Toxtyper

● Confident and Comprehensive Screening
with Simplicity and Speed

Innovation with Integrity

Rapid toxicology screening for forensics and clinical research

Today's forensic toxicology and clinical research labs are challenged by demands for fast and accurate results, along with lab efficiency and cost reduction. Further pressure results from the continuous emergence of new drugs into the market, requiring frequent updates of sample screening methods. Easy to use, flexible, and reliable screening and analysis techniques are clearly needed to address these demands.

The Toxtyper is a toxicology "push button solution" with ready to use LC-MS^n methods and a simplified, intuitive user interface for immediate use – providing full confidence in every laboratory environment. Screening and confirmation is delivered in one analysis, with the lowest rate of false positives on the market.

The Toxtyper workflow

3
Fully automated data processing including spectral library search and **PDF reporting**

1
Push button sample submission – from sample to result **in 12 minutes**

UHPLC-MS^n analysis
• UHPLC separation of sample
• MS^n spectra acquisition

2
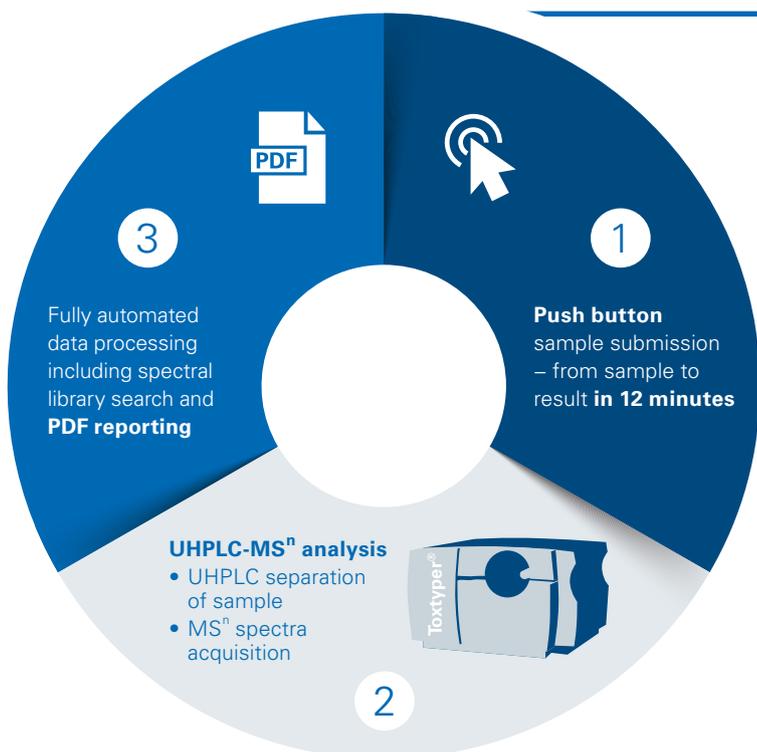
Fast and reliable identification

The screening workflows of the Toxtyper cover drugs and drugs of abuse (DOA) in various specimens including whole blood, serum, plasma, urine, and oral fluids.

Confident identifications are based on a comprehensive full scan MS^n library search using a manually curated spectral reference library of nearly 1200 compounds.

High confidence identifications

Simplicity, speed and confidence by true MS^n

Rapid and reliable detection of drugs and toxins is critical for clinical research screening and forensic applications. The Toxtyper system identifies compounds based on MS, MS^2 and MS^3 spectra plus retention time information, providing confident results and minimizing time for data mining.

Key attributes

- Tune-free, ready for use, robust LC-MS^n solution for 24/7 toxicology screening
- Easy to use software, designed for non-MS experts
- Comprehensive and confident screening results, based on high quality curated spectral libraries
- Less then 12 min from injection to report, fast polarity switching for detection of basic, acidic and neutral compounds in one run
- Allows for streamlined sample preparation – in particular for urine – without need for hydrolysis and/or derivatization
- Open library concept enabling easy and fast library updates, e.g. for new psychoactive substances (NPS)
- Provides access to semi-quantitative results

Drugs of abuse screening in urine
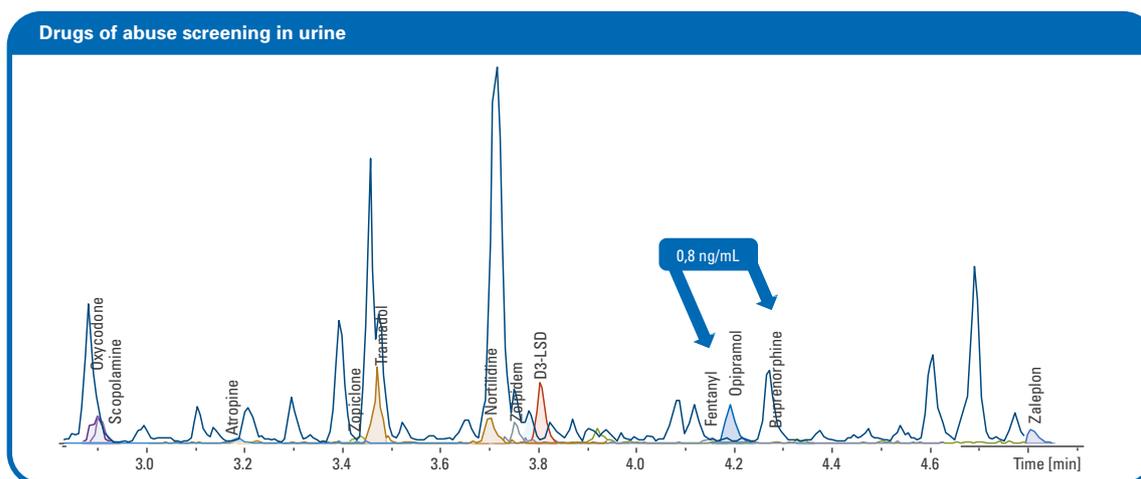
Example data demonstrating simultaneous, highly sensitive detection of eleven drugs in human urine. Following simple sample preparation (liquid-liquid-extraction) of 1 mL of urine, the Toxtyper permits detection down to 0.8 ng/mL.

Compound	ng/mL	Compound	ng/mL	Compound	ng/mL
Oxycodone	20	Tramadol	20	Opipramol	20
Scopolamine	20	Nortilidine	20	**Buprenorphine**	**0,8**
Atropine	20	Zolpidem	4	Zaleplon	4
Zopiclone	4	**Fentanyl**	**0,8**	-	-

Intuitive easy-to-use software

User interface designed for non-MS experts

Push-button sample submission and analysis requires minimal user training and allows for 24/7 operation.
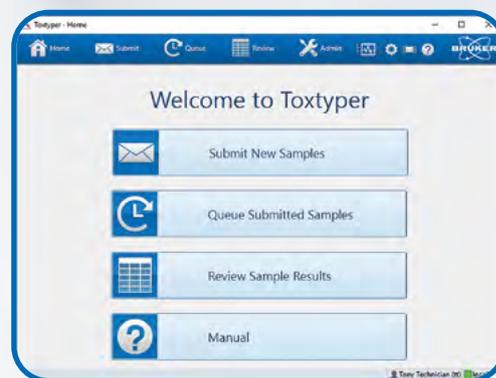
The Toxtyper software enables one click review of library search results for fast interactive result evaluation using chromatogram and MS^n spectra views. Identified compounds can be sorted by various parameters, e.g. signal intensity, retention time, or alphabetically. Color coding facilitates the review process.
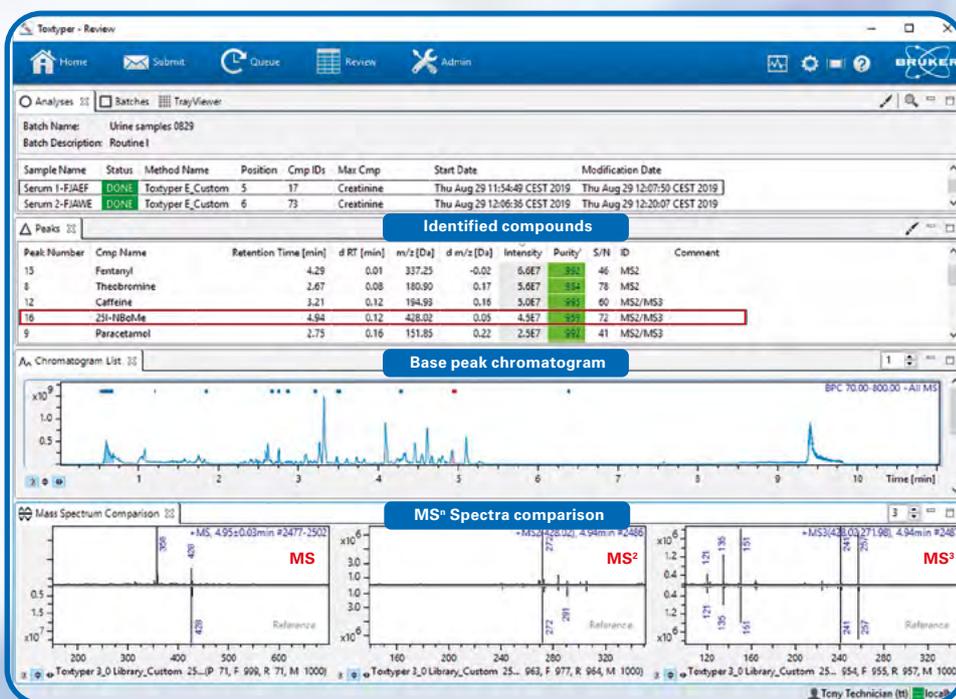
Open toxicology concept

Keep your screening and research workflows up-to-date

The appearance of new psychoactive substances, such as synthetic opiods, cannabinoids and cathinones, makes it necessary to update screening methods quickly. Toxtyper provides a ready-to-use spectral MS^n library of nearly 1200 drugs and metabolites, constantly updated through contributions from our customers and collaboration partners. User-defined library entries can be created with a few mouse clicks, allowing your laboratory to quickly respond to new patterns of illicit and licit drug misuse.

Tailor-made sub-libraries for increased sensitivity

Comprehensive screening is fast and easy. However, the use of a more specific screening method, e.g. use of the DOA method (83 compounds) instead of the classic Toxtyper method (nearly 1200 compounds) can improve detection sensitivity by targeting a lower number of compounds. This increased selectivity is based on a reduced "Scheduled Precursor List" for MS/MS acquisitions.

Targeted libraries

Targeted libraries, often with different LC gradients and thus retention times, may also be purchased for use on the Toxtyper system. These include:
• Synthetic Cannabinoids
• Psychotropics

In addition, the Toxtyper supports the Maurer/Wissenbach/Weber LC-MS^n library* containing almost 6000 drugs and metabolites.

Add new compounds with just a few mouse clicks

1

Selection of MS, MS^2 and MS^3 spectra and "Add to Library".

2

Add compound name and additional information such as molecular formula and structure.

3

The extended library is ready to use.

Reproducibility and robustness

Patented SmartFrag – the guarantee for reproducible and transferable fragmentation patterns

Amitriptyline: MS^2 results of 7 Toxtyper systems
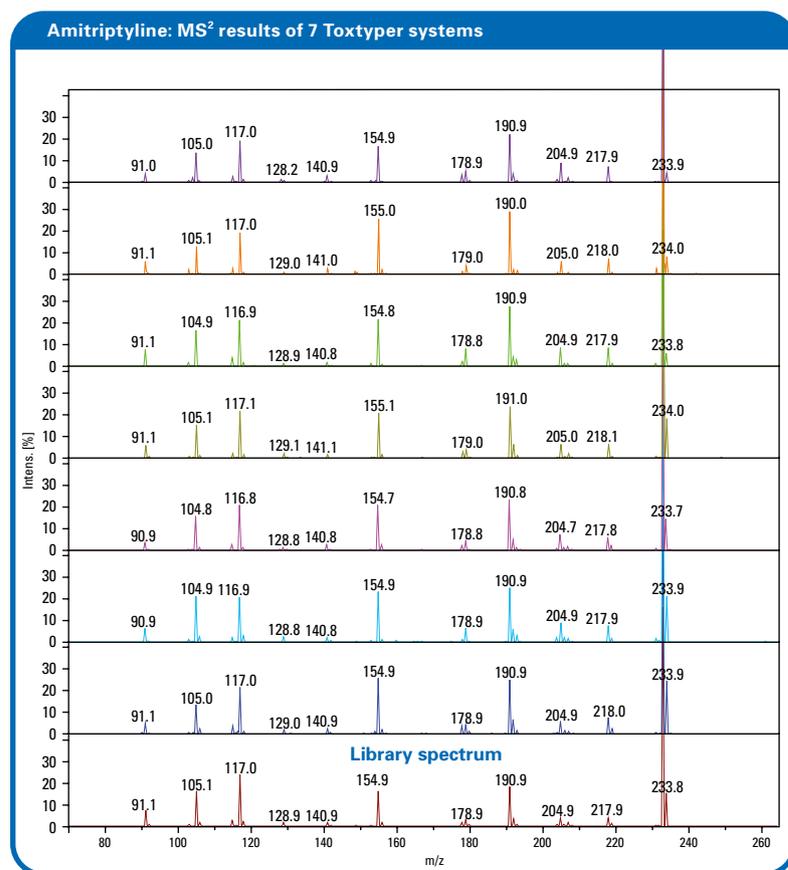
Library spectrum

Reproducible spectra recorded with multiple instruments: the sound basis for a successful spectral library approach.

Data-dependent MS^n acquisition using Bruker's patented SmartFrag technology enables the successful analysis of different types of compounds, regardless of their chemical nature, concentration, or sample matrix. With this technology, generated MS^n spectra and thus identification results are completely reproducible and transferable from instrument to instrument and lab to lab.

The Toxtyper's patented Dual Ion Funnel leads to high sensitivity, with identification limits in the low ng/mL range. With Zero Delay Alternating (ZDA™) polarity switching, both basic and acidic drugs can be detected providing the complete information in a single analysis.

MS^n data and library search results, 1000 ng/mL amitriptyline

MS^n data and library search results, 5 ng/mL amitriptyline
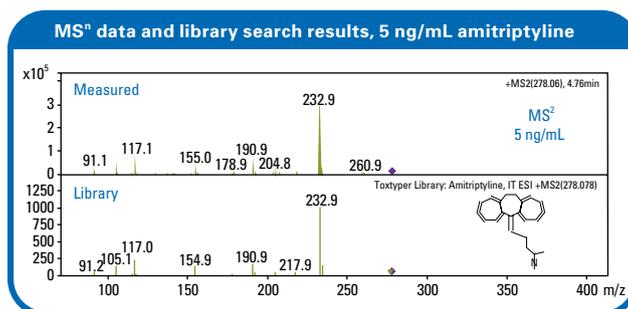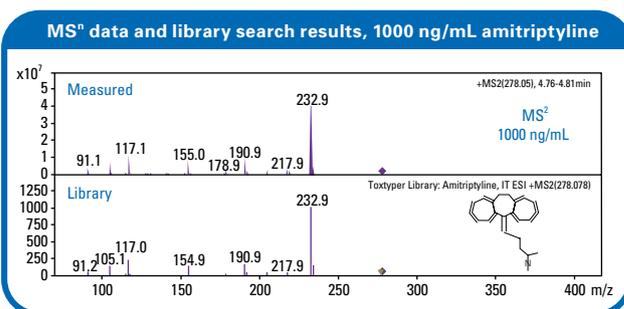
SmartFrag leads to reproducible and standardized library search results, irrespective of the compound concentration.

Semi-quantitation

Screening, confirmation, and semi-quantitation in a single run

Comprehensive screening methods reveal qualitative results. However, positive findings may require an accurate quantitation or at least an approximate concentration value for a particular compound in a given sample. To add value to the comprehensive screening, the standard Toxtyper analysis using Toxtyper and DOA libraries can be extended by semi-quantification.

After performing a one-point calibration for the target compounds using two or more internal standards, the subsequent Toxtyper analyses provide, in addition to the qualitative screening results, semiquantitive values (e.g., concentration above or below a target value).

Toxtyper® Report

Sample-ID	SQM-298GHT4198		Station	Toxtyper_3.0
Submitter	Tony Technician		Method	Toxtyper_SemiQuant (3.0E)
Analysis Name	SQM-298GHT4198_01_4018.d		Acquisition Date	5/18/2017 3:54:15 PM
Sample Description	Spiked Serum Matrix			

Base Peak Chromatogram

Library Search Results

Cmp Name	#	Purity'	RT [min]	d RT	m/z [Da]	d m/z	Int.	S/N	Semi-quant Conc.	ID	Comment
Buprenorphine	22	958	4.31	-0.11	468.33	-0.02	1.0 E8	158	38 ng/mL	MS2	
D5-Diazepam	28	984	5.76	-0.13	290.06	0.05	3.8 E7	134	68 ng/mL	MS2	
Methadone	24	967	4.72	-0.06	310.19	0.03	3.8 E7	85	17 ng/mL	MS2/MS3	
Creatinine	1	871	0.52	-0.01	114.05	0.02	2.5 E7	48		MS2	
D3-6-O-Acetylmorphine	14	981	2.88	-0.09	331.17	0.00	2.2 E7	79	39 ng/mL	MS2	
Diazepam	29	959	5.79	-0.14	285.03	0.05	1.7 E7	51	20 ng/mL	MS2	
Naproxen	26	992	5.48	-0.16	230.97	0.13	1.5 E7	66		MS2/MS3	
Trazodone	19	992	3.90	-0.17	372.17	-0.01	1.1 E7	24		MS2	
Hydrocortisone	23	974	4.46	-0.07	363.18	0.04	9.8 E6	32		MS2	
Fentanyl	21	991	4.12	-0.15	337.18	0.05	9.8 E6	24	5 ng/mL	MS2	
Warfarin	30	995	5.79	-0.16	309.06	0.05	7.3 E6	24		MS2	
Temazepam	27	844	5.57	0.06	301.13	-0.06	5.1 E6	12	tentative	MS2 unspecific	
Caffeine	15	982	3.00	-0.09	194.96	0.13	4.1 E6	9		MS2/MS3	
3-OH-Flubromazepam	25	877	4.88	-0.08	349.07	-0.07	3.7 E6	10		MS2	
Morphine	7	973	2.12	-0.07	286.07	0.08	3.1 E6	13	31 ng/mL	MS2	
Amphetamine	13	989	2.83	-0.02	135.93	0.17	2.5 E6	24	202 ng/mL	MS2/MS3	
Cotinine	6	972	1.22	0.19	176.98	0.12	2.1 E6	10		MS2	
Theophylline	11	932	2.68	-0.03	180.91	0.16	2.0 E6	7		MS2/MS3	
Theobromine	8	803	2.50	-0.09	180.99	0.08	1.9 E6	7		MS2	
9-Hydroxyrisperidone	17	900	3.68	-0.17	427.19	0.02	1.8 E6	3		MS2/MS3	
Risperidone	18	946	3.77	-0.20	411.17	0.05	1.7 E6	4		MS2/MS3	

A complete toxicology solution

Dr. Michael Böttcher, Head of Toxicology, MVZ Labor Dessau GmbH

"The Toxtyper is our fast routine workhorse solution for General Unknown Screening (GUS) in diverse matrices such as blood, urine or gastric content.

We answer demanding questions for our addictions lab customers by new Toxtyper applications like GUS in saliva."

Benefits of using Toxtyper:
"Streamlined sample throughput in our laboratory by unified, faster and easier sample preparation for urine samples and 24/7 usage of the system. Ready to use methods combined with comprehensive libraries."

George W. Hime, M.S., Assistant Laboratory Director and Elisa Shoff, Toxicologist II, Miami-Dade Medical Examiner Dept. Toxicology Laboratory, Miami, USA

"The Toxtyper has been our go-to instrument for postmortem casework containing novel substances, substances that are otherwise undetectable via GCMS, and unknown substances we have not yet seen in the lab. This instrument has been a blessing to our laboratory over the last several years of dealing with the flood of new illegal drugs in Miami. From synthetic cathinones to synthetic fentanyls we have detected and identified them all reliably and with high confidence. "

Benefits of using Toxtyper:
"Reliable, rugged, sensitivity beyond expectation, and ease of maintenance and operation are all features of this instrument. Full spectral MS^3 data at pg/mL sensitivities in postmortem whole blood or tissues cannot be beaten in our work by any other instrument."