PRODUCT NOTE

GAS CHROMATOGRAPHY / MASS SPECTROMETRY

TurboMass GC/MS Software

Today's demanding laboratory requires software that is easy to learn yet offers sophisticated instrument control, robust data handling and streamlined reporting options. TurboMass™ GC/MS software is powerful enough to meet the most demanding lab requirements and is designed for a wide variety of application needs. In addition, it is extremely easy to use and has the flexibility and power of sophisticated data-evaluation tools.

PerkinElmer has been in the GC business for more than 50 years and understands the increasing requirements facing many laboratories. Many of these challenges are fully addressed by TurboMass software. So, whether your laboratory is a QA/QC or research laboratory, consider the easy-to-use and flexible capabilities available in TurboMass software.

Key Features

- Software-upgrade paths now available for all TurboMass Gold and Clarus® GC/MS users
- Automated tuning for optimum performance
- Selected Ion and Full Ion (SIFI™) scanning technology
- Fast and powerful data review environment for evaluation of results
- Flexible standard and customized report formats
- GC detector support adds flexibility

Intuitive and comprehensive navigation

The TurboMass desktop provides an intuitive environment to manage all necessary tools for GC/MS samples. The desktop (Figure 1) is composed of a spreadsheet layout for fast sample-list generation, enabling users to utilize tools such as automated sample fills and sequencing with only a few mouse clicks. This flexible spreadsheet environment provides simple and fast building of a multitude of sample methods into one sequence. For example, you can use different GC control methods, MS acquisition methods and data processing methods on each line of a sample list for maximum flexibility.

The TurboMass desktop also provides information on the current status of the instrument, as well as a clear view of all acquisition, processing and reporting that is occurring. Lastly, the TurboMass desktop will bring you to all other essential environments through a single click. These may include the tune page, chromatogram viewer, or the reporting environment.

Automated tuning for optimum performance

Tuning the mass spectrometer is critical to providing good library-searchable spectra with superior performance. TurboMass software can automatically tune the mass spectrometer using a new-generation proprietary tune with an electron ionization (EI) source, providing enhanced stability and reproducibility. UltraTune™ calculates settings for the tuning parameters until they are optimized for intensity, resolution and peak shape.

Mass calibration can also be included to complete the setup. For special situations, the starting conditions can be varied to provide a customized tune, not only for general use, but for your specific samples.

Improve detection limits with SIFI scanning

With a powerful process called Selected Ion and Full Ion (SIFI) scanning, a Selected Ion Monitoring (SIM) scan is obtained while simultaneously acquiring data in the full-scan mode (Figures 2 and 3). First implemented by PerkinElmer in 1998, SIFI enhances your analytical productivity by allowing you to:

- Acquire SIM detection limits and full-scan library searching in a single run.
- Receive more information in less time: provides information from both full scan and SIM in one chromatographic run. Up to 32 full scan and/or SIM acquisition functions can be acquired in parallel, in series, or in combination.
- Detect and quantify compounds difficult to determine at low levels with greater accuracy and sensitivity.
- Save time and money on costly solvents: labor-intensive pre-concentration and sample cleanup steps may be reduced or eliminated.
- Increase the throughput of your lab: reduces the number of analyses by combining a wider range of analyte responses in a single chromatographic run.

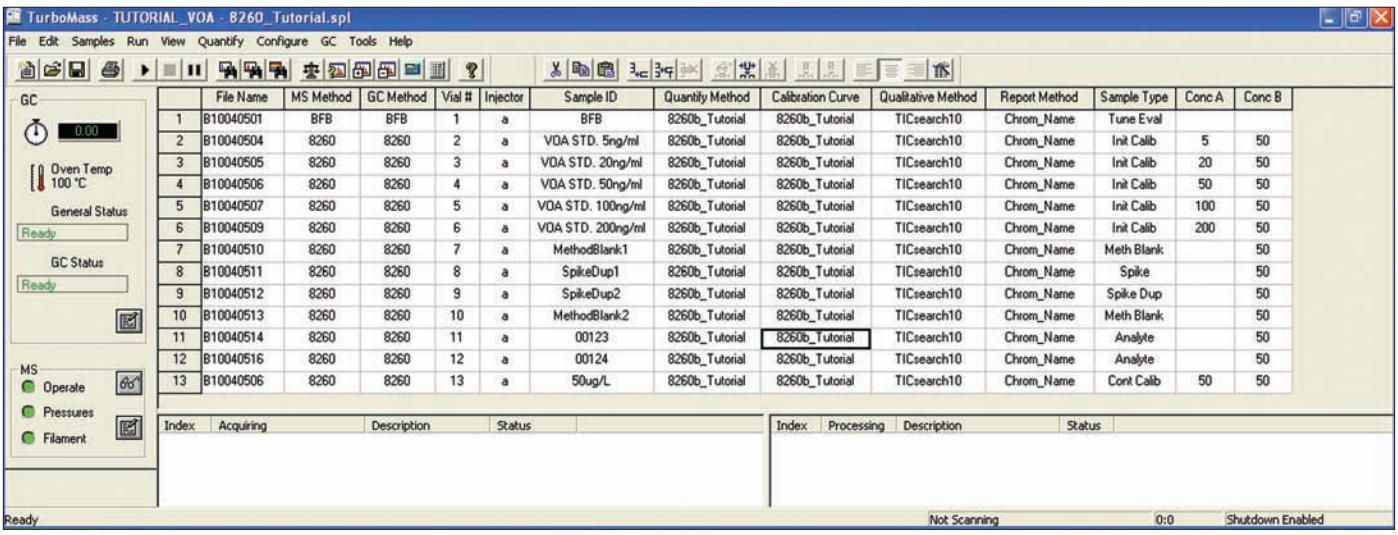

Figure 1. Top-level TurboMass software desktop provides easy navigation.

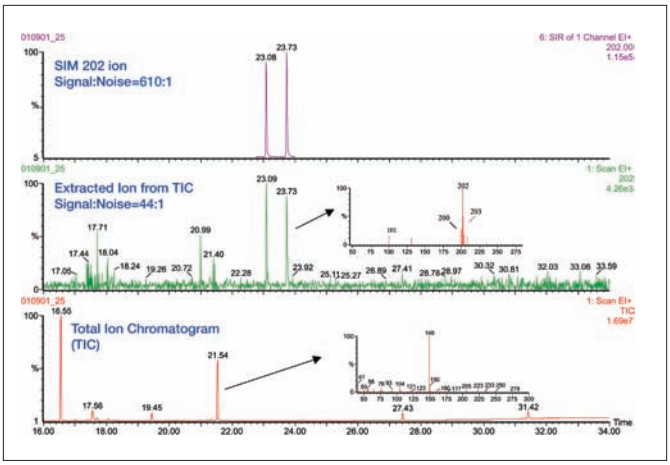

Figure 2. SIFI scanning ensures accurate identification, while simultaneously providing enhanced quantifiable sensitivity from the selected ion signal.

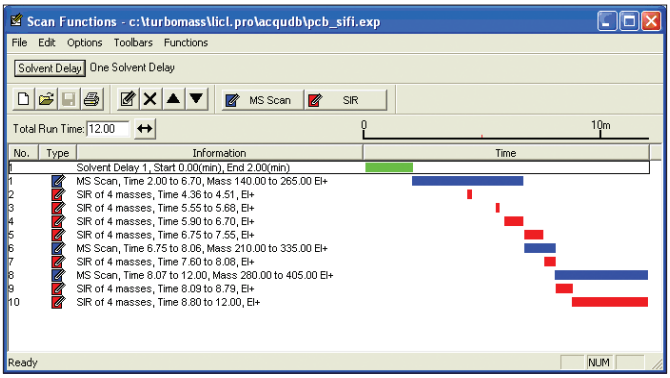

Figure 3. TurboMass software's SIFI collection method offers quick and easy setup.

AutoBuild delivers quick and easy method development

AutoBuild is a tool designed to speed the development of quantitative methods. It is accessible directly from the chromatogram-review environment with just a few clicks and the necessary information is transferred to the quantitative method. This intelligent feature automatically searches spectral libraries and imports information into the quantification method. Names, retention times, spectra and quantification ions of the respective peaks are automatically imported. This automated tool saves you time in building complex, multi-component methods from scratch.

Powerful interactive data review and evaluation

Data evaluation is an important preliminary step to ensure that only correctly integrated and identified peaks are used in quantitation and for further evaluation. The data review page (Figure 4) can speed this step of the process with windows organized to show the most important information for each compound of interest in an easy-to-use format. Peaks can be evaluated in the most efficient way and effective decisions rapidly implemented, if adjustments are required.

Figure 4. Data review environment, showing enhanced rapid viewing features.

Integrated environmental sample processing and reporting package

Typical environmental methods have strict quality-control requirements to demonstrate that a method is in compliance throughout the entire analytical run. A key purpose of these requirements is to demonstrate the instrument is operating properly and in calibration prior to the analytical run. Further data-quality checks are made within the chromatographic run and at the end. These checks require accurate and rapid evaluation after the run is completed to ensure the method criteria are met before the data are delivered to a Laboratory Information Management System (LIMS) or a report is printed locally. TurboMass software offers the tools to execute these performance checks quickly and with ease.

Intelligence tools deliver easy sample setup and processing

The software offers unprecedented ease-of-use in entering data required for an environmental evaluation. A sample "wizard" expedites entry of sample-specific information such as date received, date extracted and information based on analysis, matrix and level. Figure 5 shows an example of the wizard during data entry for a group of water samples.

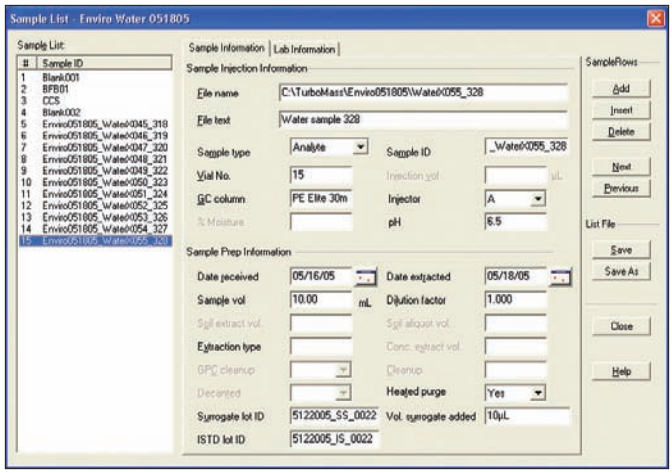

Figure 5. Sample wizard during data entry for a water sample group.

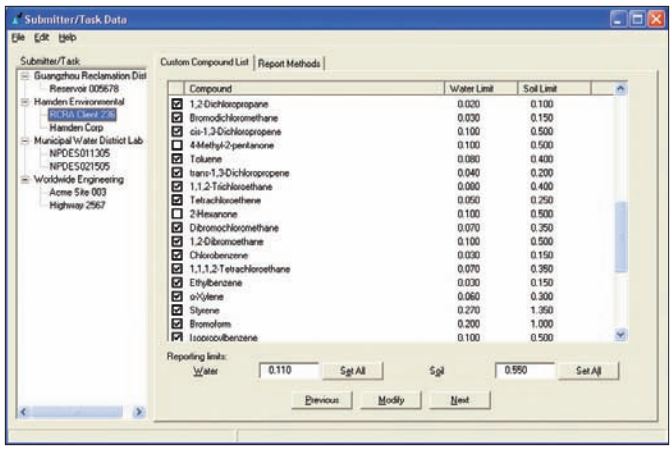

Figure 6. Easy-to-create custom compound lists for client reports.

Laboratories require high productivity and one way to ensure this is to run full sample groups to use the instrument most efficiently. Several clients' samples may have similar requirements and be run in the same batch. The custom compound list allows the user to rapidly choose which analytes should be reported for each client. Multiple lists of compounds are possible for each client and reporting thresholds can be created for each compound using the same quantification method and calibration curve. Figure 6 shows the easy-to-use interface for this important task.

When all of the information is entered and the data collected, the operator can choose which runs of the sample list to include in the evaluation. For example, Figure 7 shows a selection of sample candidates chosen for reporting. Included in the evaluation may be sample blanks, tune samples, calibration samples, spiked samples, QC checks and customer samples. The software will intelligently pick which samples are associated with each environmental form and fill in the information. The data is presented in a logical manner in a series of tabbed data sheets, based on the U.S. Environmental Protection Agency (EPA) Contract Laboratory Program (CLP) forms. Reports may include items such as initial calibration response factors, concentrations of the target compounds and tentatively identified compounds (TIC).

The pane at the bottom of the screen lists intelligently-detected inconsistencies in the choice of samples for the requested reports. The errors are cleared when the inconsistencies are resolved.

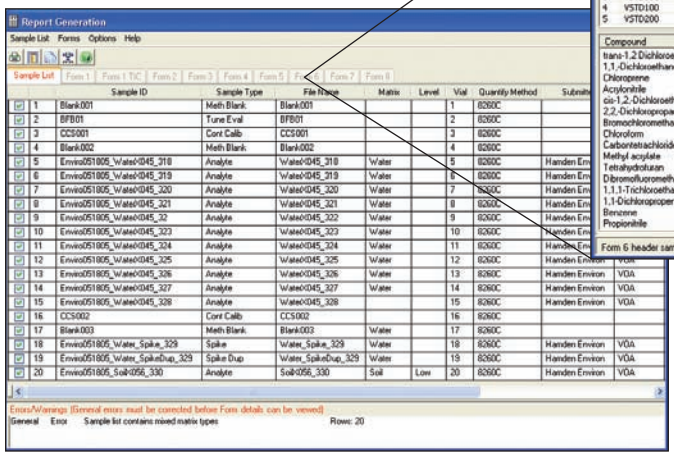

Figure 7a. Intelligent error detection in choosing samples for evaluation.

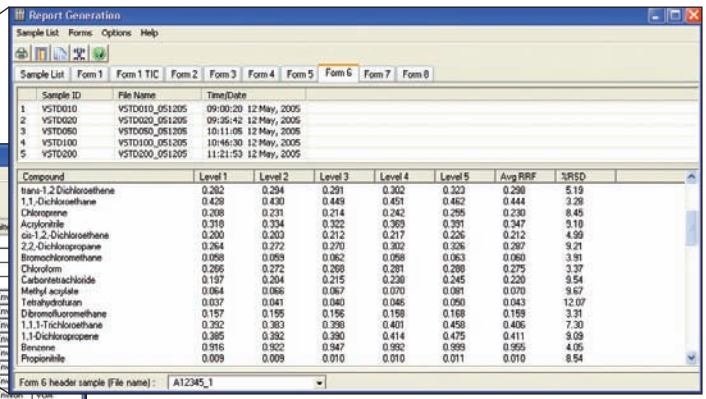

Figure 7b. Form 6 (initial calibration curve), shown by clicking a tab once errors are resolved.

The sample-centric software is intuitive to learn and provides easy setup of stored methods for the routine user. The software is organized around projects, collecting all the necessary method information and data in one place, facilitating archiving. Data can be collected using a simple checklist – just check off the desired steps and press the "OK" button to initiate data collection. Coupled with rapid scanning and the widest mass range for a quadrupole GC/MS, data collection for a range of applications is easily achieved.

Multiple-ion-ratio review

Also available in TurboMass software is multiple-ion-ratio capability. Multiple-ion ratio (often called "3-ion ratio" for historical reasons) is a mass spectrometry technique where specific selected ions of a mass spectrum are ratioed to determine if they match a reference spectrum within certain pre-defined tolerances. Only if the calculated ion ratios are within user-defined limits is the peak "identified" as the presumptive target compound. A match adds additional certainty to a compound confirmation, beyond that available through only a GC retention time and the presence of a peak at a single mass. TurboMass software will allow the user to:

- Define up to four qualifier ions (per compound)
- Specify relative intensities of qualifier ions (to target ion or base peak)
- Specify tolerances of qualifier ions
- Define ratio calculation method (absolute, relative, ISO)
- Update method ratios and retention times from standard chromatogram
- Integrate qualifier ions
- Use qualifier ion ratios in peak identification
- Use full spectrum match value as a figure-of-merit for the match

Fast and simple reporting completes the process

Many laboratories need to put their data into an attractive, standardized format for reporting to internal or external clients. Routine reports can be easily printed from more than 70 standard templates supplied with TurboMass software. Standard templates for specific applications are included. Examples are forensic and environmental CLP-like reports, which make reporting easy. Customized with your logo, they provide an instant report for many clients. Very little training is required and these reports can be generated by analysts of many skill levels. For many laboratories, this is sufficient for their needs and relieves the burden of using an additional software package for report generation.

Laboratories with clients requiring customized reports can also be accommodated by the reporting functionality in TurboMass software. The software offers a wide variety of design elements that can be used to create exactly the report the client desires (Figure 8).

The user can customize the report to include the laboratory or organization logo, chromatograms, spectra, calibration plots, a quantification report, library-search reports, page header and footer. The ultimate benefits for the user include the ability to plot the total ion chromatogram and/or selected ions and to overlay target and qualifier multiple-ion traces. Additionally, the user can plot multiple full scan and SIM acquisition functions and plot target compounds with associated internal standards showing integration baselines.

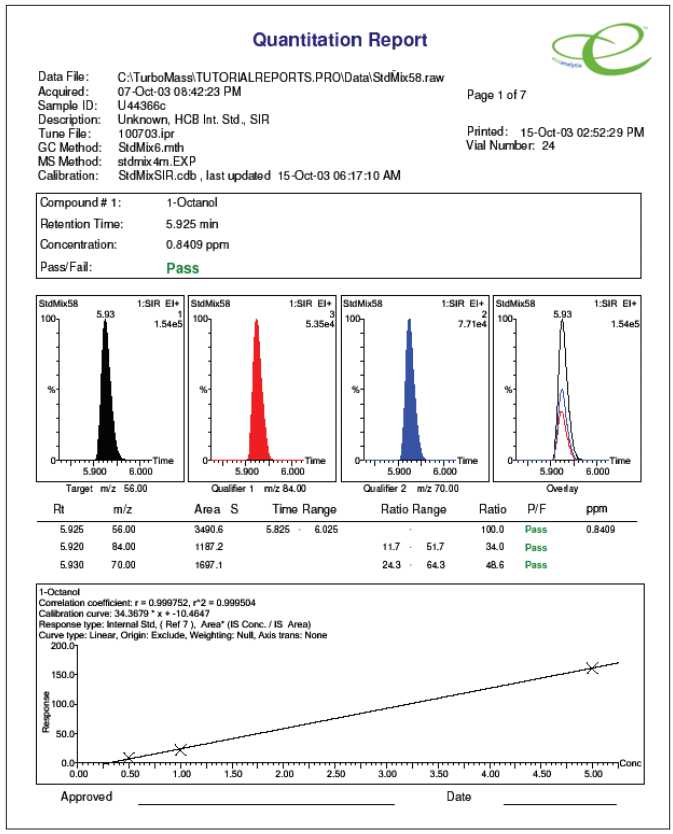

Figure 8. Example of an included report showing multiple-ion-ratio validation.

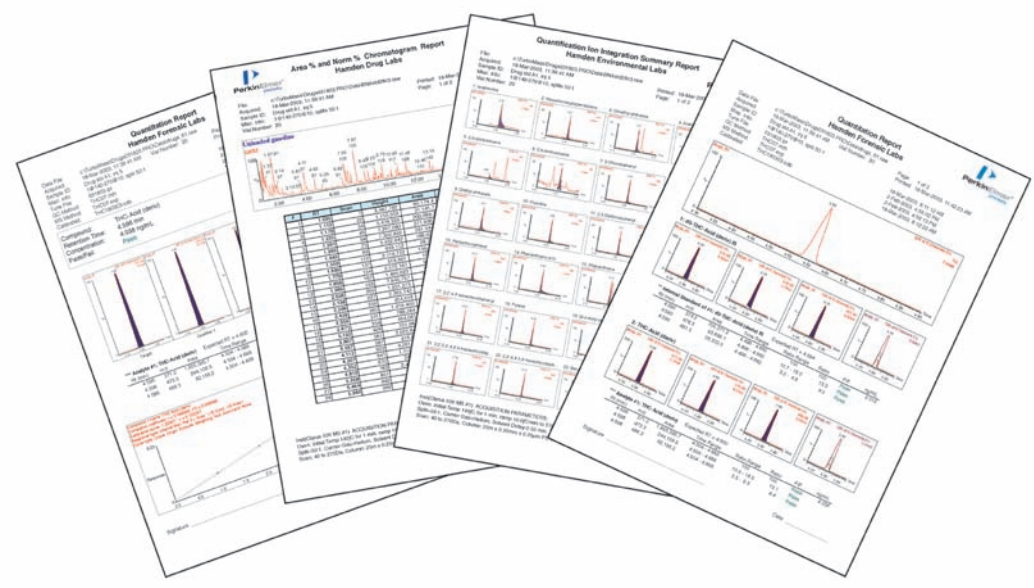

Figure 9. TurboMass GC/MS software provides standard and customized report templates.

TurboMass software also allows spectra to be printed, including spectra from multiple acquisition functions with optional automatic background subtraction or "AutoRefine", a type of spectral deconvolution. Especially useful for multiple-ion-ratio reporting, TurboMass software provides the ability to print out quantitative calibration plots with the data. Quality-control reports can also be generated to check the validity of compound calibrations.

GC detector support adds flexibility

Two additional detectors can be used simultaneously with your Clarus GC/MS system. All acquisition, display and quantitation for the detectors can be performed by TurboMass software – or you have the option of using TotalChrom® Workstation software for these processes.

Optional tools

There are many optional tools that are available to add to your TurboMass package. For example, sample lists can be downloaded from the Laboratory Information Management Systems (LIMS) and data uploaded back to the LIMS. Mass spectral data can be imported from or exported to industry-standard AIA format. In addition, a variety of mass spectral libraries for compound identification are available, including NIST, Wiley, and Maurer/Pfleger/Weber. Translation software is also available to convert data from other MS systems or libraries, and optional deconvolution GC/MS software for target compounds in complex matrices is also available. Contact your local PerkinElmer sales representative for more information.

Software-upgrade paths

Software-upgrade paths are available for most existing users of TurboMass GC/MS software. Please contact your local PerkinElmer sales or service representative for more information or a quotation.

Continuing a 50-year tradition of GC innovation, PerkinElmer is the only GC supplier that manufactures and sells a complete single-vendor solution – from sample handling to data handling.

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006811C_01 KG040803 Printed in USA