[C_{15}H_{11}ClN_2O_2+H]^+$= 287.058182




2. Chromatographic peak check. If more than one, matched with correct retention time.




3. Verification via diagnostic ions: in-source and bbCID fragments, isotopes, and adducts.




4. Scoring based on four criteria: Mass accuracy, retention time, diagnostic ions, and isotopic pattern.

| MRSQ | Score |
|---|---|
| | ++++ |
| | +++ |
| | +++ |
| | + |
| | + |
| | + |
| | + |


**M** Mass accuracy
**R** Retention time
**S** Isotopic pattern
**Q** Diagnostic ions

5. Quantitation: Concentrations of confirmed compounds are instantaneously calculated.

# TASQ for Rapid Screening AND Quantitation

*Screening Review perspective in TASQ*

Bruker's intuitive TASQ software is uniquely fitted to provide screening and quantitation of targeted compounds in one continuous workflow. Screening result review is supported by simplified color coding of matched parameters, and detailed information on individual diagnostic ions is just a click away.

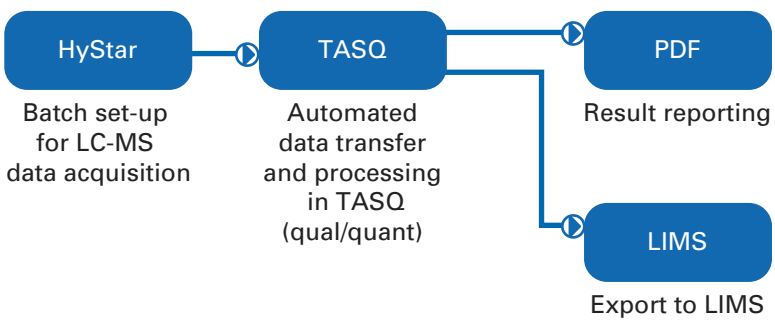
*Quantitation perspective in TASQ*

TASQ enables full quantitation, for an unlimited number of targets, within the same graphical user interface. Pre-defined rules, which can be adapted and extended to meet a laboratory's specific interests or requirements, flag "alarm" levels of targets. If desired, single-point and legacy calibration functions are applicable within the software.

# Automated and Integrated

## From data acquisition to direct export of results to PDF or LIMS

Supporting demands of time and priority interests in routine laboratories, the modern client-server architecture of the TASQ software allows multiple users to access the same server for parallel data acquisition and evaluation, all with seamless integration and direct reporting and/or data export to LIMS.

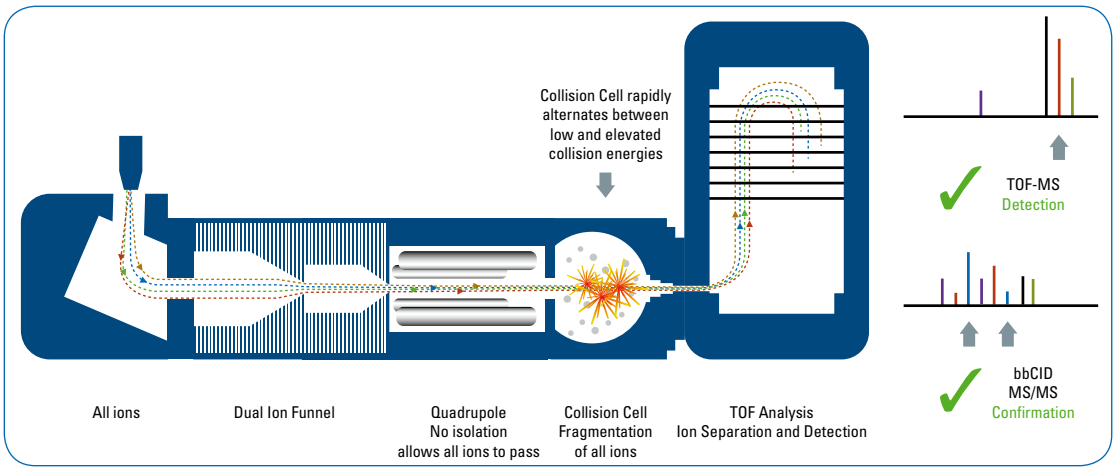


# “All of the Data, All of the Time”

## Alternating full scan MS and broadband CID

Bruker’s TargetScreener workflow uses alternating collection of full scan MS data and broadband CID MS/MS. This unbiased approach, with an elevated collision energy and no isolation of specific precursor ions during bbCID data acquisition, provides a clear analytical advantage, enabling:

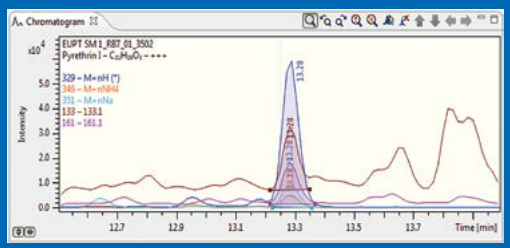
- Wide discriminatory capacity for the detection of an unlimited number of targets over a large dynamic range
- Detection of trace compounds that, due to their low intensity, failed to be selected as precursors in standard data-dependent acquisition modes
- In-depth retrospective screening and discovery workflows, especially useful when new targets are added to the database
- Suspect compound screening based on accurate mass determination and isotope pattern fit, without the need for reference standards




*Schematic of TargetScreener bbCID data acquisition*

# Food Safety: Confident detection of pesticide residues in spinach

Participating in European Proficiency Test Screening Methods in Fruits and Vegetables in 2016 (EUPT-FV-SM-08), a French lab using the TargetScreener solution detected and simultaneously quantitated residual concentrations of pesticides in a blinded spinach homogenate, and was one of 12 of 83 participating laboratories correctly detecting all 15 pesticides.



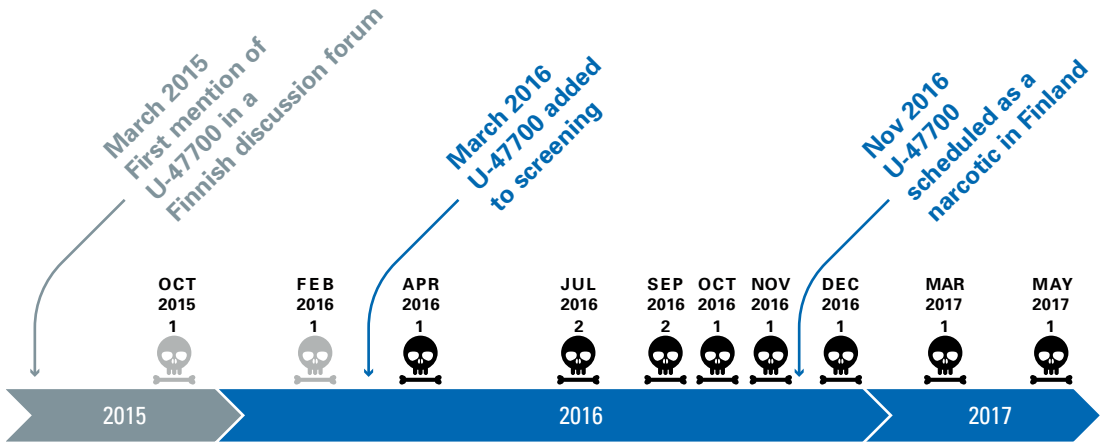

*Detection of Fenpyrazamine (0.060 mg/kg) including five qualifier ions*

# Facilitating retrospective and secondary analyses beyond the conventional known unknown screening

As target databases are expanded with the discovery of new emerging threats or the regulation of new suspect compounds, the unrestricted nature of MS and MS/MS fragmentation data collected via the TargetScreener workflow is ideal for retrospective analyses. No additional data collection is required, even for low abundant compounds. This approach offers a significant analytical advantage for a wide array of applications, including:

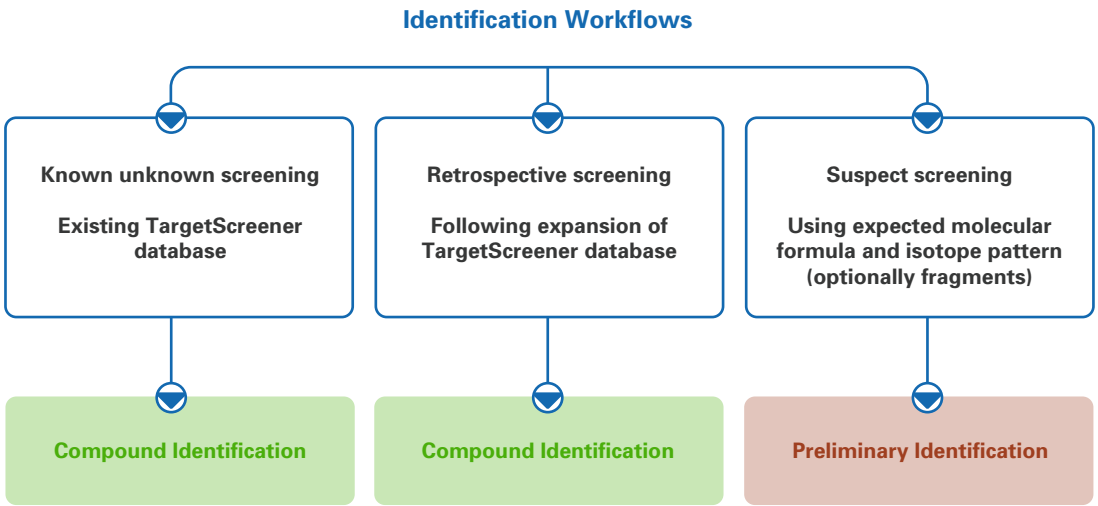
- ✔ Food safety: Unexpected food contamination or adulteration (e.g., new veterinary drugs in meat, melamine in milk products)
- ✔ Environmental studies: Pesticides and pharmaceuticals in waste or river water
- ✔ Forensics: Emergence of new psychoactive subtances (NPS), criminal investigations, and post-mortem analyses
- ✔ Sports toxicology: Performance-enhancing substances (doping control)

In particular, forensic laboratories need to quickly adapt their screening methods to keep pace with the constant emergence of new psychoactive substances (NPS). Retrospective analysis is a valuable tool for identifying new drugs in unexplained deaths without having to reanalyze samples.




*Post-mortem cases in Finland due to U-47700. Death cases before March 2016 were subjected to retrospective analysis after addition of the NPS U-47700 to the TargetScreener database. (Reference: https://www.sciencedirect.com/science/article/pii/S0379073819301707)*

If no reference substances are available, a suspect screening can be performed with the Target-Screener. A suspected compound can be searched using only the molecular formula (and optionally, predicted fragment information) by virtue of the mass accuracy and the 'True Isotopic Pattern' of the detected signals.

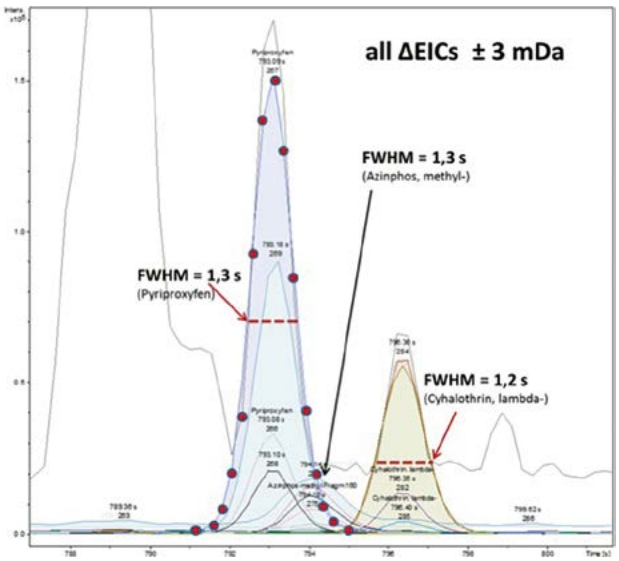


# Extended Scope of Detection Capabilities

## Supporting environmental, food, and feed safety workflows

The addition of Bruker's GC-APCI II source to the TargetScreener offers a powerful expansion of target scope, including volatile and non-polar pesticides, and persistent organic pollutants (POPs).

Easy switching between the LC-ESI and GC-APCI sources enables configuration flexibility depending on your laboratory's analytical requirements. The complete setup is fully software integrated.



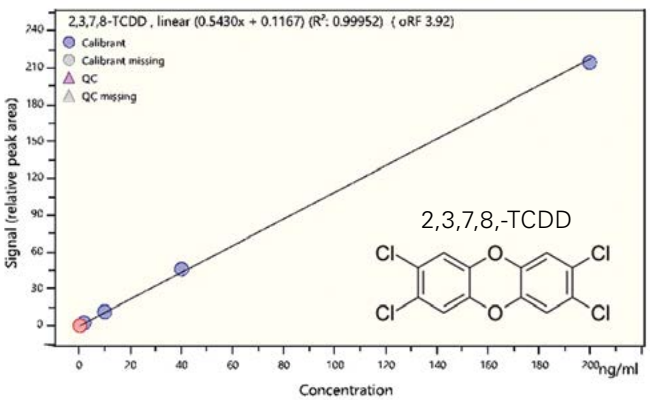

In complex matrixes with a great variety of substances, efficient separation and confident detection is achieved through the combination of excellent GC peak resolution and fast MS scanning (>8 Hz) rates, and is well matched to meet EU and US EPA (Environmental Protection Agency) requirements.

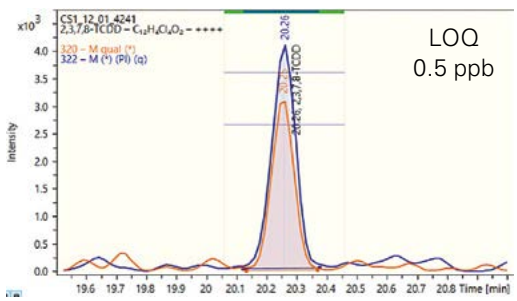
As in the HPLC TargetScreener workflow, the complete (data independent) collection scheme supports the detection and quantitation even of trace amounts.

*The high scanning speed of the GC-APCI TargetScreener delivers more than 10 points per peak for accurate quantitation.*

### Dioxin analysis using GC-APCI with high resolution QTOF

Even residual levels of pesticides and POPs can have toxicological effects on human and animal health and damage natural ecosystems. With LODs of 0.1-1 ppb, PCBs, PCDDs, and PCDFs (among other targets) can be clearly identified and quantitated from food, water, soil, and air samples.



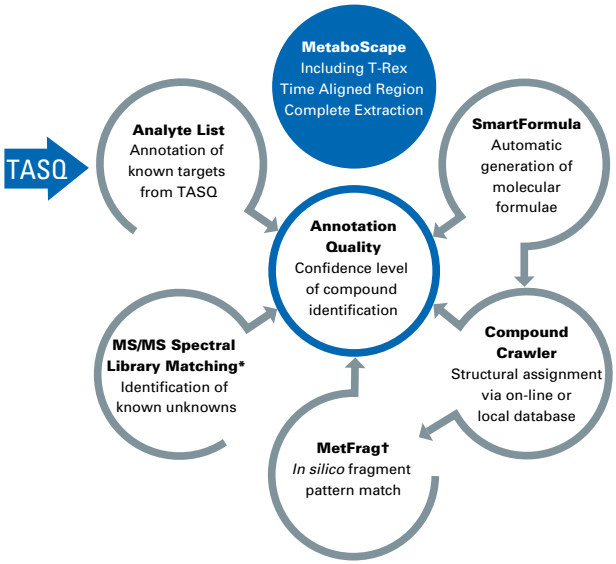




*Calibration curve (left) from 0.5 to 200 ppb and extracted ion chromatograms (above) at 0.5 ppb (LOQ) for 2,3,7,8,-TCDD ("Seveso toxin").*

# Beyond Target Screening

## From Unknown to Known Target Discovery using MetaboScape

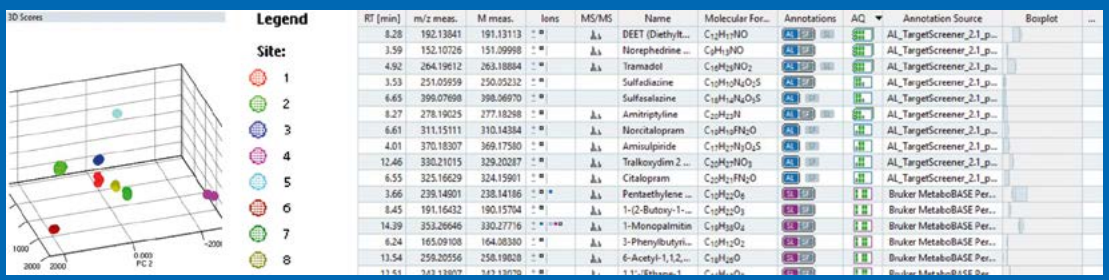
The comprehensive information gained from accurate mass MS and MS/MS data allows for the discovery of analytes that go far beyond the original compounds covered by targeted screening. The optional add-on Bruker MetaboScape software expands the capabilities to identify known compounds and investigate true unknowns with confidence and ease by using multiple tools for seamless annotation. In addition, MetaboScape enables both univariate and multivariate statistical analysis to mine complex sample sets and detect differences for exploring potentially new targets.




*Compound identification in Bruker's MetaboScape software (*Including the MetaboBASE Personal Library with more than 100,000 compounds, derived from the METLIN library of the Scripps Research Institute; † Sebastian Wolf, Stephan Schmidt, Matthias Müller-Hannemann and Steffen Neumann, BMC Bioinformatics 2010, 11:148)*

# Environmental Monitoring: Analysis of River Water

The River Clun (Wales, UK) was found to be in failure of the environment standards of the EU's Water Framework Directive. A ten-month study was conducted to determine which chemical compounds, likely resulting from the discharge of wastewater treatment plants, were responsible. Passive sampling devices were deployed for four-week periods at eight sampling points along the river. In addition to the detection of known targets (using the TargetScreener workflow) various unknowns were detected and identified using MetaboScape PCA models and annotation tools.



# What Our Customers Are Saying...

*Prof. Dr. Volker Auwärter, Institute of Forensic Medicine, University of Freiburg*
*"Whenever a more in-depth analysis is required in our laboratory, the TargetScreener is our go-to solution. Providing full scan and bbCID high resolution mass information, also allowing for fully retrospective data evaluation, it is ideally suited for cases dealing with 'general unknown screening'. It is a valuable tool for identifying new psychoactive substances (NPS) and their metabolites, assisting with their structural elucidation and analytical characterization. The TargetScreener also proved to be very useful for comprehensive drug screening in alternative matrices, especially hair samples."*

*Dr. Anthony Gravell, Natural Resources Wales, UK*
*"The TargetScreener with the impact II has become our routine solution for target, suspect and unknown screening in diverse matrices such as water, effluents, passive sampling extracts and sediments. We can quickly and efficiently identify pesticides and other chemical pollutants which may have detrimental effects on river ecology; a powerful tool for investigative monitoring under the Water Framework Directive". Benefits of using TargetScreener: "Efficient sample throughput combined with excellent sensitivity, dynamic range and selectivity for LCMS screening of environmental samples using comprehensive mass spectral libraries."*

*Prof. Nikolaos Thomaidis, Laboratory of Analytical Chemistry,*
*National and Kapodistrian University of Athens, Greece*
*"TargetScreener is our one-stop solution for our research or routine screening purposes. Either for emerging contaminants in the environment or food contaminants, TargetScreener provides high quality bbCID high resolution MS/MS information, increasing substantially the identification confidence. Both LC-ESI-QTOFMS and GC-APCI-QTOFMS high quality libraries, along with TASQ software enables the quick and reliable identification and quantitative determination of important contaminants in environmental and food matrices, a perfect tool also for routine analysis for food industry. It is an extremely valuable tool for identifying pesticides, pharmaceuticals, illicit drugs and new psychoactive substances (NPS) and their metabolites in sewage epidemiology research projects. Data generated by both LC-ESI- and GC-APCI-QTOFMS is also available for fully retrospective data evaluation, making full use of the potential of HRMS general screening for suspects."*

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