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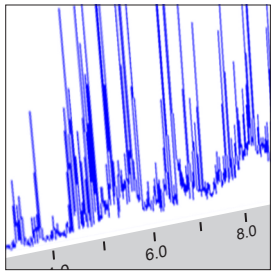
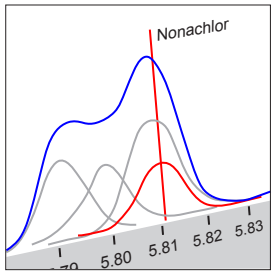
THE QUEEN'S AWARDS FOR ENTERPRISE: INTERNATIONAL TRADE 2015

TargetView

Easy-to-learn software for identifying compounds in complex GC–MS profiles





Target compound	CAS No.
Benzene	71-43-2
Toluene	108-88-3
Furfural	98-01-1
Heptanal	111-71-7
Benzaldehyde	100-52-7
	108-95-2

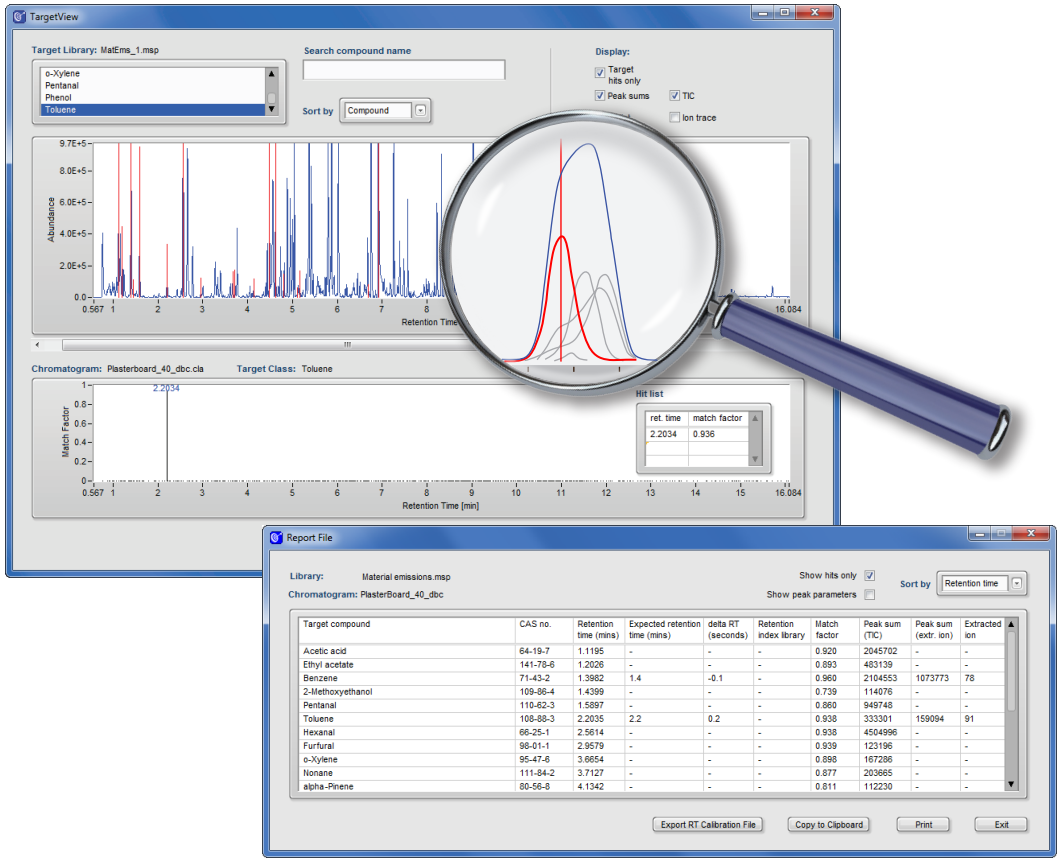
TargetView™

TargetView is a time-saving software package that confidently identifies both target and 'unknown' compounds in GC–MS profiles.

Using data in a variety of common file formats, TargetView processes complex chromatograms and displays information on the key compounds present in easy-to-understand graphical and tabular formats.

With TargetView, you'll be able to quickly identify trace-level analytes – even if they're apparently lost in complex background or hidden under co-eluting peaks.

Importantly, you don't need to be a GC–MS or statistics expert to get accurate, reliable results, because TargetView is far less complicated than other software platforms.



Target compound	CAS no.	Retention time (mins)	Expected retention time (mins)	delta RT (seconds)	Retention index library	Match factor	Peak sum (TIC)	Peak sum (extr. ion)	Extracted ion
Acetic acid	64-19-7	1.1195	-	-	-	0.920	2045702	-	-
Ethyl acetate	141-78-6	1.2026	-	-	-	0.893	483139	-	-
Benzene	71-43-2	1.3982	1.4	-0.1	-	0.960	2104553	1073773	78
2-Methoxyethanol	109-86-4	1.4399	-	-	-	0.739	114076	-	-
Pentanal	110-62-3	1.5897	-	-	-	0.860	949748	-	-
Toluene	108-88-3	2.2035	2.2	0.2	-	0.938	333301	159094	91
Hexanal	66-25-1	2.5614	-	-	-	0.938	4504996	-	-
Furfural	98-01-1	2.9579	-	-	-	0.939	123196	-	-
o-Xylene	95-47-6	3.6654	-	-	-	0.898	167286	-	-
Nonane	111-84-2	3.7127	-	-	-	0.877	203665	-	-
alpha-Pinene	80-56-8	4.1342	-	-	-	0.811	112230	-	-

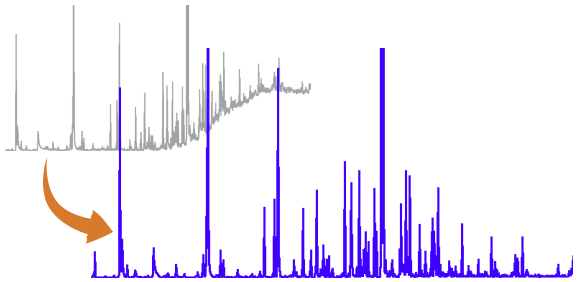
> "TargetView's clear report saves me a lot of time by rapidly confirming the presence of target compounds in complex samples"

Dr Amado Enrique Navarro Frómeta
Universidad Tecnológica de Izúcar de Matamoros, Mexico

Compound identification made easy

Using TargetView is easy. There are no complex settings to optimise, and results are delivered in a matter of minutes.

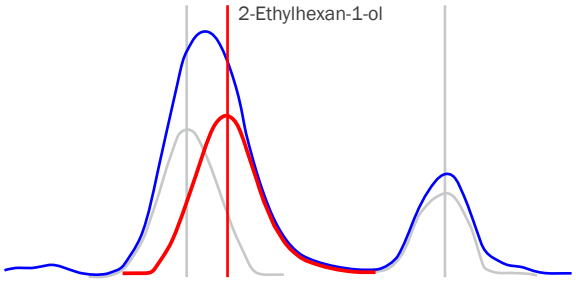
1 Import your chromatogram



Unify your laboratory procedures by using TargetView to intelligently remove unwanted baseline interference from chromatograms acquired using a variety of GC–MS platforms:

- BenchTOF-Evolve™ (.lsc)
- ChemStation® (.d)
- Xcalibur™, Chromeleon™ and TraceFinder™ (.raw)
- TurboMass™ (.raw)
- ANDI/netCDF (.cdf).

2 Run TargetView



Behind the scenes, TargetView's deconvolution algorithms work quickly and accurately to identify the compounds hidden in your dataset against your chosen library – whether a custom list of targets or the entire NIST database.

3 Output your report

Target compound	CAS No.	Retention time (min)	Match factor	Peak area
Benzaldehyde	100-52-7	17.273	0.915	133797
2,4-Dimethylheptane	2213-23-2	17.511	0.743	466333
beta-Pinene	127-91-3	17.598	0.894	156723
Octanal	124-13-0	17.732	0.773	41416
2-Ethylhexan-1-ol	104-76-7	18.051	0.869	64671
Benzyl alcohol	100-51-6	18.471	0.879	140629
Limonene	138-86-3	18.494	0.888	776248
gamma-Terpinene	99-85-4	18.955	0.810	42230

Fully automated report generation means you see your results straight away – and can export them to Excel® with a single mouse-click.

> "TargetView's ability to process multiple file types saves us significant time because one technician can process data from three different GC–MS systems"

Kieran Kilcawley
Teagasc Food Research Centre
Cork, Republic of Ireland

Reliable results – for targets *and* unknowns

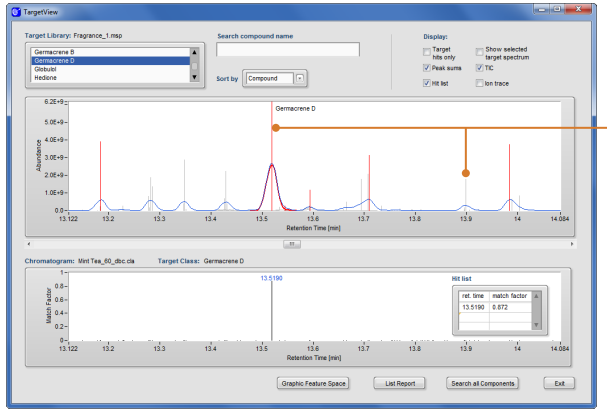
Whether you're looking for a discrete set of compounds in a specialist library, or want to interrogate your sample against large commercial databases, TargetView will give you results you can depend on, in the shortest possible time.

Quick, powerful searching against spectral libraries

If you're looking for a defined set of compounds, use TargetView's **target-searching capability** to quickly tell you whether or not they're present.

Routine searches are complete in a matter of minutes, and the results – viewable either as the interactive chromatogram or as a table – make it easy to see the compounds that are present.

In addition, creation of TargetView libraries is simple, whether from in-house datasets, or using data from a NIST-format library.

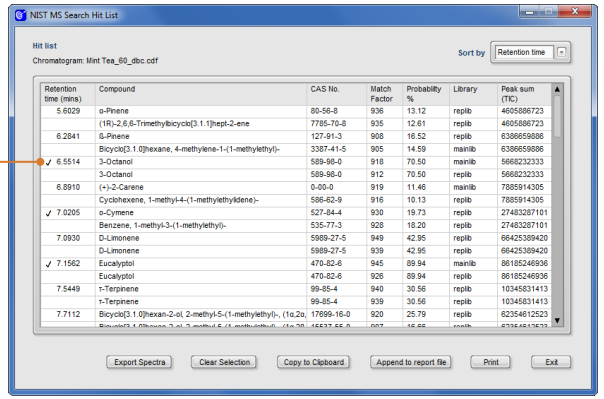


TargetView's interactive chromatogram distinguishes between targets (red bars) and non-targets (grey bars), for at-a-glance understanding. The heights of the bars themselves provide a quick indication of relative abundance.

TargetView's **ability to identify non-target compounds** by querying them against libraries is a powerful way of dealing with 'unknowns'.

When analysing a new type of sample, or simply wishing to identify as many relevant compounds as possible, use an 'all-component' search to screen against any NIST-format database.

Hits from an 'all-component' search are easily added to a target library.



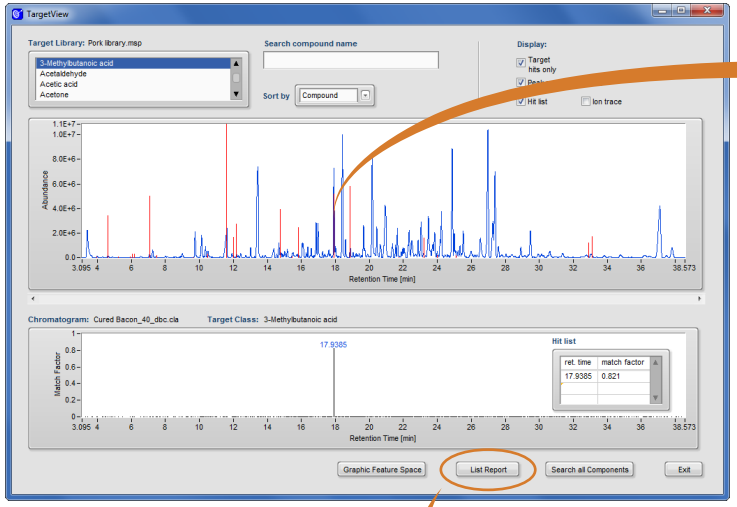
From complexity to clarity

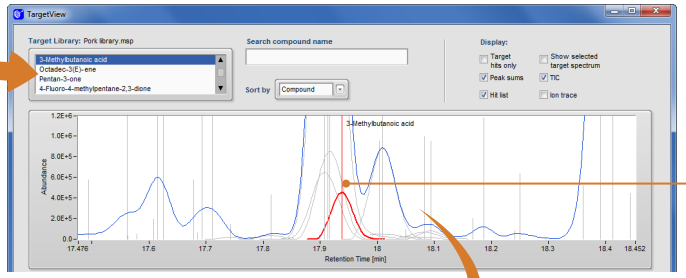
TargetView's interactive chromatogram allows you to delve into the results as much as you want – from a simple 'yes/no' confirmation that a particular compound is present, to detailed examination of elution profiles or comparison of mass spectra.

Processing multiple files?

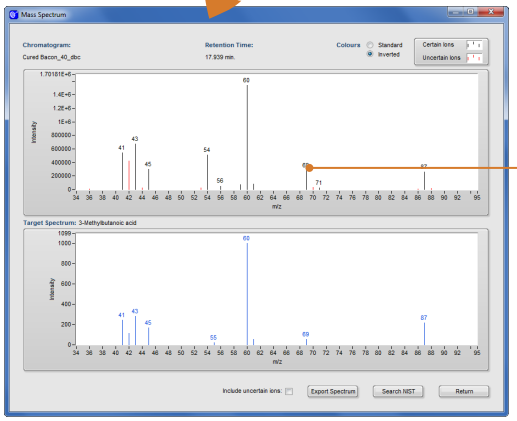
TargetView makes it easy to batch-process files against a single target library.

Diverse functionality from a single interface

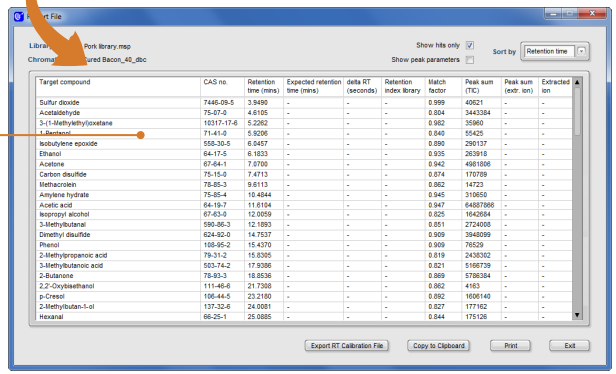




Simply clicking on a peak pulls up the deconvolved profiles of the target peak and those nearby, enabling you to visualise minor components hidden under other peaks.



The acquired mass spectrum of an individual compound (top) is readily compared against the library spectrum (bottom), for visual confirmation of the quality of the match.



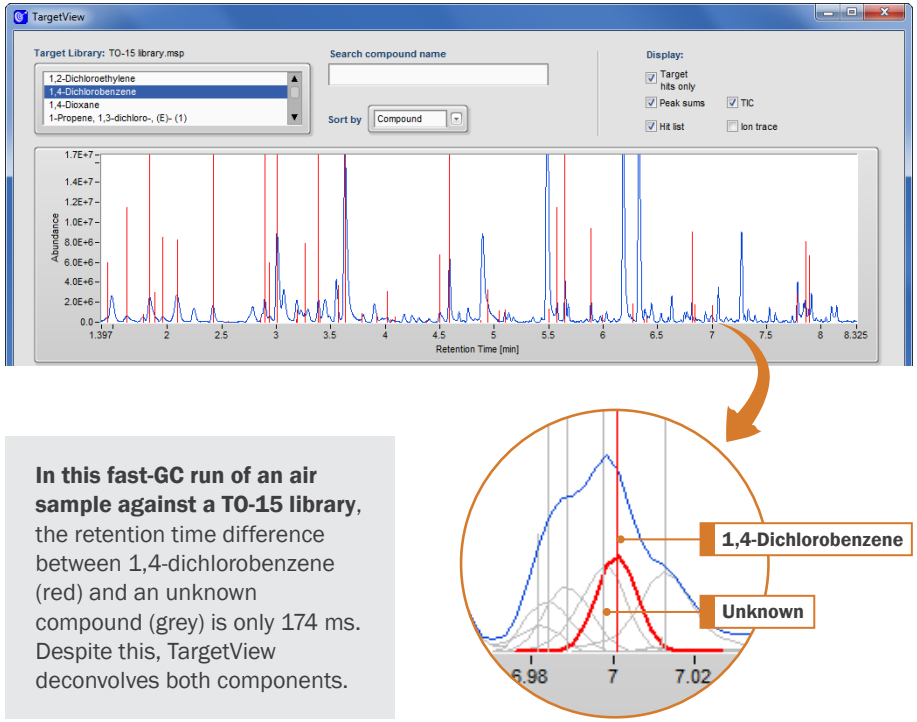
The easy-to-understand results listing provides key information such as retention time, match coefficient and peak areas. It can also be re-ordered on-screen for easier scanning, or exported to spreadsheet format for more in-depth processing.

Perfect for every application

TargetView's capability to identify both targets and unknowns makes it valuable to GC–MS analysts in every field. Below are just a few examples.

Air monitoring using high-speed chromatography

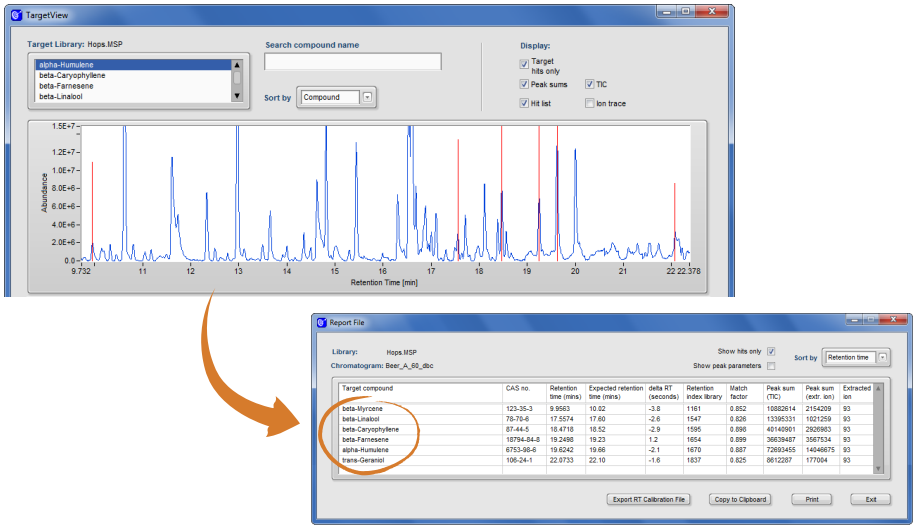
High-speed chromatography offers significant time savings for the busy laboratory, but co-elution can be a problem for complex samples. TargetView is a powerful tool in such cases – as illustrated by its ability to resolve pollutants in this air sample, despite a run time of less than 9 minutes.



In this fast-GC run of an air sample against a TO-15 library, the retention time difference between 1,4-dichlorobenzene (red) and an unknown compound (grey) is only 174 ms. Despite this, TargetView deconvolves both components.

Confidently identifying flavour components in beer

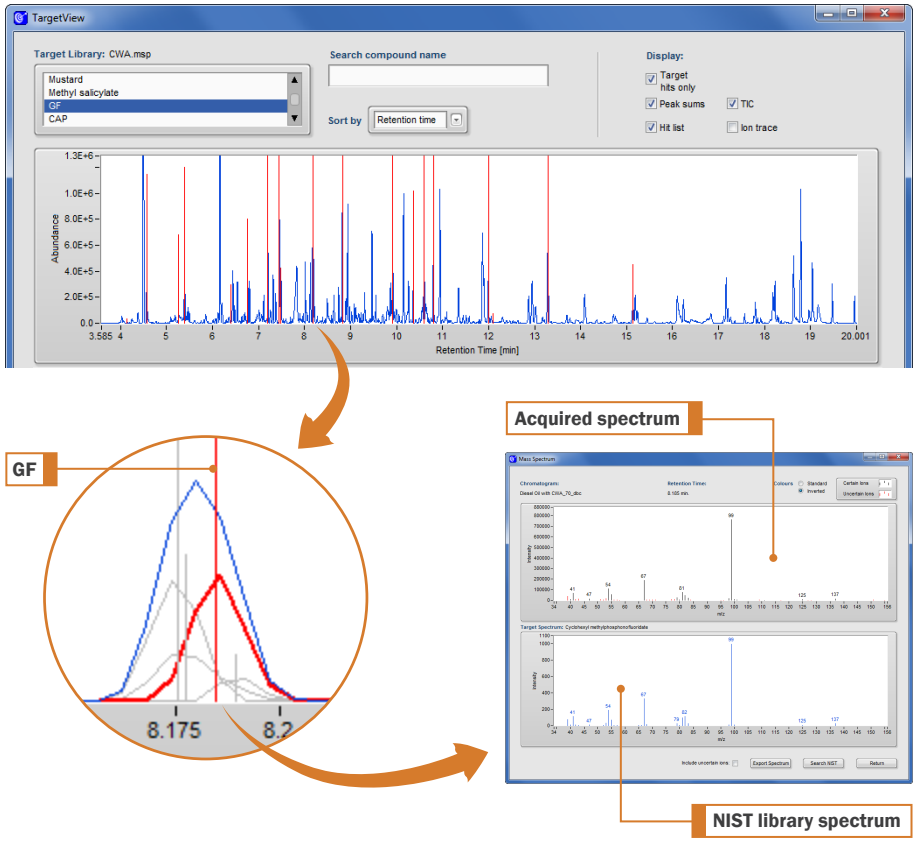
Retention indices generated by TargetView aid rapid, confident identification of challenging analytes, such as the hop-derived aroma compounds in this beer sample. Such compounds typically occur at low/sub-ppb concentrations, and play a key role in the characteristic flavours of beer.



Six target terpenes and sesquiterpenes at low-ppb concentrations were detected by TargetView within a beer sample using sorptive extraction and thermal desorption–GC–TOF MS analysis. Retention index values calculated by TargetView assist in compound confirmation and are listed in the final report.

Finding chemical warfare agents in a complex matrix

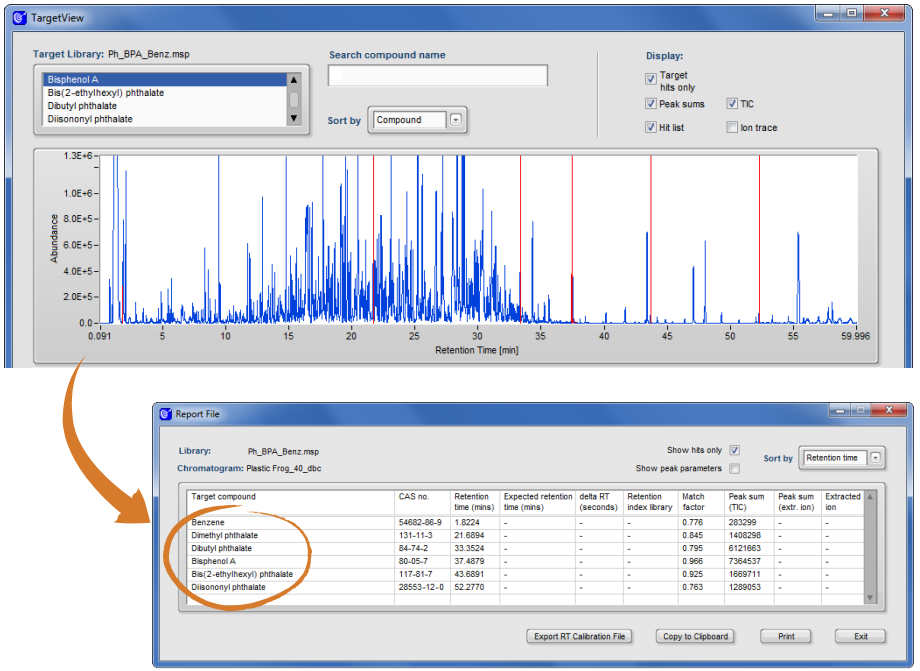
Identification of trace-level chemical warfare agents is highly challenging, and in this example we set up a worst-case scenario by mixing a selection of them with diesel oil. However, even presented with this challenge, TargetView is able to identify 'GF' (cyclosarin) with a high degree of confidence, despite significant co-elution.



Confident identification of 'GF' (cyclosarin) in a sample of diesel oil is possible despite the complexity of the original chromatogram and the presence of co-eluting compounds (whose profiles are shown in grey in the inset).

Detecting potentially hazardous components in plastic toys

TargetView is ideal for quickly flagging up the presence of target components in complex chromatograms, as shown by this example. The analysis reveals significant levels of phthalates and bisphenol A – endocrine disruptors that are present in a wide range of consumer goods, and are increasingly the focus of regulation.



TargetView's report easily identifies a number of potentially hazardous components in the VOC profile of a toy plastic frog – including benzene, bisphenol A and several phthalates.

For more examples of the application of TargetView, visit www.markes.com

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Markes International Ltd

Gwaun Elai Medi-Science Campus
Llantrisant
RCT, CF72 8XL
UK

T: +44 (0)1443 230935
F: +44 (0)1443 231531
E: enquiries@markes.com
W: www.markes.com

Markes International, Inc.

11126-D Kenwood Road
Cincinnati
Ohio 45242
USA

T: 866-483-5684 (toll-free)
F: 513-745-0741
E: enquiries@markes.com
W: www.markes.com

Markes International GmbH

Schleussnerstrasse 42
D-63263 Neu-Isenburg
Frankfurt
Germany

T: +49 (0)6102 8825569
F: +49 (0)6102 8825583
E: enquiries@markes.com
W: www.markes.com