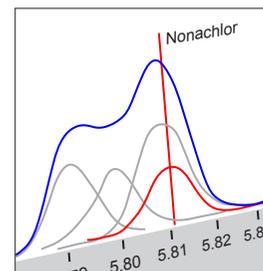
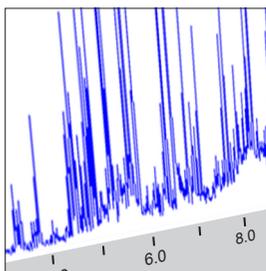


TargetView

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

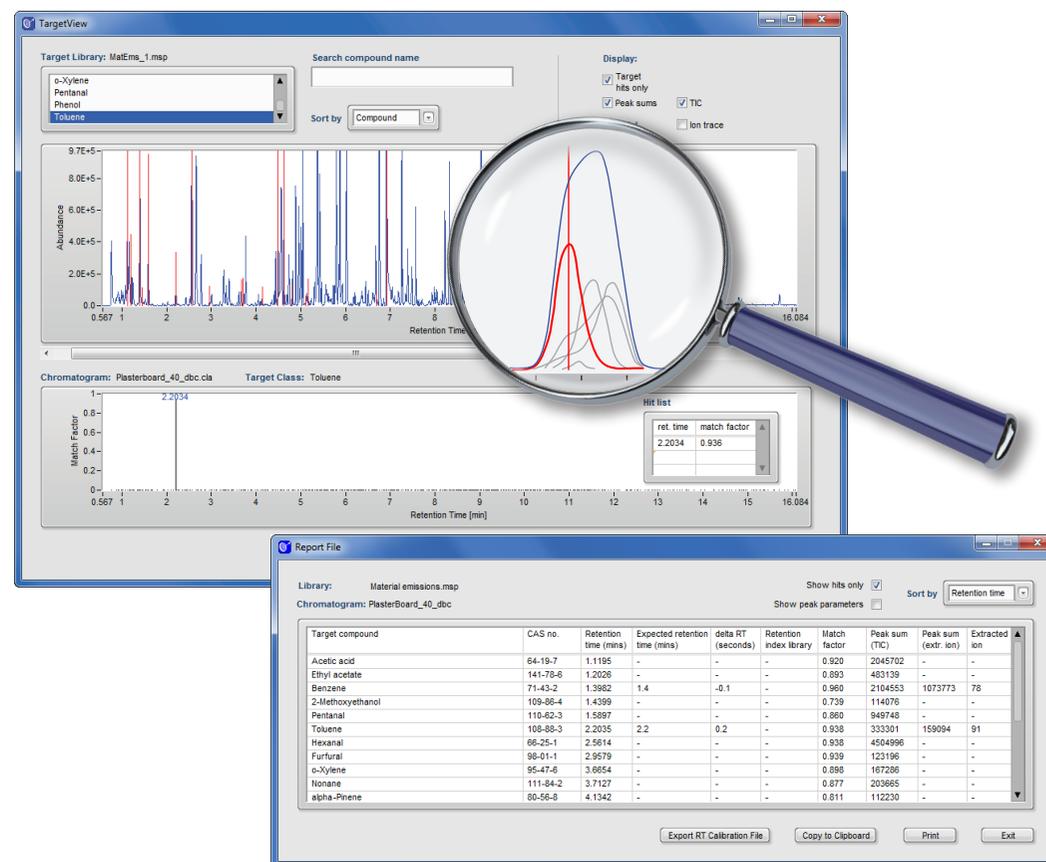
TargetView™

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.



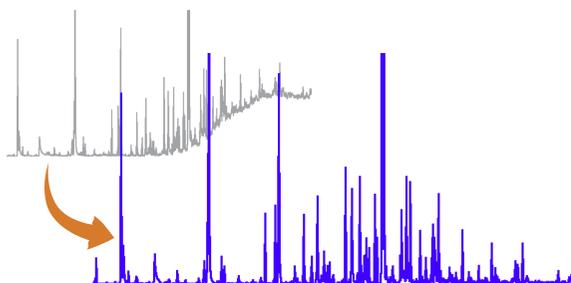
“TargetView’s clear report saves me a lot of time by rapidly confirming the presence of target compounds in complex samples”

Dr Amado Enrique Navarro Frómata
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.

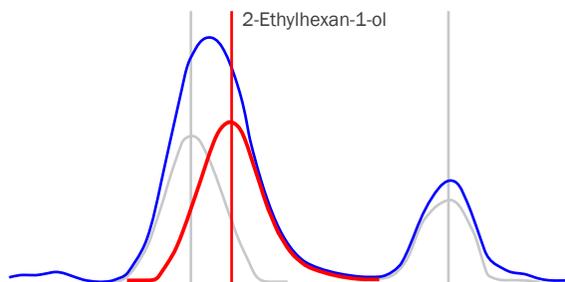
1 Import your chromatogram



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
Octenal	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.

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.

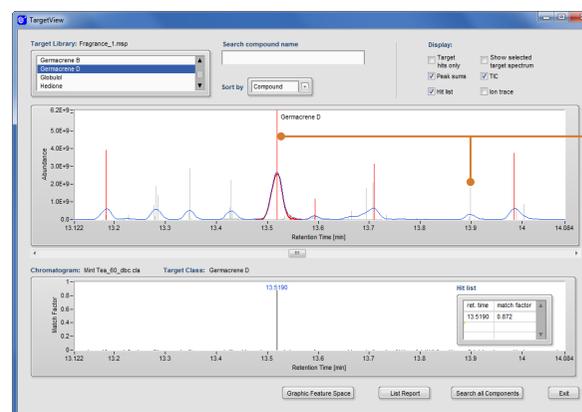
Routine searches are complete in a matter of minutes, and the results – viewable either as the interactive chromatogram or as a table – make it easy to see the compounds that are present.

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

TargetView's **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.

Quick, powerful searching against spectral libraries



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.

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

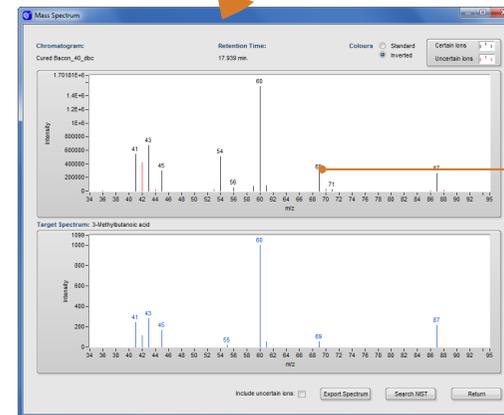
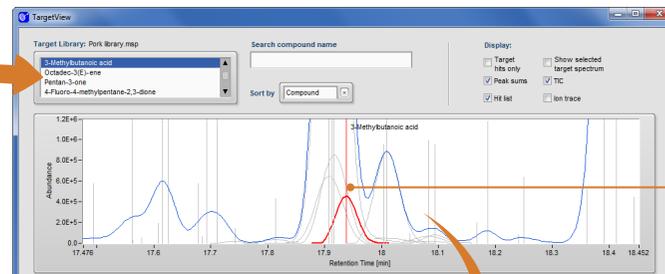
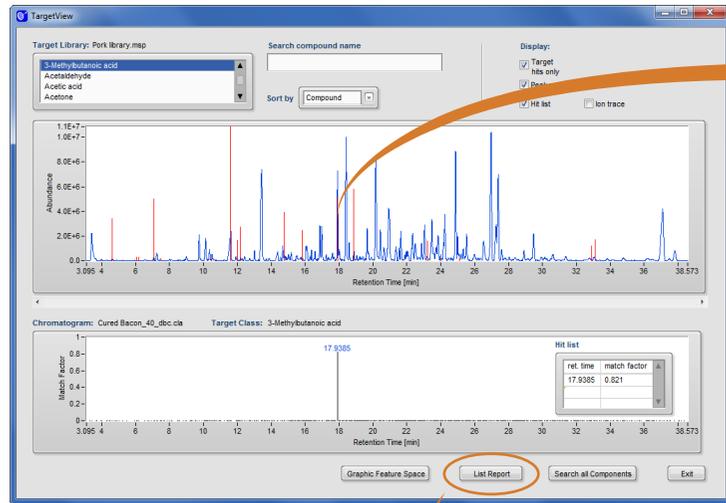
The screenshot shows the NIST MS Search Hit List window. It displays a table of search results. The table has the following columns: Retention time (min), Compound, CAS No., Match Factor, Probability, Library, and Peak sum (TIC). The table is sorted by Retention time. The first few rows are:

Retention time (min)	Compound	CAS No.	Match Factor	Probability	Library	Peak sum (TIC)
5.6029	o-Pinene	80-56-8	936	13.12	replib	4605586723
	(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	7795-70-8	935	12.61	replib	4605586723
6.2841	β-Pinene	127-91-3	908	16.52	replib	638659898
	Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)-	3387-41-5	905	14.59	manlib	638659898
6.5514	3-Octanol	589-86-0	918	79.86	manlib	589823233
	3-Octanol	589-86-0	912	79.50	replib	666232333
6.8910	(+)-2-Carene	0-00-0	919	11.48	manlib	7885914305
	Cyclohexene, 1-methyl-4-(1-methylethylidene)-	586-82-9	916	10.13	replib	7885914305
7.0205	o-Cymene	627-84-4	930	19.73	replib	27483287101
	Benzene, 1-methyl-3-(1-methylethyl)-	535-77-3	928	18.20	replib	27483287101
7.0930	D-Limonene	5989-27-5	949	42.95	replib	66425389420
	D-Limonene	5989-27-5	939	42.95	replib	66425389420
7.1582	Eucalyptol	470-82-6	945	89.94	manlib	8618246936
	Eucalyptol	470-82-6	928	89.94	replib	8618246936
7.5449	1-Terpinene	99-85-4	940	30.56	replib	1034531413
	1-Terpinene	99-85-4	939	30.56	replib	1034531413
7.7112	Bicyclo[3.1.0]hexan-2-yl 2-methyl-5-(1-methylethyl)-	10,20, 17699-16-0	920	25.79	replib	62354912523
	Bicyclo[3.1.0]hexan-2-yl 2-methyl-5-(1-methylethyl)-	10,20, 17699-16-0	907	16.68	replib	62354912523

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.

Diverse functionality from a single interface



Processing multiple files?

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

Simply clicking on a peak pulls up the deconvolved 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.

The screenshot shows a detailed results listing table with columns for Target compound, CAS no., Retention time (mins), Expected retention time (mins), delta RT (seconds), Retention index, Match factor, Peak sum (TIC), Peak sum (extr. ion), and Extracted ion.

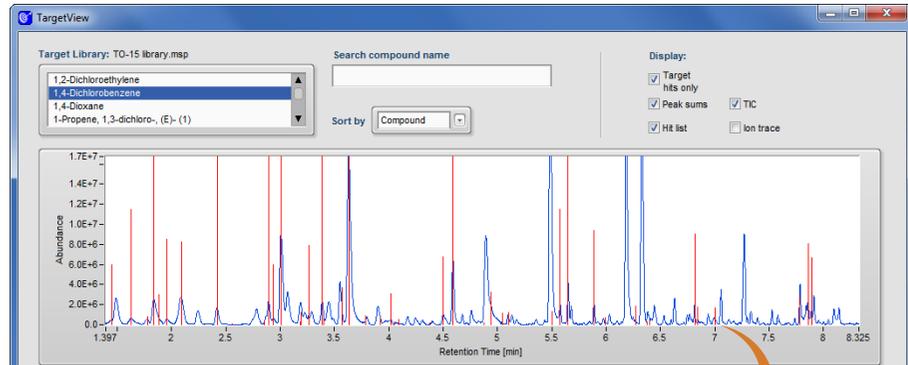
Target compound	CAS no.	Retention time (mins)	Expected retention time (mins)	delta RT (seconds)	Retention index	Match factor	Peak sum (TIC)	Peak sum (extr. ion)	Extracted ion
Sulfur dioxide	7446-09-5	3.9489	-	-	0.999	40251	-	-	-
Acetaldehyde	75-07-8	4.6105	-	-	0.804	5443384	-	-	-
3-1-Methylcyclohexane	10317-17-6	5.2262	-	-	0.962	55960	-	-	-
3-Butene	71-41-9	5.9206	-	-	0.949	55425	-	-	-
Isobutylene epoxide	558-35-5	6.9457	-	-	0.890	290137	-	-	-
Ethanol	64-17-5	6.1823	-	-	0.926	283918	-	-	-
Acetone	67-64-1	7.0709	-	-	0.942	4891696	-	-	-
Carbon disulfide	75-15-9	7.4713	-	-	0.874	179779	-	-	-
Diethaceton	78-85-3	9.6113	-	-	0.982	14723	-	-	-
Alkyne hydrate	75-85-4	10.4544	-	-	0.945	310665	-	-	-
Acetic acid	64-19-7	11.6194	-	-	0.947	64037966	-	-	-
Isopropyl alcohol	67-63-0	12.0959	-	-	0.825	1603064	-	-	-
3-Methylbutanal	595-85-3	12.1893	-	-	0.851	2724000	-	-	-
Dimethyl disulfide	624-82-0	14.7537	-	-	0.909	3948099	-	-	-
Phenol	108-95-2	15.4370	-	-	0.909	78529	-	-	-
3-Methylpropanoic acid	79-31-2	15.6395	-	-	0.819	2436302	-	-	-
3-Methylbutanoic acid	503-74-2	17.9386	-	-	0.821	5166739	-	-	-
2-Butanone	78-93-3	18.8038	-	-	0.969	9798384	-	-	-
2,2-Oxyethanol	111-46-8	21.7398	-	-	0.862	4183	-	-	-
p-Cresol	108-44-3	23.2180	-	-	0.892	1883148	-	-	-
2-Methylpropan-2-ol	137-32-6	24.0981	-	-	0.827	177162	-	-	-
Hexanal	66-26-1	25.0885	-	-	0.844	175128	-	-	-

Perfect for every application

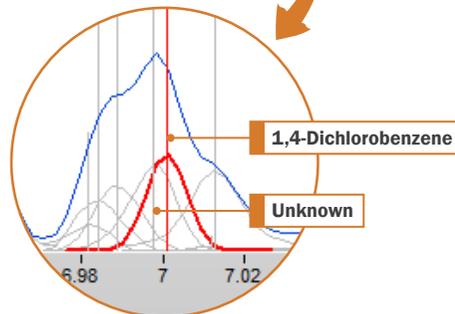
TargetView's capability to identify both targets and unknowns makes it valuable to GC-MS analysts in every field. Below are just a few examples.

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.

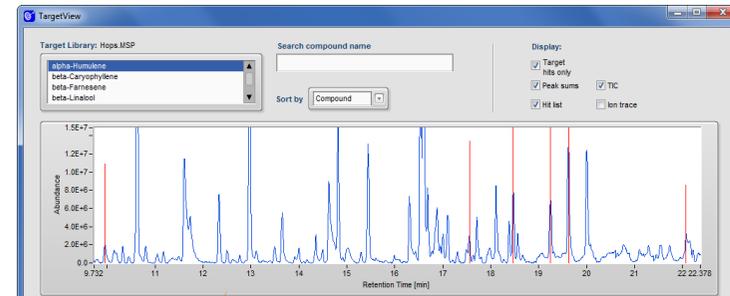


In this fast-GC run of an air sample against a TO-15 library, the retention time difference between 1,4-dichlorobenzene (red) and an unknown compound (grey) is only 174 ms. Despite this, TargetView deconvolves both components.



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.



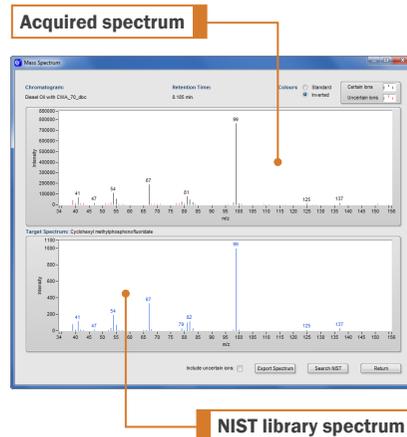
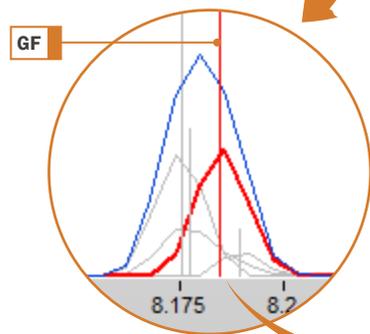
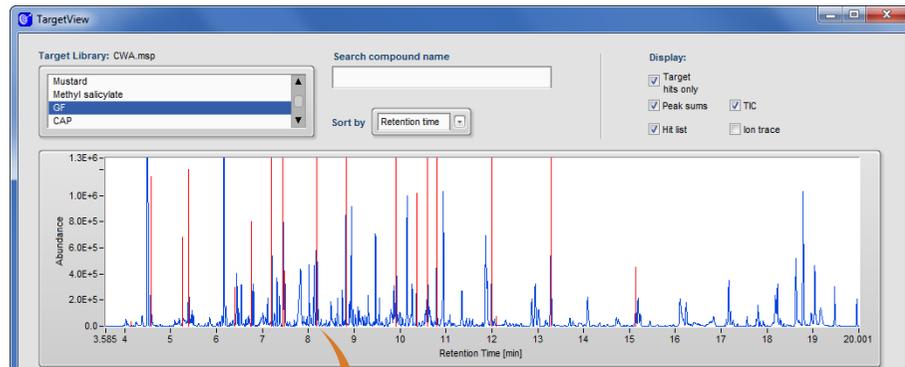
Target compound	CAS no.	Retention time (min)	Expanded retention time (min)	delta RT (seconds)	Retention index (TC)	Match factor	Peak sum (TIC)	Peak sum (ext. ion)	Extracted ion
beta-Myrcene	123-35-3	9.9563	10.02	-3.8	1161	0.852	11082814	2154209	93
beta-Linalool	78-79-6	17.5274	17.60	-2.6	1547	0.838	13368331	1021528	93
beta-Caryophyllene	87-44-5	18.4710	18.52	-2.9	1585	0.898	40149801	2928983	93
beta-Farnesene	19794-04-8	19.2480	19.23	1.2	1654	0.899	36839487	3687534	93
alpha-Humulene	6753-96-6	19.8242	19.68	-2.1	1670	0.887	73820445	1468875	93
trans-Geraniol	106-24-1	22.0753	22.10	-1.6	1837	0.825	8612287	177004	93

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.

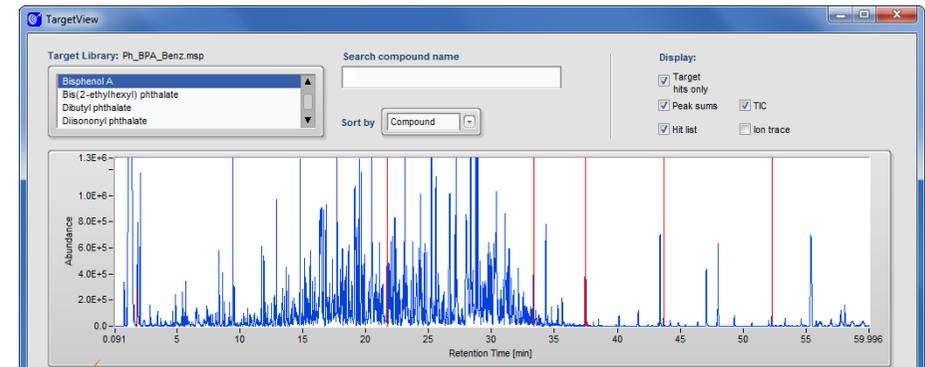


Confident identification of 'GF' (cyclosarin) in a sample of diesel oil is possible despite the complexity of the original chromatogram and the presence of co-eluting compounds (whose profiles are shown in grey in the inset).

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.



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
Benzene	54682-95-9	1.8224	-	-	-	0.776	283299	-	-
Dimethyl phthalate	131-11-3	21.6894	-	-	-	0.845	1402268	-	-
Dibutyl phthalate	84-74-2	33.3524	-	-	-	0.795	6121663	-	-
Bisphenol A	80-05-7	37.4879	-	-	-	0.966	7364537	-	-
Bis(2-ethylhexyl) phthalate	117-81-7	43.6891	-	-	-	0.925	1668711	-	-
Diisononyl phthalate	28553-12-0	52.2770	-	-	-	0.763	1289053	-	-

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

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

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