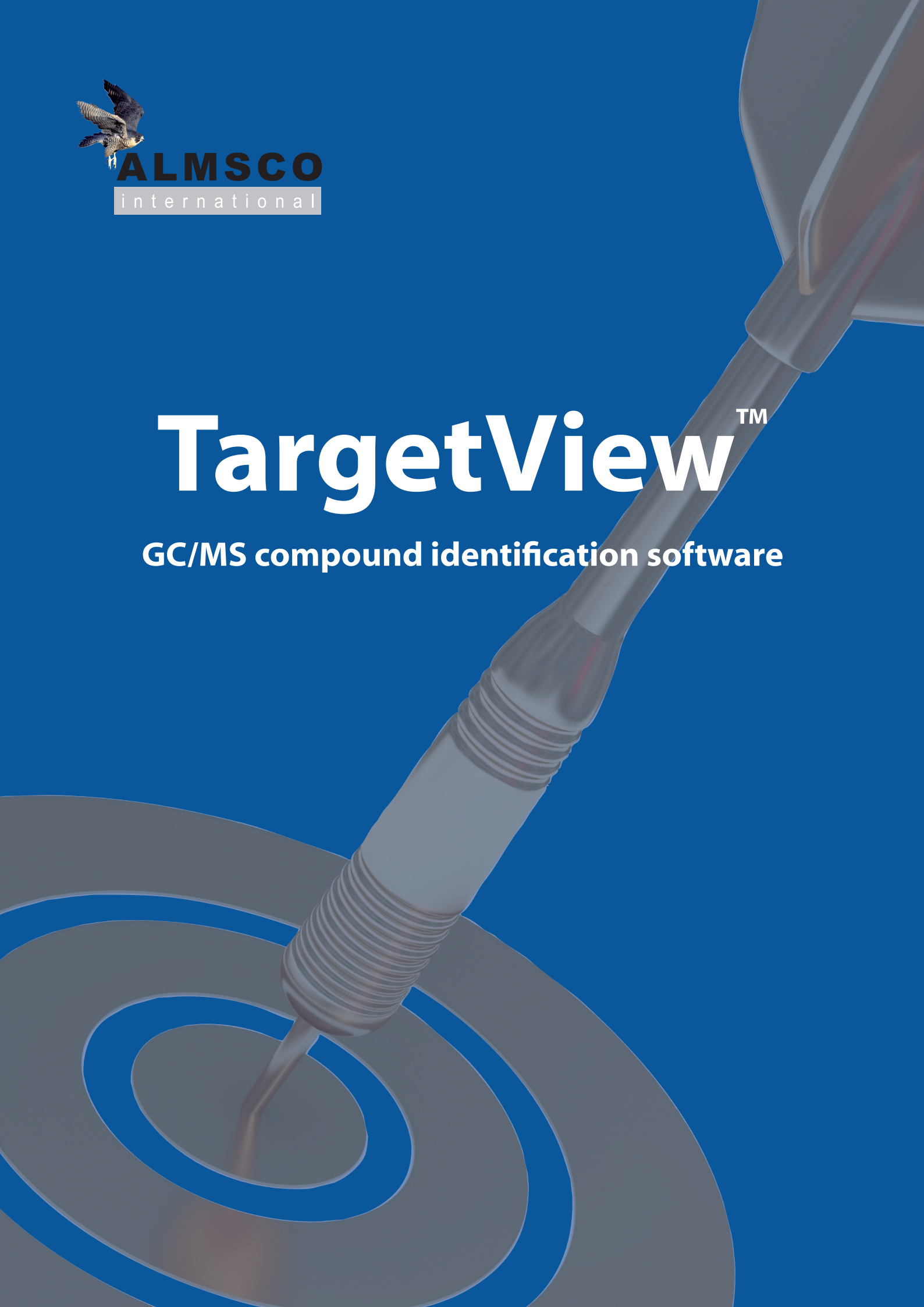




**ALMSCO**  
international

# TargetView<sup>TM</sup>

GC/MS compound identification software

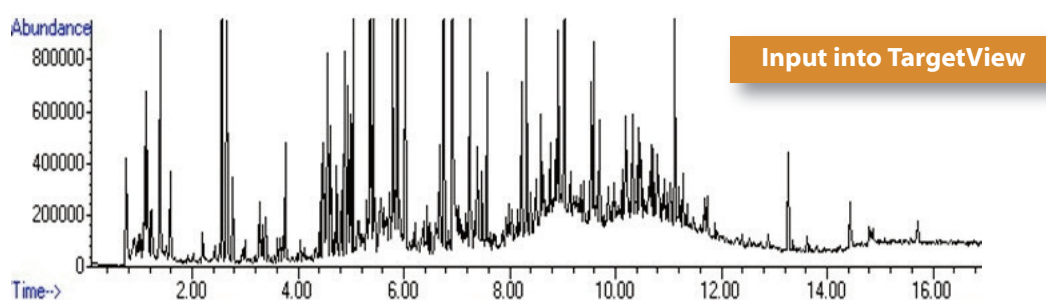


# TargetView™

## What is TargetView?

TargetView is a time-saving software package allowing accurate identification of both target and non-target ('unknown') compounds in GC/MS profiles. It is easy to learn and simple to operate, and compatible with GC/MS files produced by all major brands of GC/MS instruments.

TargetView is ideal for GC/MS analysts who need to rapidly screen chromatograms against compound libraries, or those who are looking for trace-level analytes apparently lost in complex background. TargetView also offers automated identification of unknown compounds, making it suitable for all GC/MS applications.



Report File

Library: MatEms\_1.msp  
Chromatogram: PlasterBoard\_40\_dbc

☒ Show hits only    Sort by: Matching coefficient

Target compound	CAS no.	Retention time (mins)	Expected retention time (mins)	delta RT (seconds)	Retention index library	Matching coefficient	Peak sum (TIC)	Peak sum (extr. ion)	Extracted ion
1-Methoxy-2-propyl acetate	108-65-6	3.3248	-	-	-	0.991	404805	-	-
Ethanol, 2-phenoxy-	122-99-6	6.9138	-	-	-	0.960	6582164	-	-
Heptanal	111-71-7	3.7599	-	-	-	0.956	1155717	-	-
Phenol	108-95-2	4.6142	-	-	-	0.953	1346286	-	-
Benzene	71-43-2	1.3941	1.4	-0.4	-	0.952	2031643	1073683	78
Benzaldehyde	100-52-7	4.4853	-	-	-	0.948	1152502	-	-
Toluene	108-88-3	2.1995	2.2	-0.0	-	0.948	328793	160233	91
Dibutyl phthalate	84-74-2	11.7265	-	-	-	0.946	448206	-	-
Furfural	98-01-1	2.9531	-	-	-	0.939	125357	-	-
Hexanal	66-25-1	2.5559	-	-	-	0.931	4482918	-	-
Ethyl Acetate	141-78-6	1.1970	-	-	-	0.910	462123	-	-
Nonane	111-84-2	3.7074	-	-	-	0.906	222766	-	-
Benzene, 1,2,4-trimethyl-	95-63-6	4.7993	-	-	-	0.901	157435	-	-

Copy to Clipboard    Print    Exit

TargetView data-mines a complex chromatogram, producing a simple report showing the compounds identified.

## What TargetView offers the GC/MS analyst

---

TargetView offers several benefits to the user compared with other data-mining software packages or manual processing.

### TargetView at a glance:

- Easy to learn and simple to operate
- Identifies both target compounds and non-targets ('unknowns')
- Rapidly screens chromatograms against compound libraries
- Deconvolves co-eluting compounds
- Eliminates background interferences
- Produces a simple report allowing at-a-glance assessment
- Easy exporting of data to Microsoft Excel®
- Produces an interactive chromatogram that makes detailed interpretation of results easy
- Compatible with files produced by all major brands of GC/MS instruments
- Processes chromatograms rapidly, saving time and money
- Interfaces with commercial or custom-made spectral libraries
- Retains original chromatograms for future reference

**For faster, simpler and more accurate analysis  
of compounds in complex GC/MS profiles**

## The three main stages of the TargetView process

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### 1 Import files



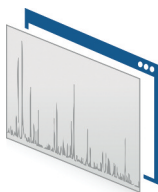
During file import, TargetView removes background interference from your imported chromatogram and deconvolves the data into individual analyte peaks.



### 2 Compare data



TargetView either compares each peak against a target library, or identifies as many compounds in the chromatogram as possible by searching against a NIST mass spectral library.



### 3 Report results



A report is produced that allows analytes to be identified, matches to be cross-checked against NIST, and compounds to be added to libraries.

## Using TargetView

### Identifying target compounds

Every TargetView library search starts by selecting the chromatogram and spectral library to be analysed. A single mouse-click then starts the TargetView process, which extracts the mass spectra of individual component peaks, and compares them against those in the library.

A report is produced that allows you to see instantly which compounds are present. It can also tell you which compounds in the library have *not* been found (this is useful if a sample is being screened to ensure that it doesn't contain certain compounds).

The screenshot shows the 'Report File' window from TargetView. It displays a table of identified compounds with the following columns: Target compound, CAS no., Retention time (mins), Expected retention time (mins), delta RT (seconds), Retention index library, Matching coefficient, Peak sum (TIC), Peak sum (extr. ion), and Extracted ion. The table lists several compounds, including 1-Methoxy-2-propyl acetate, Ethanol, 2-phenoxy-, Heptanal, Phenol, Benzene, Benzaldehyde, Toluene, Dibutyl phthalate, Furfural, Hexanal, Ethyl Acetate, Nonane, and Benzene, 1,2,4-trimethyl-. Callouts point to various features: 'Chemical name' points to the 'Target compound' column; 'A CAS number identifies the compound unambiguously' points to the 'CAS no.' column; 'A check-box toggles the display to show either those compounds found, or all compounds in the target library' points to the 'Show hits only' checkbox; 'A peak sum is calculated to aid determination of peak areas' points to the 'Peak sum (TIC)' column; 'Entries can be sorted by retention time, compound name, match coefficient, or peak sum' points to the 'Sort by' dropdown menu; 'Matches can be penalised where the retention time of the peak differs from an inputted value' points to the 'delta RT (seconds)' column; 'If present in the library data, the retention index is displayed' points to the 'Retention index library' column; 'A match coefficient indicates the quality of the target match' points to the 'Matching coefficient' column; and 'An ion can be defined in the library for improved determination of peak areas' points to the 'Extracted ion' column.

Target compound	CAS no.	Retention time (mins)	Expected retention time (mins)	delta RT (seconds)	Retention index library	Matching coefficient	Peak sum (TIC)	Peak sum (extr. ion)	Extracted ion
1-Methoxy-2-propyl acetate	108-65-6	3.3248	-	-	-	0.991	404805	-	-
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Heptanal	111-71-7	3.7599	-	-	-	0.956	1155717	-	-
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Dibutyl phthalate	84-74-2	11.7265	-	-	-	0.946	448206	-	-
Furfural	98-01-1	2.9531	-	-	-	0.939	125357	-	-
Hexanal	66-25-1	2.5059	-	-	-	0.931	4482918	-	-
Ethyl Acetate	141-78-6	1.1970	-	-	-	0.910	462123	-	-
Nonane	111-84-2	3.7074	-	-	-	0.906	222766	-	-
Benzene, 1,2,4-trimethyl-	95-68-6	4.7893	-	-	-	0.901	157435	-	-

**TargetView's simple report** shows the compounds that have been found.

Compound identification is carried out purely on the basis of similarity of the mass spectra, so it does not matter what GC platform, capillary column, or instrument setup was used. The report can be opened in a spreadsheet for more in-depth processing.

Individual peaks (whether identified as targets or not) can be searched against a NIST library on a case-by-case basis – either to provide confirmation of a target match identified using an in-house library, or to identify an unknown compound.

## Identifying unknown compounds

When analysing a new type of sample, or simply wishing to identify as many relevant compounds as possible, TargetView's ability to identify non-target compounds is indispensable – whether automated or manual.

### Automated searching

The easiest way to search a sample for all components is to use TargetView's automated matching capability, in conjunction with a large spectral database such as a NIST library.

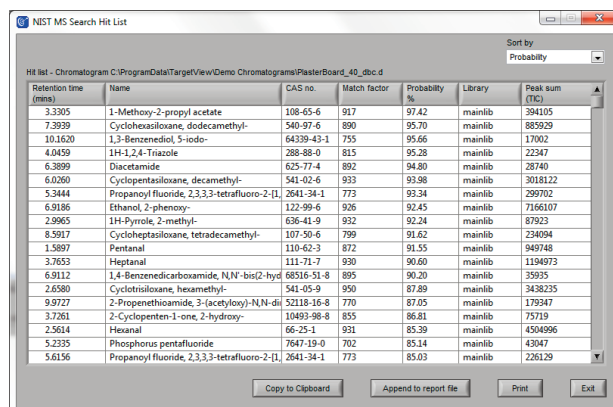
With the chromatogram selected, search criteria are confirmed by the user, and within a few minutes, TargetView will have produced a report detailing all components found. This can be carried out before or after a normal target search.

Results can be re-ordered on-screen for easy identification of relevant compounds, or can be opened in a spreadsheet for more in-depth processing.

Unknown compounds of interest can be selected to form part of a new library by simple tick-box selection. This spectral library can then be combined with others to screen subsequent samples – greatly speeding up the process of target identification.

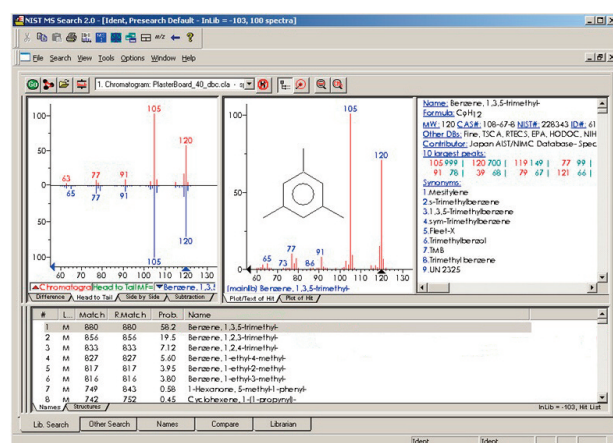
### Manual searching

The same search can also be performed on a case-by-case basis, so if just a single peak is of interest, a search against the NIST library can be undertaken, and a list of likely compounds returned.



Retention time (min)	Name	CAS no.	Match factor	Probability %	Library	Peak sum (TIC)
3.305	1-Methoxy-2-propyl acetate	108-65-6	917	97.42	mainlib	394105
7.3939	Cyclohexisiloxane, dodecamethyl-	540-87-6	880	95.70	mainlib	885929
10.1620	1,3-Benzenediol, 5-iodo-	64339-43-1	755	95.66	mainlib	17002
4.0459	1H-1,2,4-Triazole	288-88-0	815	95.28	mainlib	22347
6.3899	Diacetamide	625-77-4	892	94.80	mainlib	28740
6.0260	Cyclopentasiloxane, decamethyl-	541-02-6	933	93.98	mainlib	3018122
5.3444	Propanoyl fluoride, 2,3,3,3-tetrafluoro-2-[1,	2641-34-1	773	93.34	mainlib	299702
6.9186	Ethanol, 2-phenenyl-	122-99-6	926	92.45	mainlib	7166107
2.9965	1H-Pyrole, 2-methyl-	638-41-9	932	92.24	mainlib	87923
8.5917	Cycloheptasiloxane, tetradecamethyl-	107-50-6	799	91.62	mainlib	234094
1.5897	Pentalan	110-62-3	872	91.55	mainlib	949748
3.7653	Heptanal	111-71-7	930	90.60	mainlib	1194973
6.9112	1,4-Benzenedicarboxamide, N,N'-bis(2-hyd	68516-51-8	895	90.20	mainlib	35935
2.8389	Cyclotrisiloxane, hexamethyl-	541-05-9	950	87.89	mainlib	3438235
9.9727	2-Propenethiolamide, 3-(acetylonyl)-N,N-di	52118-16-8	770	87.05	mainlib	179347
3.7261	2-Cyclopenten-1-one, 2-hydroxy-	10493-98-8	855	86.81	mainlib	75719
2.5614	Hexanal	66-25-1	931	85.39	mainlib	4504996
5.2335	Phosphorus pentafluoride	7647-19-0	702	85.14	mainlib	43047
5.6156	Propanoyl fluoride, 2,3,3,3-tetrafluoro-2-[1,	2641-34-1	773	85.03	mainlib	226129

TargetView can query the NIST database and return a list of matches for all peaks in the chromatogram, whether in the target library or not.

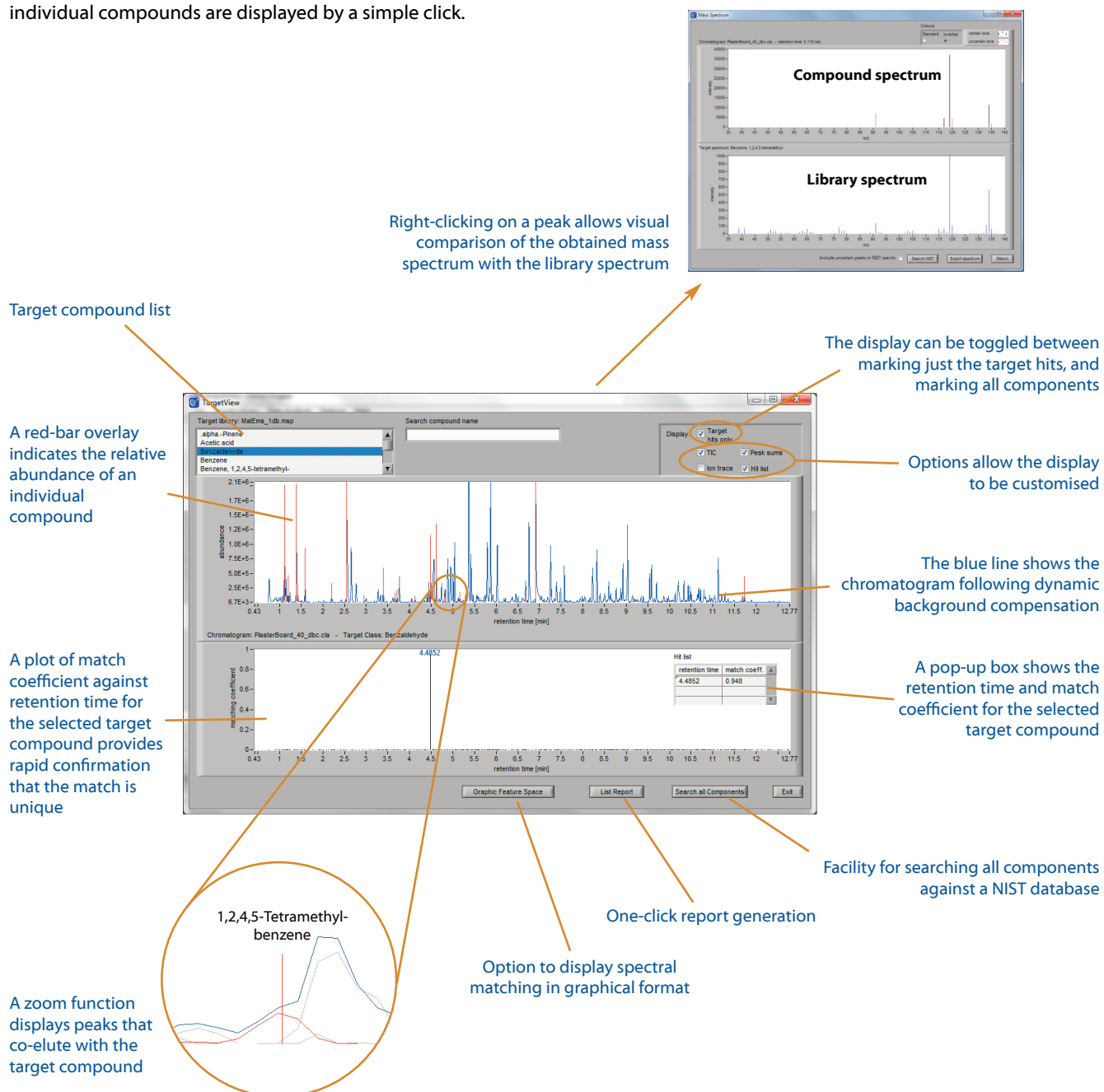


TargetView allows an individual peak to be searched against the NIST database.

# Accurate and reliable identification of target compounds *and* unknowns

## Interactive chromatogram

TargetView's interactive chromatogram allows the user to see instantly the outcome of the target-matching process. Zoom capability allows every detail to be examined, while match details and mass spectra of individual compounds are displayed by a simple click.



**TargetView's interactive chromatogram** shows the compounds identified in the sample, with a range of features that allow in-depth examination of the results.

## Creating libraries

Creation of TargetView libraries is simple, whether from in-house datasets or using spectra imported from databases such as NIST.

In addition, TargetView can be used to save deconvolved spectra of unknown compounds to a bespoke library. This is useful where the spectra are not in a commercial library and need to be experimentally determined, or where you need that extra confidence that comes from acquiring a spectrum on the instrument to be used for subsequent analyses.

## Determination of peak areas

All TargetView peak abundance data is determined after the application of algorithms that minimise interference from baseline anomalies and overlapping components, making it ideal for semi-quantitative determination of peak areas.

It is also possible for the user to specify an extracted ion for each target compound and generate a peak sum for that ion.

## Batch processing

TargetView's batch processing mode makes it easy to process multiple files against a single target library, saving time for busy laboratories.

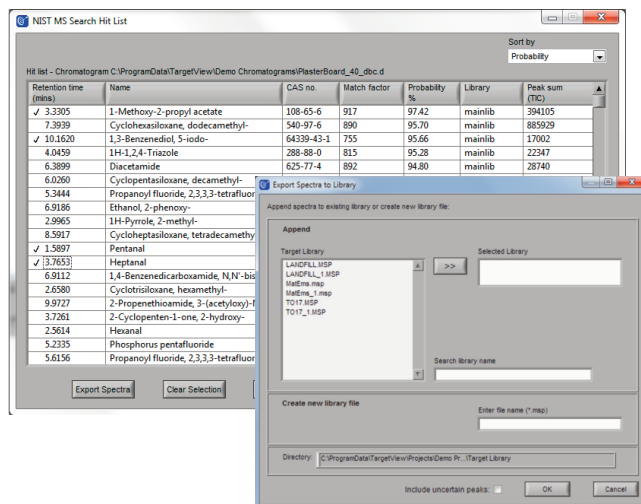
## File preview

Double-clicking a file icon for a chromatogram, library or report in the main project window is a convenient way of previewing the file content.

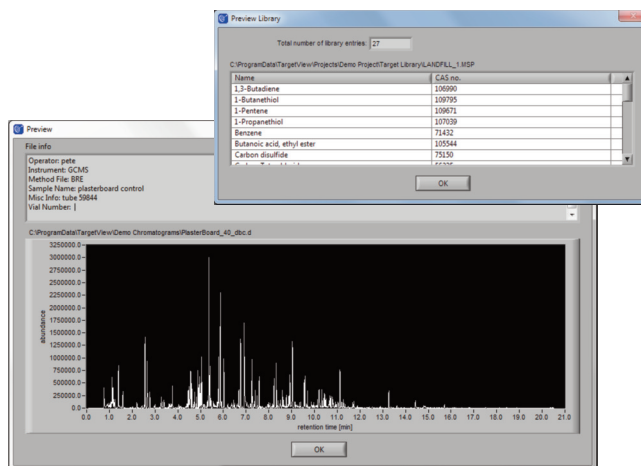
## File formats accepted

The following GC/MS file formats are supported by TargetView: ChemStation® (\*.d), ALMSCO (\*.lsc) and ANDI/netCDF (\*.cdf).

In addition, native file formats from many other GC/MS data systems can be easily converted to \*.cdf format for analysis by TargetView.



Creating a library or adding to an existing library is simple and straightforward.

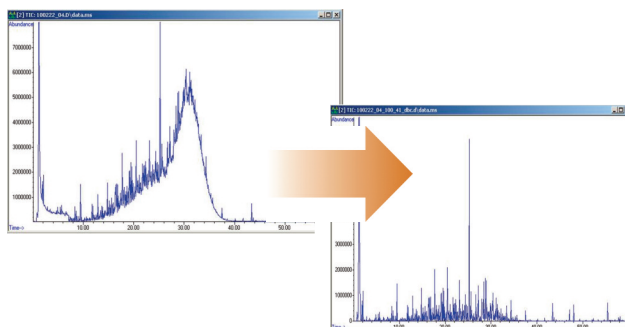


The file preview function is a convenient way of viewing the contents of chromatograms, libraries and reports.

## How TargetView works

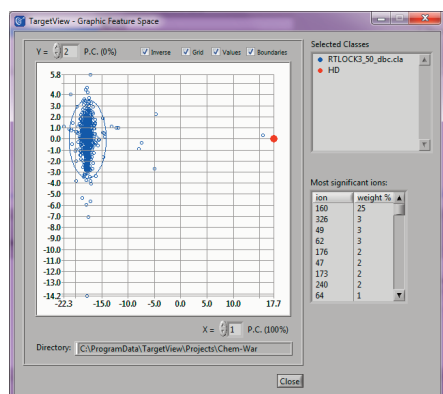
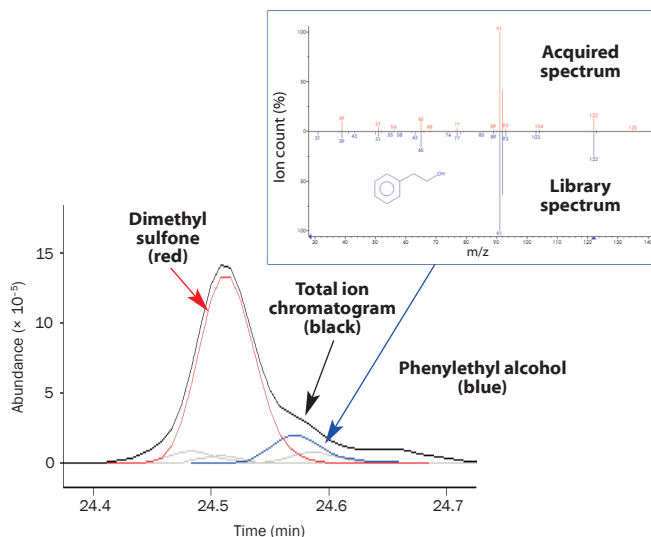
### 1 Elimination of background noise

TargetView uses **dynamic background compensation (DBC)** to selectively eliminate ions that contribute to chromatographic background noise (e.g. column bleed). This minimises interference in the chromatogram, improving the reliability of the subsequent component identification and target matching processes.



### 2 Deconvolution of component spectra

A **deconvolution algorithm** is applied to locate components that have a distinct mass spectrum, and distinguish between those components that co-elute.



### 3 Identification of targets by spectral matching

TargetView then applies **principal components analysis** to compare the spectra of individual components with those in the target library, and find the best match. An option is available that allows the outcome of this matching process to be visualised graphically.

Easy to learn and simple to operate,  
but harnessing powerful algorithms

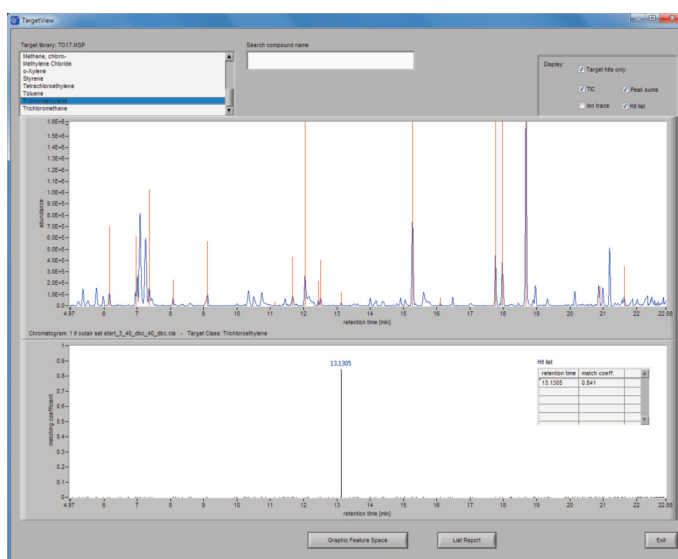
## Application examples

TargetView's capability to identify both targets and unknowns makes it valuable to GC/MS analysts in nearly every field. Below are a few examples that demonstrate TargetView's capabilities – for more information, download our Application Notes from the ALMSCO website.

### 'Air toxics' in semi-rural air

TargetView was used to identify which of a list of 62 'air toxics' (hazardous air pollutants) was present in a sample of semi-rural air.

Improvement of the signal-to-noise ratio by TargetView's background compensation process greatly improved the prospects for successful analysis. Nineteen compounds of wide-ranging abundance were detected in this particular air sample, as indicated in the interactive chromatogram.

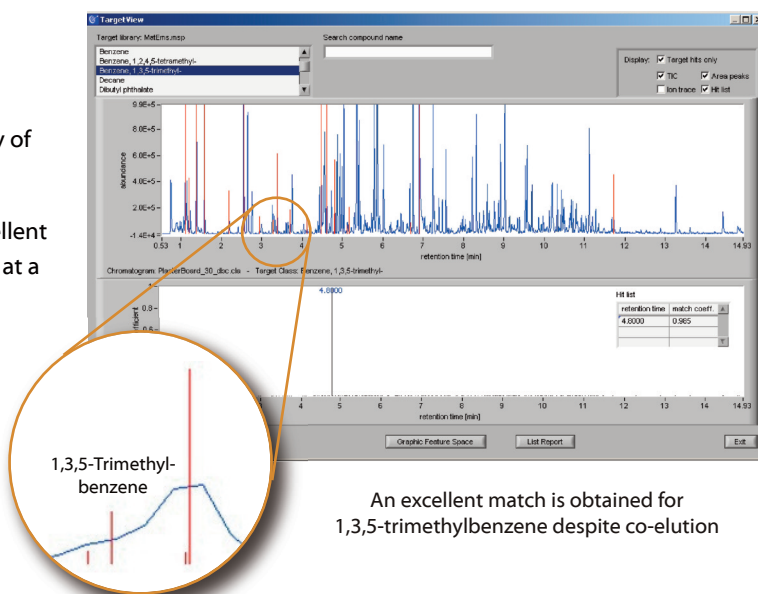


The red lines in the interactive chromatogram allow the user to rapidly visualise the 19 compounds detected

### Hazardous compounds in plasterboard

TargetView was used to match a chromatogram of emissions from plasterboard (drywall) against a library of over 600 regulated compounds.

Over 60 compounds were detected, including an excellent match for 1,3,5-trimethylbenzene, even though it was at a low concentration and was eluting with several other compounds.



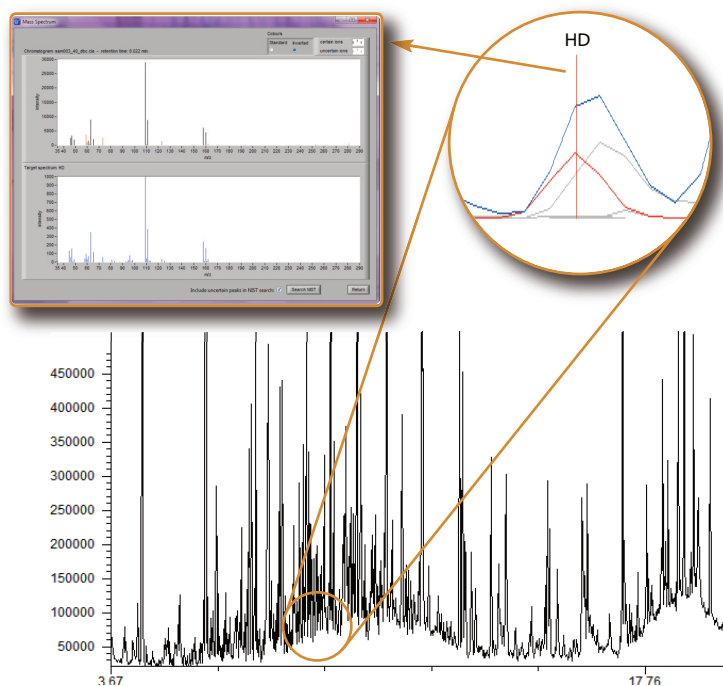
An excellent match is obtained for 1,3,5-trimethylbenzene despite co-elution

Confident identification of HD is possible despite co-elution and the complexity of the original chromatogram (bottom)

## Chemical warfare agents in diesel

Identification of trace-level chemical warfare agents is highly challenging, and in this case we set up a worst-case scenario by mixing a selection of them with diesel oil.

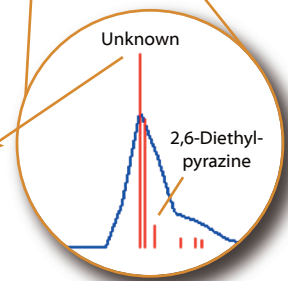
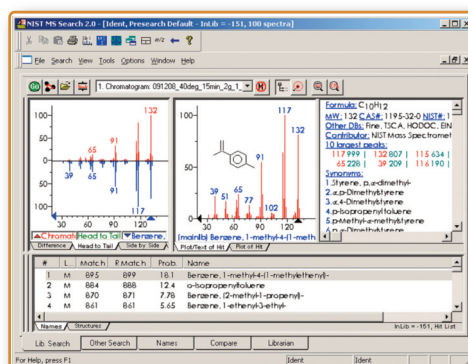
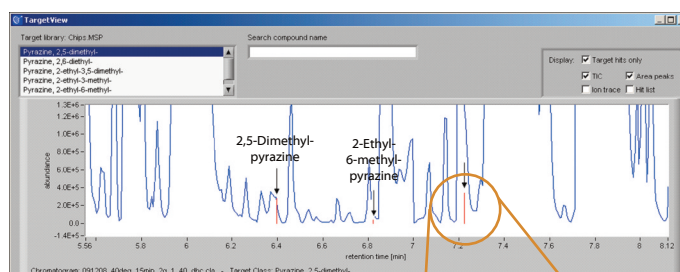
However, even in this challenging case, TargetView is able to identify mustard ('HD') with a high degree of confidence, despite the presence of co-eluting compounds (whose profiles are shown in grey in the inset).



## Pyrazines in crisps

TargetView was used to analyse a sample of crisp headspace for pyrazines – compounds that are responsible for flavour in a variety of foods.

Three pyrazines were found using a target library. A compound that nearly overwhelmed one of these pyrazines in the original chromatogram was searched against the NIST database, leading to its confident identification as *p*-isopropenyltoluene.



Changing the display to show all components indicates that five compounds co-elute with the target compound 2,6-diethylpyrazine

A NIST search on one of the 'unknown' co-eluting compounds identifies it as *p*-isopropenyltoluene

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