Multiplelabs
Turnkey Laboratories Solutions

Analytical®
Technologies Limited

GCMS 3068i

EPCC / PRODUCTS / APPLICATION / SOFTWARE / ACCESSORIES / CONSUMABLES / SERVICES

Analytical Technologies Limited

An ISO 9001 Certified Company

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Product Introduction

GC has been designed for use with single quadrupole mass-spectrometric detector. The GC has a small footprint to save on laboratory bench space. It features proprietary design Electronic Pneumatic Control to maintain very stable flow to the MS detector during temperature programmed GC separation cycles offering excellent Retention Time stability. Column backflash feature is available, supported by built-in backflash calculator.

System Overview

The new improved single channel version of GC has split/splitless inlet that offers low reactivity to labile samples. The inlet is made compatible with range of automated liquid and headspace samplers. The inlet features consumable items that are common to other GC models from market leaders, eliminating the need to maintain consumable items of different sizes and types.

A standard 78.5 mm glass liner of various diameters and internal configurations is used in the inlet. The septum and liner O-ring are also standard sizes and these consumable items may be used interchangeably with other compatible GCs.

The inlet heater provides uniform heating across the liner, to avoid cold spots and condensation of the sample vapor once heated, and a cooler septum cap to reduce bleed and prolong septum life.

Proprietary design EPC supports a wide variety of method conditions and sample applications, which may require either a split or splitless mode of operation. The EPC with capillary columns provides 4 column flow control modes: constant pressure, ramped pressure, constant flow, ramped flow. Column average linear velocity is calculated. Atmospheric pressure and temperature compensation is provided.

Sensitive LCD touch screen on GC front panel has user selectable menu options to display required information instantly by a «finger click». Easy access to maintenance and service modes directly from the touch screen display keeps GC manual away from workplace. GC system control can be done from touch screen display or via a networked data system. Display of GC and ALS user set points is effected on GC touch screen or through the Data system.

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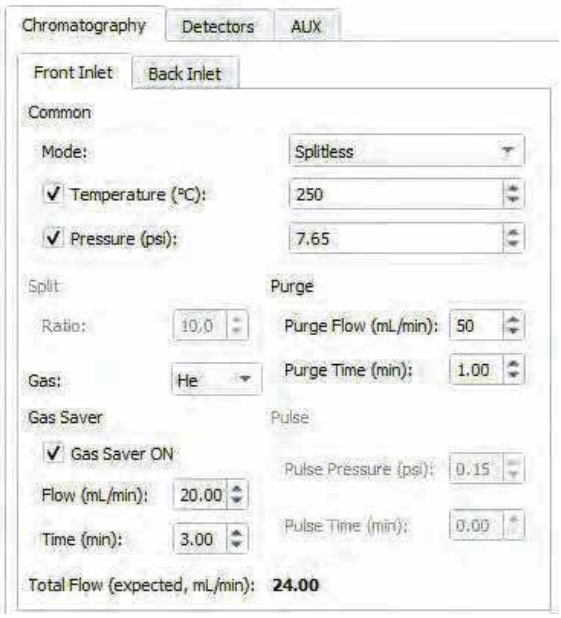
Split/splitless (S/SL) inlet module

The inlet operates in Split, Splitless, Pulsed Split, Pulsed Splitless injection modes as per the user settings in GC method.



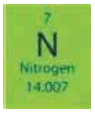
All flows and gas types are set by the user in the GC control method, allowing for reproducible and resettable pneumatic conditions from run-to-run.

Broad pressure control range upto 150 psig permits use of all available GCMS column sizes.

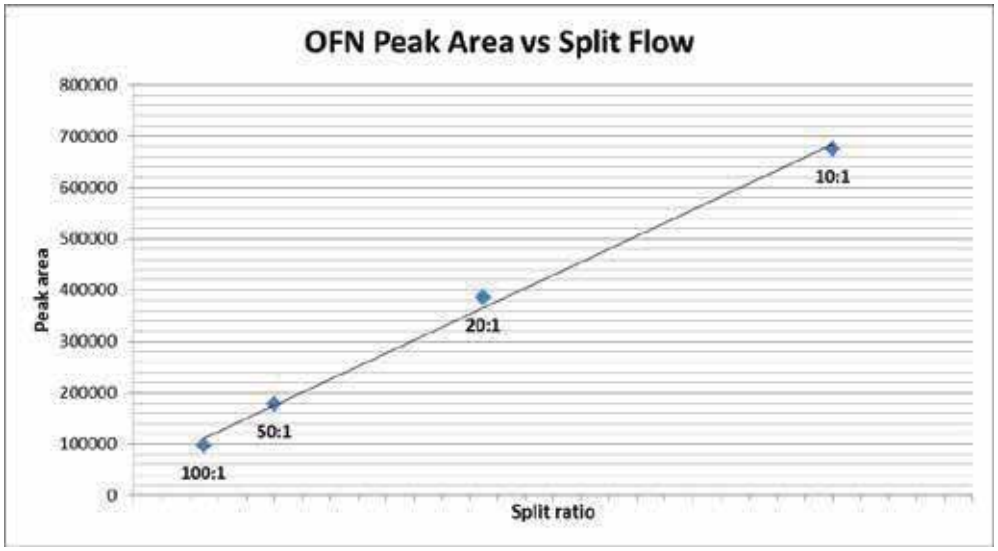
The Maximum inlet operating temperature can be set upto 400°C.

Total flow setting range depends on carrier gas and is settable in ranges:

- 0 to 550 ml/min for He or H_2
- 0 to 225 ml/min for N_2

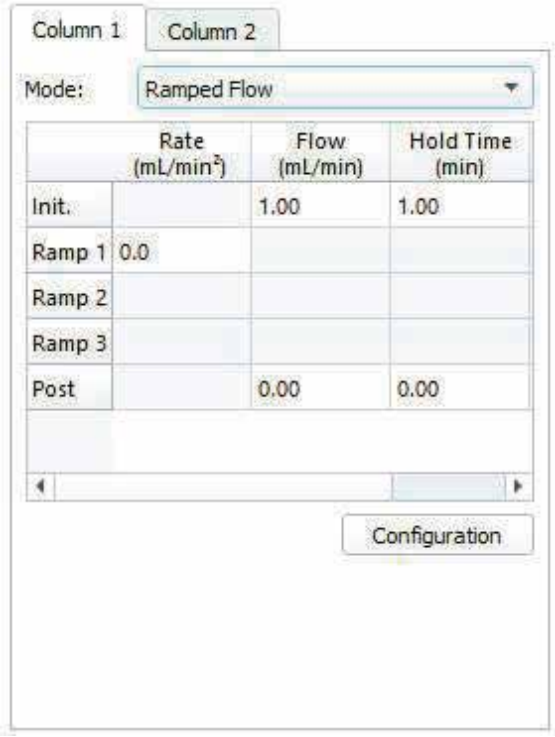
or


Operating in Split mode the maximum ratio can be set as high as 800:1 while split linearity is excellent over the entire range of split flow.



Electronic Pneumatic Control (EPC)

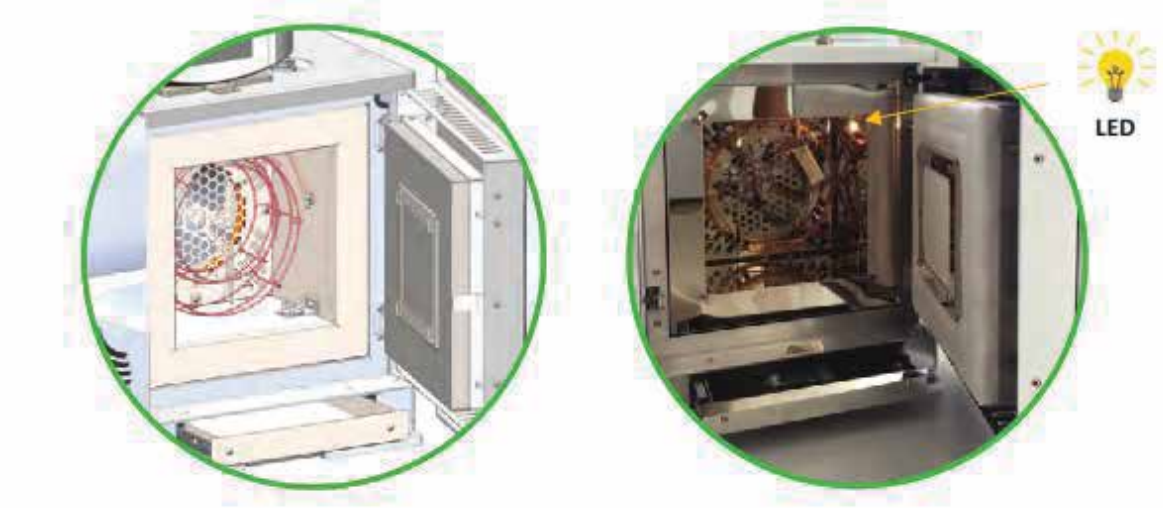
Carrier gas can be controlled over range of flows and/or pressures, used in mass-spectrometric methods and depending on column size. The EPC technology allows for control of 3 types of carrier gas He, H_2 and N_2 by pressure, flow or linear velocity. Whichever parameter is selected as the control, it is maintained at that set point and the other two parameters are recalculated accordingly by the system. Compensation for barometric pressure and ambient temperature changes is automatically provided.



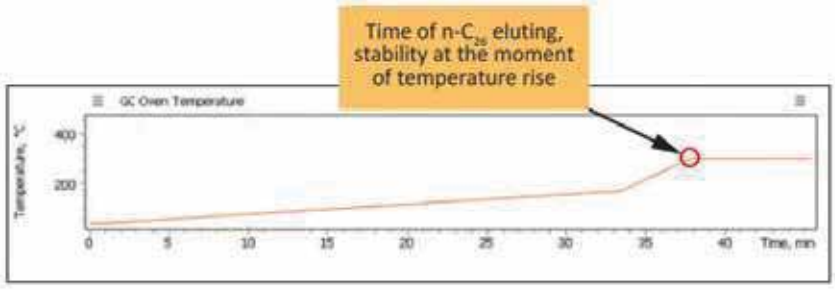
- Pressure/flow ramps are available.
- In the Split mode of operation, the split vent flow is regulated by an EPC module to maintain a constant Split ratio throughout the run automatically. The septum purge gas is also EPC controlled at user specified flow regardless of the pressure in the inlet.
- Pressure units can be set in psi, kPa bar.

Column Oven

While compact in size with thin punched walls to reduce its thermal mass the oven has enough space to accommodate a capillary GC column of any length on 5” and 7” racks.



• The oven operating temperature range is suitable for all MS compatible columns and can be set as high as +400°C with temperature set point resolution of 0.1°C.
• The oven program supports 42 oven ramps, negative ramps are allowed. Thanks to its low thermal mass, the maximum temperature ramp rate is 300°C/min, while cool down time from 310°C to 50°C is less than 5 minutes at ambient 22°C in the lab.
• LED illumination inside the oven makes the column installation convenient.
Press-in drawer located underneath the oven has a space for maintenance tools and some consumables while its front surface is never too hot to touch.

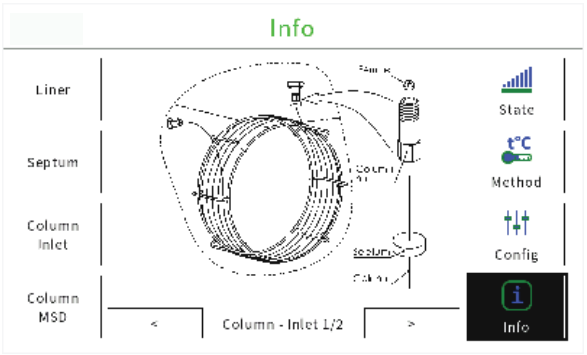


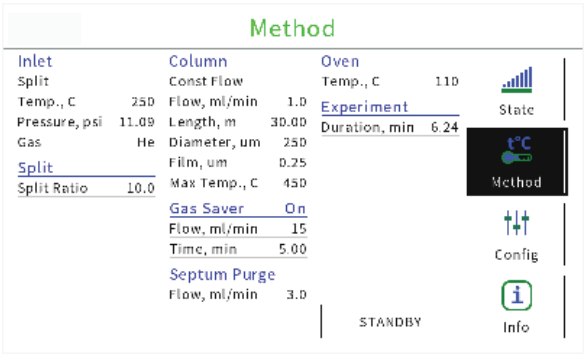
To demonstrate the GC performance a series of injections of ann-hydrocarbon mix from n-C_{23} to n-C_{30} was made to establish Retention Time repeatability in the split mode of operation.Relative standard deviation (%RSD) was calculated for Retention Time of n-C_{26} eluting during oven temperature ramp, to be as low as 0.015% as shown in the table.

Repeat C_{26}	RT, min
1	39.7475
2	39.7457
3	39.7394
4	39.7318
5	39.7348
6	39.7353
7	39.7346
RSD, %	0.015

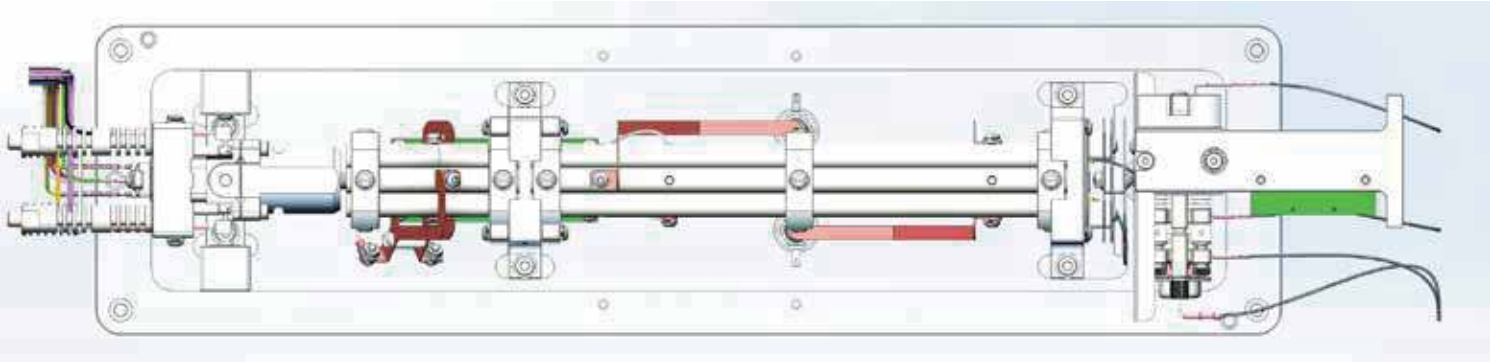
Touchscreen Graphical User Interface

- 7 inch TFT display; Resolution: 800 x 600;
- Multi-language support (English, Chinese);
- Real-time graphical display of temperature and pneumatic programs;
- Built-in Column pressure/flow/velocity calculator;
- Meaningful error/alarm messages;
- Log file;
- Status-summary screen.





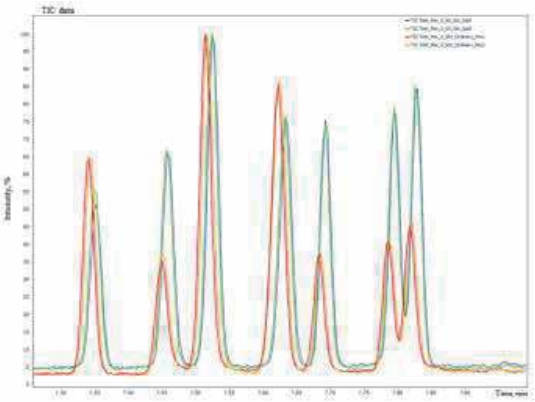
Remote system status monitoring via smartphone application operated under iOS or Android is an instant and secure loop-up access to instruments in your lab wherever you are at the moment.



Exceptionally robust inert ceramic ion source

Ion source operates at high emission current values resulting in high ion currents.

- Inert ceramic ion source designed to tolerate long series of high matrix samples and complex extracts of biological origin.
- Inert ceramic ion source designed to tolerate long series of high matrix samples and complex extracts of biological origin.
- A novel ceramic inner surface ensures high ionization efficiency of nitro compounds.



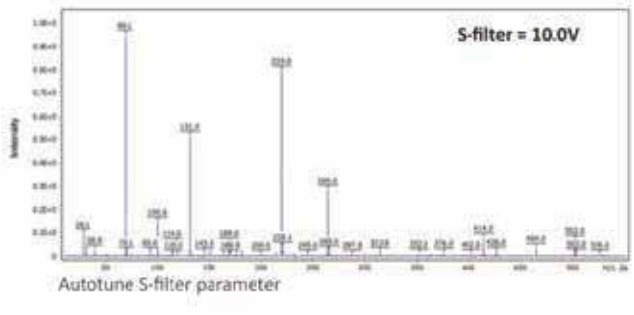
Trifluralin compound response for the inert source.

Trifluralin compound response for the conventional ion source.

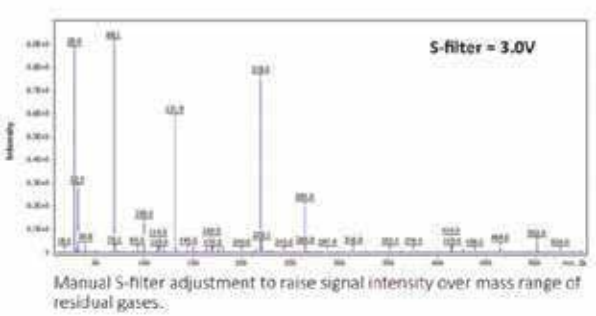
S-filter provides complete removal of photon noise from spectra

The S-filter forms a retaining electric field that guides ions into quadrupole and then onto the detector while filtering neutrals away.

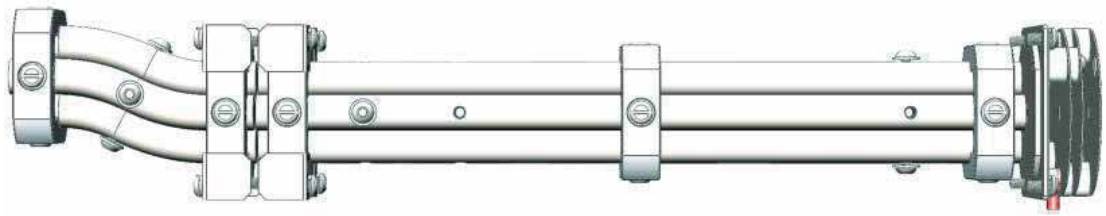
• Changing the voltage on the S-filter allows operator to further adjust signal intensity over different ranges of analyzed masses.



Autotune S-filter parameter

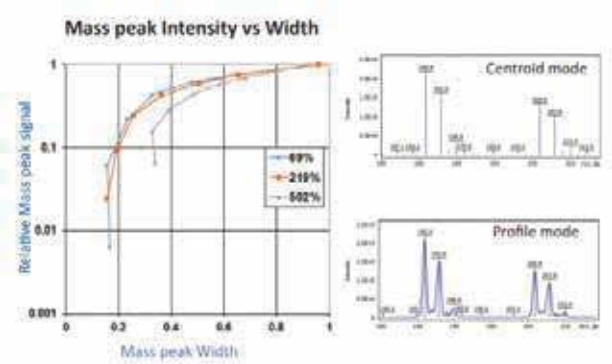


Manual S-filter adjustment to raise signal intensity over mass range of residual gases.



- High-precision quadrupole filter for separating ions by their mass-to-charge ratio

The utmost fabrication precision of the quadrupole permits to hold a high-intensity ion beam even with a mass-peak width below 0.4 Da.



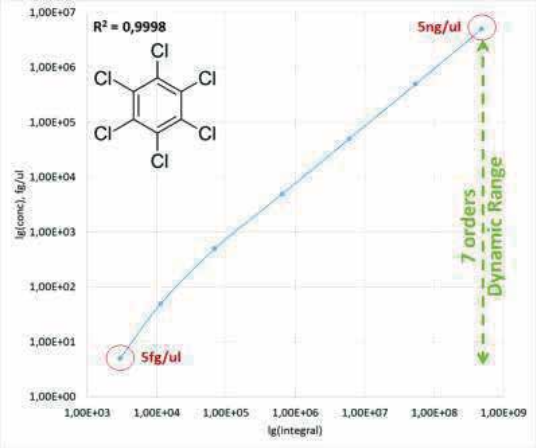
• Regardless of the data collection mode, the data for each experiment can be provided in both Centroid (one peak per integer mass), and Profile (raw signal) modes.

The newest ion detection options

PMT – photo electron multiplier (PMT) with extended dynamic range.

• PMT operates in dual mode automatically switching between photon counting and analog signal to extend the dynamic range of the detector signal (up to 10^8 orders).

Linearity of the HCB signal (PMT's)

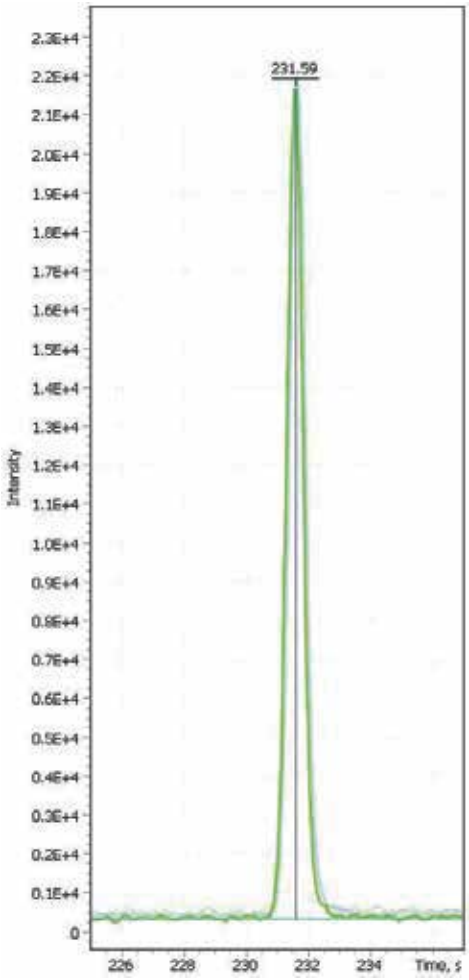


• PMT lifetime is known to reach beyond lifetime of the instrument itself.

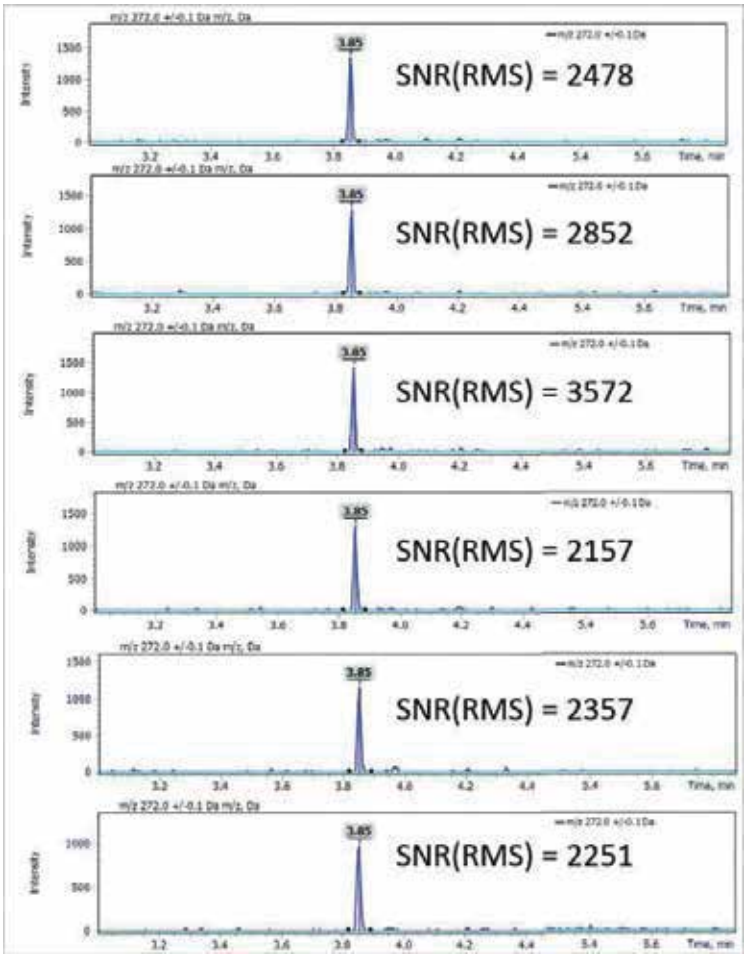
• EM – electron multiplier remains a default detector option.

System Specifica ons

100 ppt, octafluoronaphthalene
EIC@272 Da (+/- 0.1 Da), SIM



1 ppb, octafluoronaphthalene
EIC@272 Da (+/- 0.1 Da), SCAN

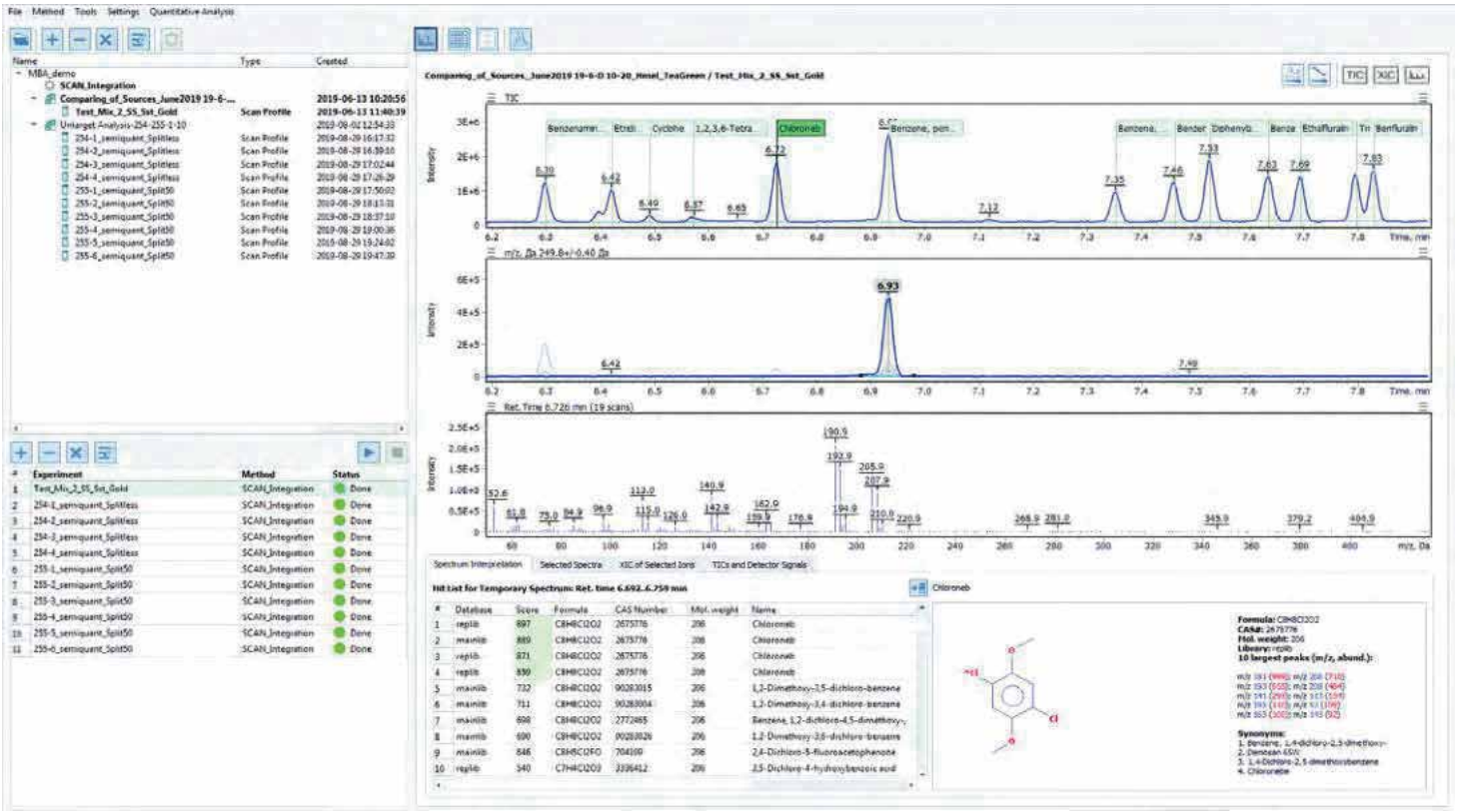


System Technical Specifications

Mass range: 15 – 1200 amu.
Scan rate: upto 20000 amu/sec
SCAN sensitivity: SNR > 1800:1 (OFN@272)
SIM sensitivity: IDL < 10 fg (OFN@272)
Linear dynamic range: $5^{\wedge}10^{6}$
Mass axis stability: < 0,1 amu/48 hrs
Turbomolecular pumps: 85 L/sec or 300 L/sec
GLP features: OQ/IQ/PV protocols available
FID Detection Limit: $2x10^{-12}$ qC/sec for n-hydrocarbons or propane $1,1\times10^{-12}$ qC/sec(optional)

Easy to use, state-of-the-art-software with highly automated auxiliary algorithm architecture

- "Easy to use" - is a fundamental principle that has been used in development of software.
- The software combines many automatic algorithms for configuring ion scanning methods to achieve maximum sensiticvity and quality of data, as well as many auto-maticc algorithms for processing the acquired data.
- The software works under Windows, Linux, operaticng systems.
- The software is designed to be translated into different languages.

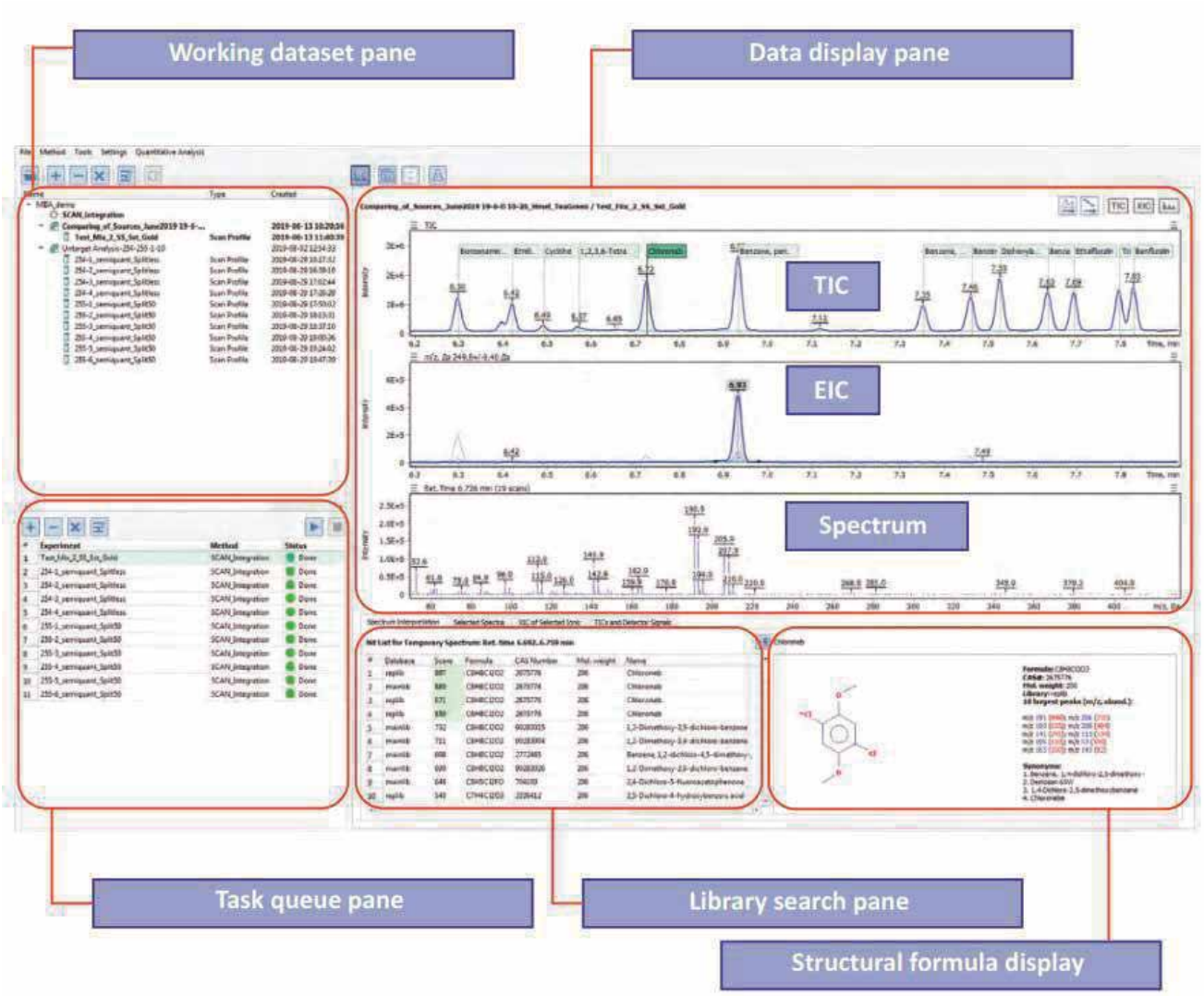


Windows

Linux

The software

«Easy to use» - is a fundamental principle that is used in the development of software. It has become a modern software product much appreciated for convenience and ease of operation, having all the necessary tools at hand on a single screen.

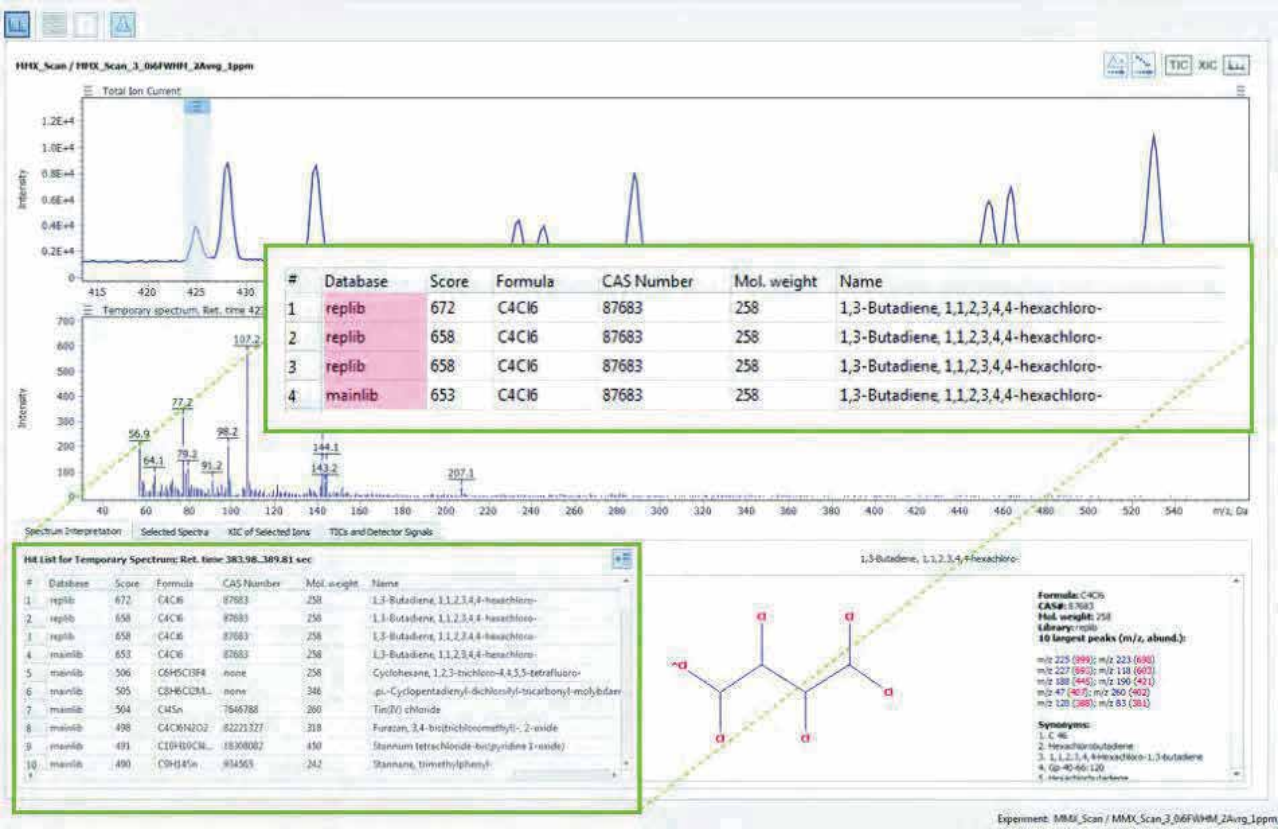


- Instant result of spectral library search*;
- Simultaneous use of multiple libraries.

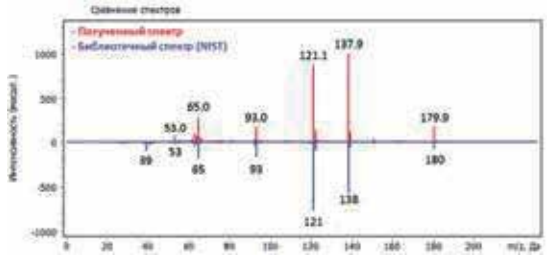
Software tools, for processing data acquired in full scan mode (Scan)

The software package uses a variety of algorithms that enable an operator to quickly and easily review chromatograms obtained in full scan mode (Scan). The software supports all known commercial libraries: NIST, Wiley, Pfleger-Maurer-Weber etc.

«On-line» scanning the chromatogram profile with simultaneous data matching in multiple libraries.



#	Database	Score	Formula	CAS Number	Mol. weight	Name
1	replib	672	C4Cl6	87683	258	1,3-Butadiene, 1,1,2,3,4,4-hexachloro-
2	replib	658	C4Cl6	87683	258	1,3-Butadiene, 1,1,2,3,4,4-hexachloro-
3	replib	658	C4Cl6	87683	258	1,3-Butadiene, 1,1,2,3,4,4-hexachloro-
4	mainlib	653	C4Cl6	87683	258	1,3-Butadiene, 1,1,2,3,4,4-hexachloro-

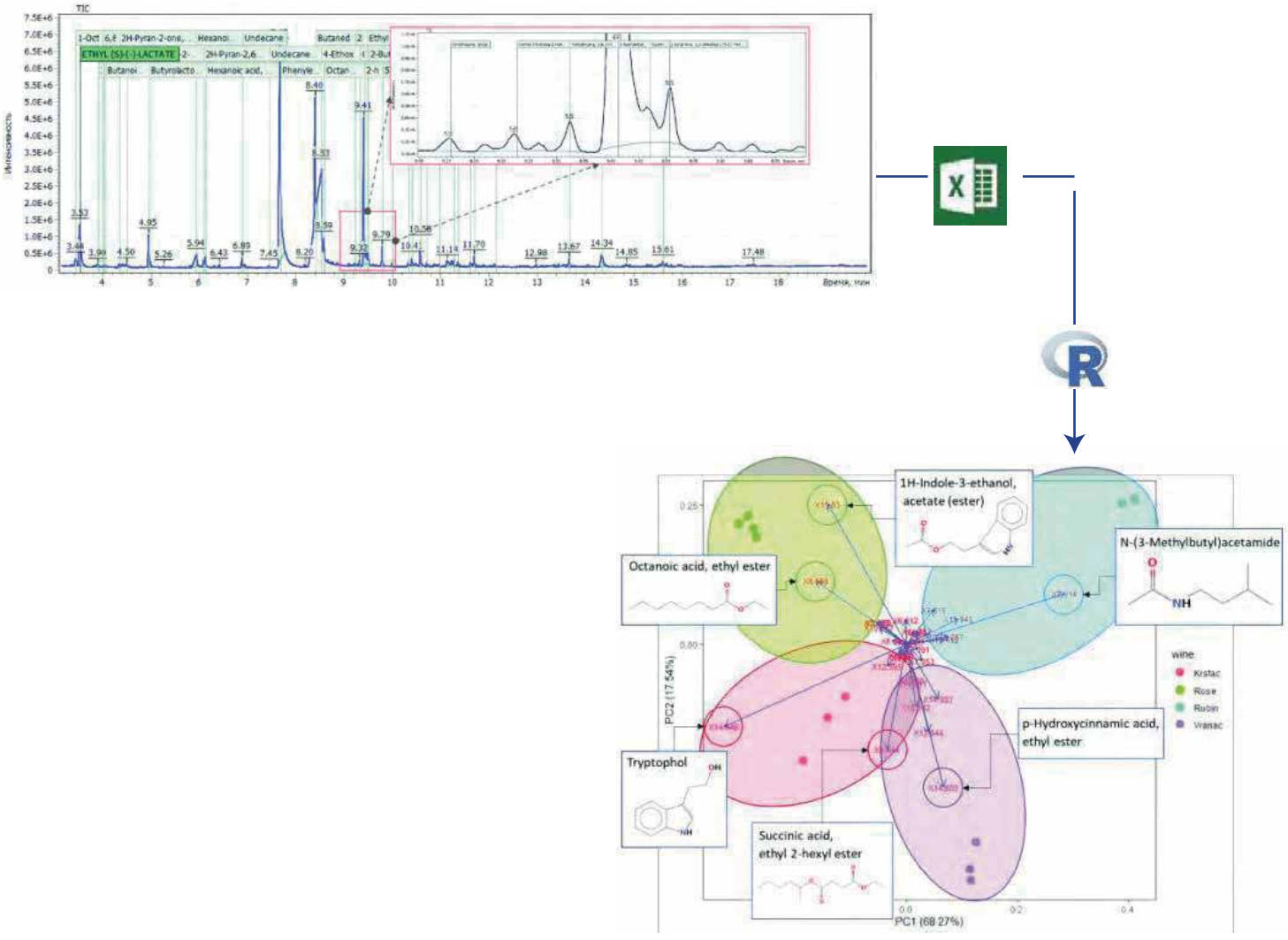


- The software supports all known commercial libraries: NIST, Wiley, Pfleger-Maurer-Weber etc.

- The feature to compare spectra "Head-to-Tail" is implemented directly in the program.

Transfer data to any external software for further processing

The integration results in the software can be easily exported to any external software for further processing while charts and plots are as easily exported to text editors. This feature is particularly very useful for writing scientific articles, publications, as well as calculating the "raw" data in any other external specialty software.

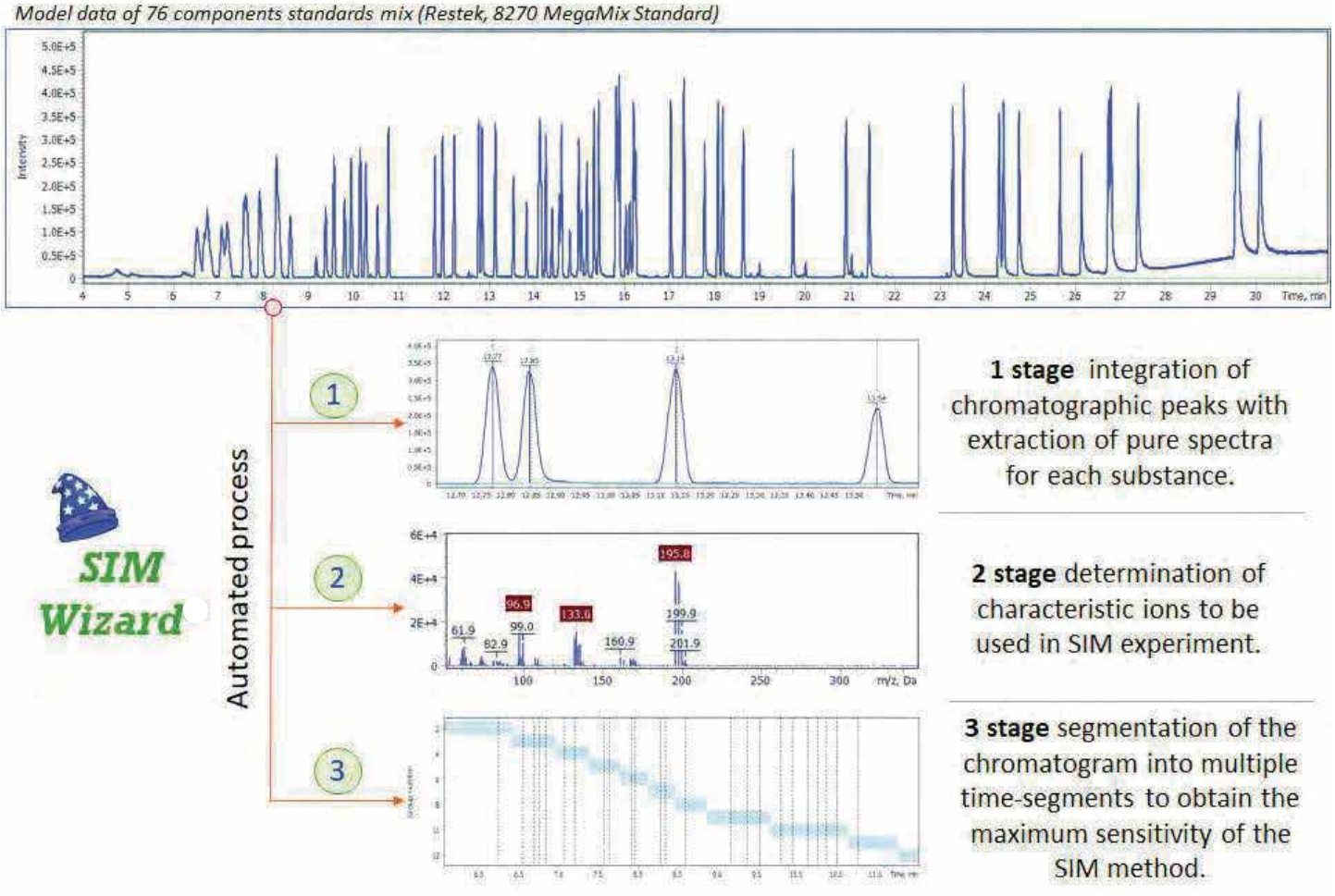


Automatic integration of chromatographic peaks with subsequent transfer of the data array to an external data processing environment allowed the use of the principal component method (PCA) in the computing environment R. As a result of data analysis, it is possible to identify unique components for different types of wines and clearly describe the chemical difference between those sorts of wine.

Automatic SIM method development algorithm “SIM Wizard”

The innovative software tool "SIM Wizard" is an algorithm for automated construction of the SIM-experiment program, based on the SCAN data from the experiment run on analyte standards.

Model data of 76 components standards mix (Restek, 8270 MegaMix Standard)



1 stage integration of chromatographic peaks with extraction of pure spectra for each substance.

2 stage determination of characteristic ions to be used in SIM experiment.

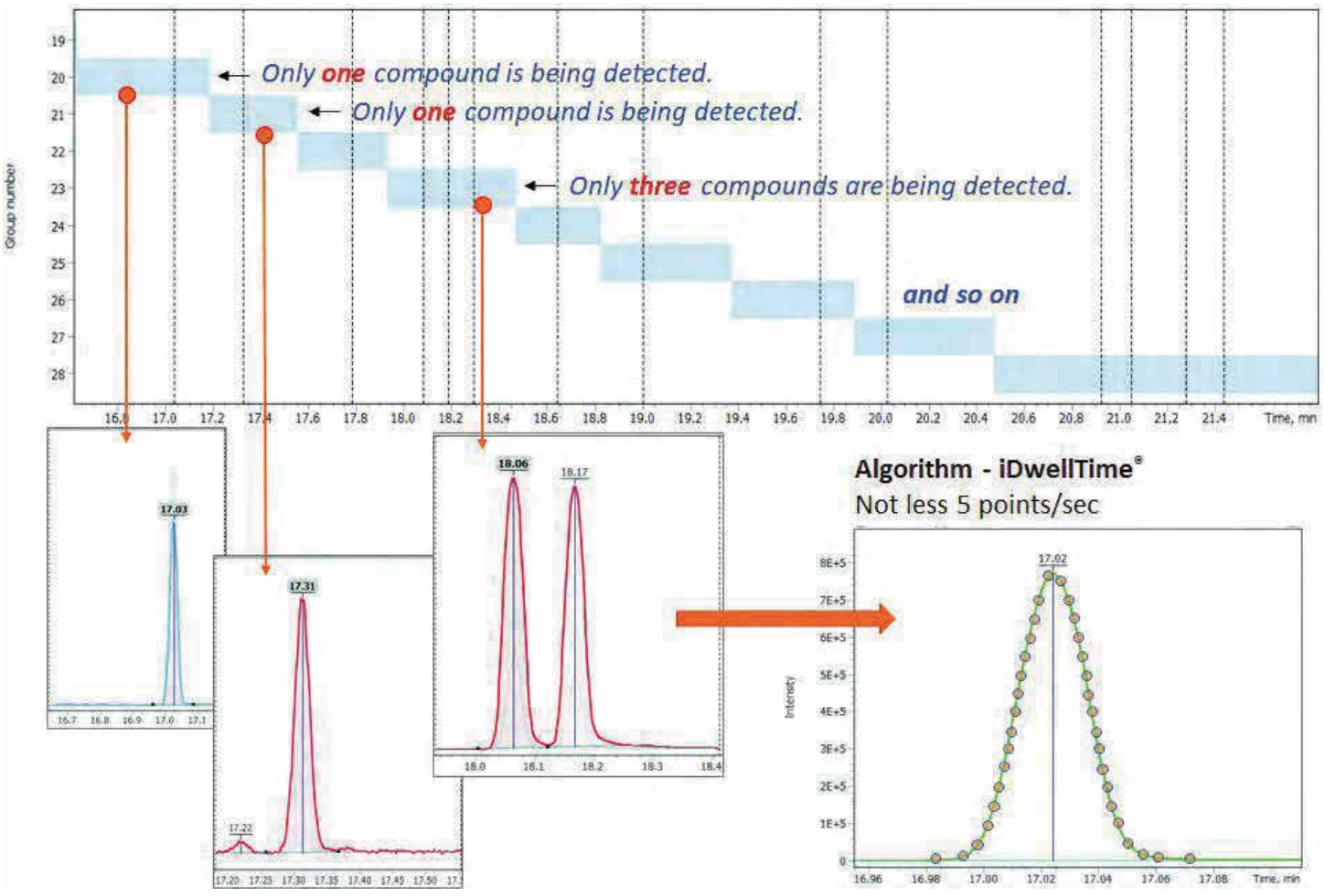
3 stage segmentation of the chromatogram into multiple time-segments to obtain the maximum sensitivity of the SIM method.

Algorithm for automatic calculation of analyze time for each ion in SIM mode - “iDewll Time”

The process of developing the SIM method involves not only making a list of individual and characteristic ions for monitoring, but also seting up a strategy for scanning them.

Quality recording of a complete chromatographic peak requires at least 10 data points to be stored over the entire width of the detected peak. However, the frequency of data point collection must meet this requirement for both narrow and wide chromatographic peaks.

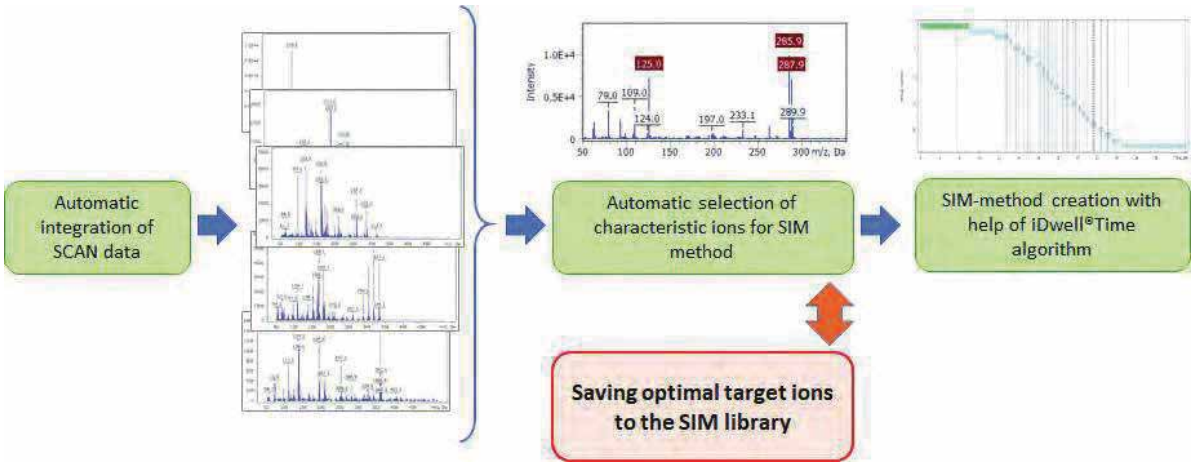
The software has a built-in innovative iDwell Time algorithm, which automatically divides the chromatogram into optimal time segments of scanning, calculates the optimal dwell time for each ion to provide data collection frequency of at least 5 points/sec, thereby achieving maximum sensitivity of the method, its stability, as well as the correct algorithm for data integration



SIM-Library

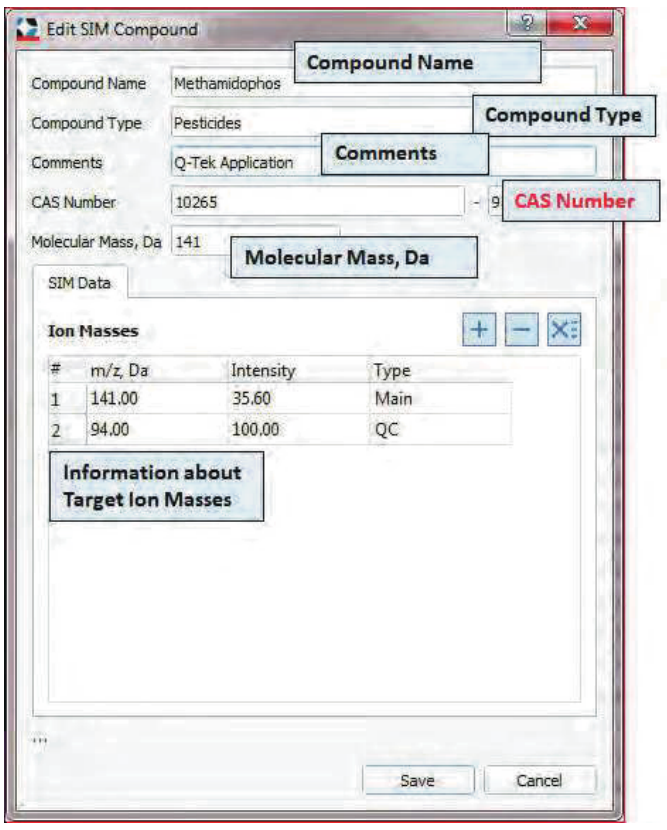
The software contains an integrated library of characteristic SIM ions for several hundred different organic compounds.

The data source for this library was both experimental data obtained from a variety of literary sources, and our own experiments. SIM-library is a great help for an operator in development of a new SIM method at maximum sensitivity and lowest detection limits. An expert level operator can edit this library to add or delete certain compounds or their relevant ions.



Each compound added to the SIM ion library is described in an "individual information card". The card displays the main relevant information of the compound:

- molecular weight of the compound,
- compound name,
- compounds type,
- the unique numerical identifier of the substance-CAS.

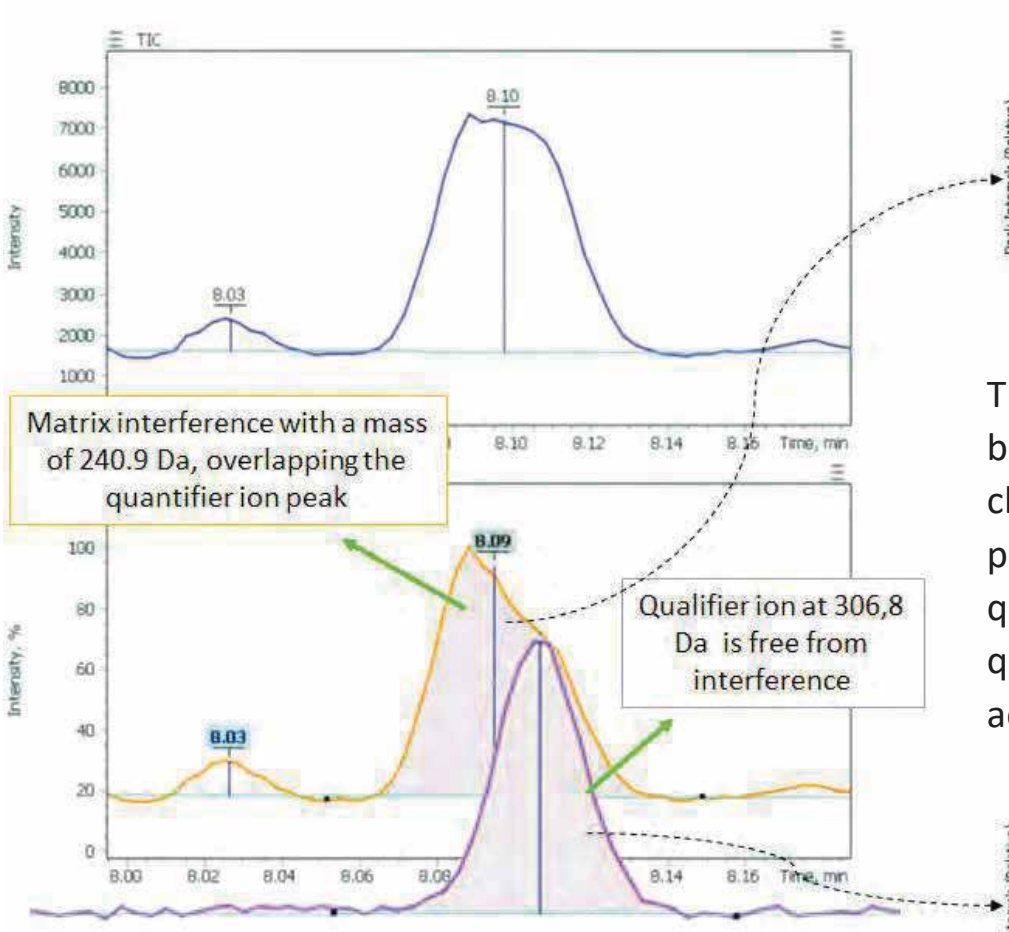


CAS-number is used as a main reference. If the CAS number of the detected compound matches compound CAS number from the SIM library, the "SIM-Wizard" algorithm will suggest using the library data set by default. Otherwise, the selection of target ions will be facilitated by the "SIM Wizard" algorithm.

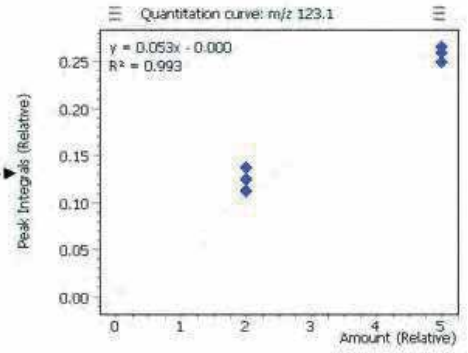
Innovative post-run data proccesing algorithm «Flexible SIM» for reliable quantification

The so-called "matrix effects" are interfering sample matrix components that impede correct detection of the target compounds in the sample. Those matrix components are detected at retention times same a those of the analytes imposing difficulties of analyte's correct identification and quantitation.

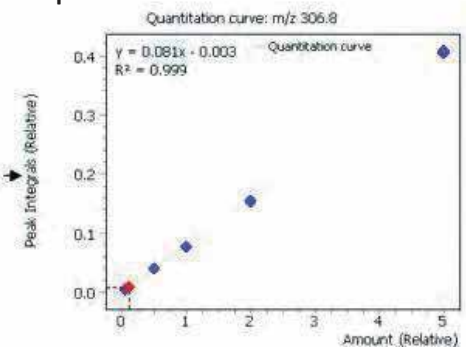
• Software contains a "Flexible-SIM" post-processing algorithm to minimize matrix effects in complex matrix extracts by changing quantitation ions. By a mouse-click an operator can swap quantifier and qualifier ions and build and new calibration curve with a free from interference qualifier without running additional experiments.



The problem of matrix influence in detecting the target ion of endosulfan ether.



The "Flexible SIM" algorithm built calibration levels for all characteristic ions and made it possible to quickly change the quantifier ion to perform quantitative analysis after data acquisition.

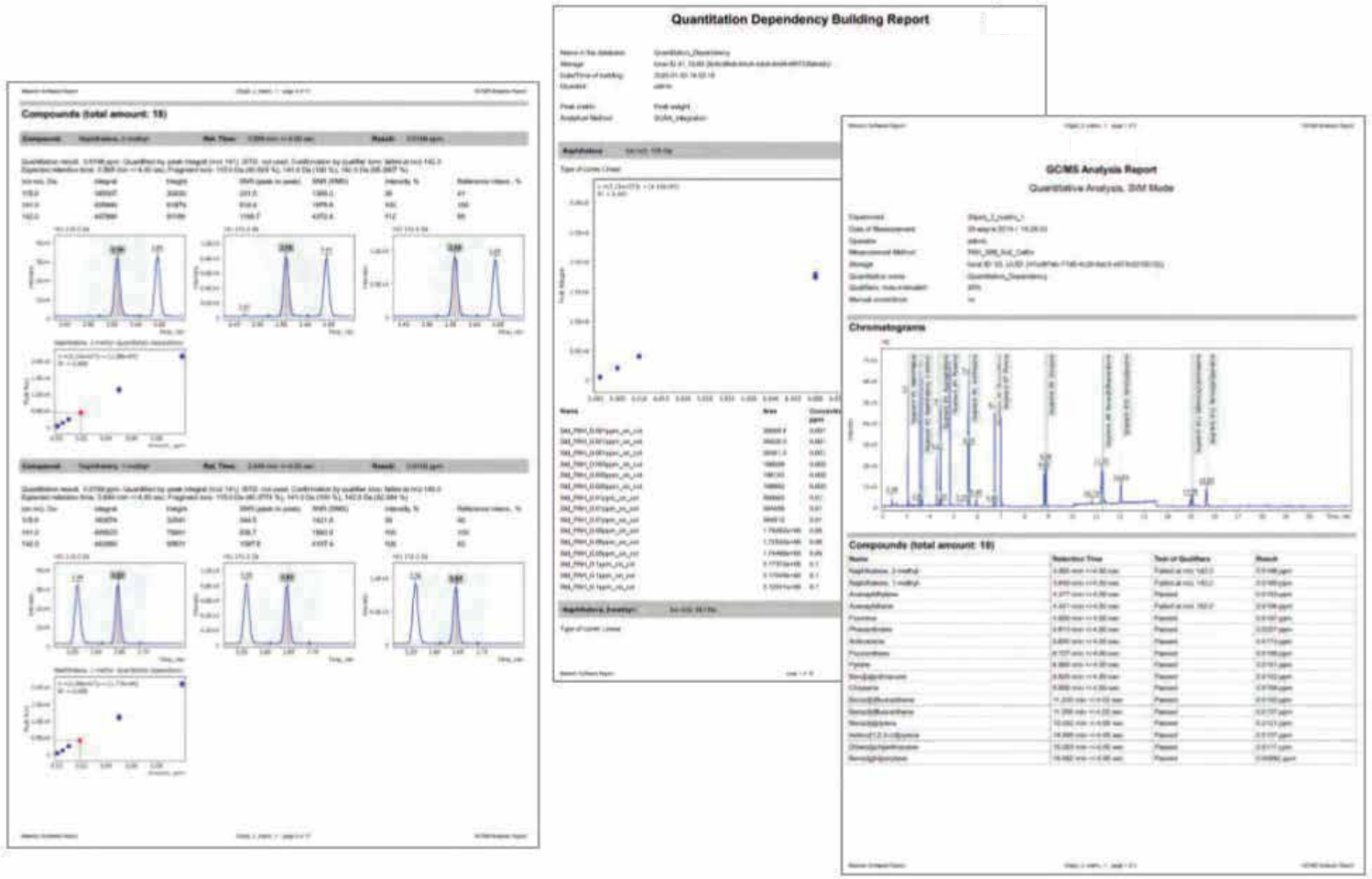


Ready-made report templates

• Software includes selection of standard report templates:

1. Report on library search on selected spectra.
2. Qualitative analysis report.
3. Quantitative analysis report.
4. Custom reports.

• There are also many templates offered to an operator for displaying chromatograms and calibration curves based on laboratory needs and current practices.



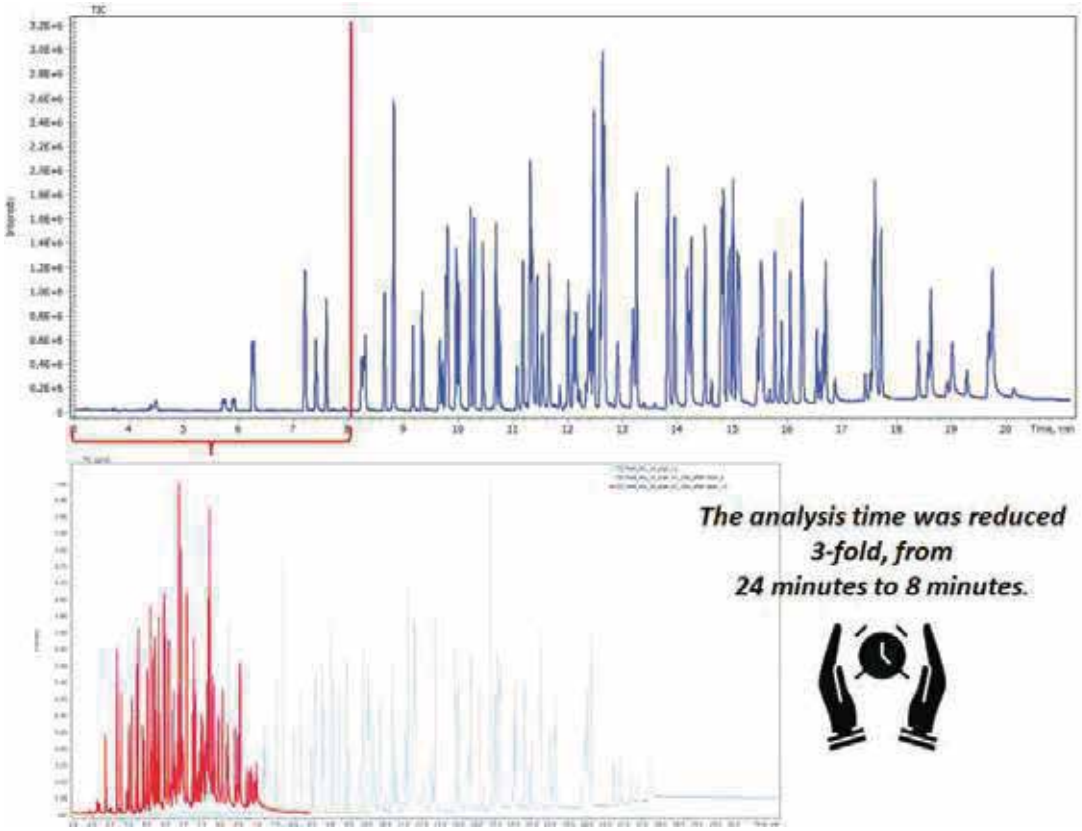
The results of quantitative and qualitative analysis can also be uploaded to *.xml format and used in any other external data processing module. In particular, an operator can export experimental GC-MS data to Excel and combine it with the data obtained with another technique for a personal report or comparison.

Using hydrogen as a carrier gas

The design of the ion source of the mass detector is optimized for both helium and hydrogen as a carrier gas and does not require modification or replacement of any ion source hardware components.

The advantages of using hydrogen are as follows:
- the speed of chromatography significantly increases (due to the higher linear velocity of the hydrogen carrier gas, compared with helium);
- therefore, the time for one analysis is reduced;
- hydrogen can be produced by a hydrogen generator;
- Besides, hydrogen is known to maintain emission properties of the electron multiplier, thus extending its lifetime.

Thorough testing have shown excellent reliability, safety and reproducibility of the MS-detector when using hydrogen as a carrier gas.



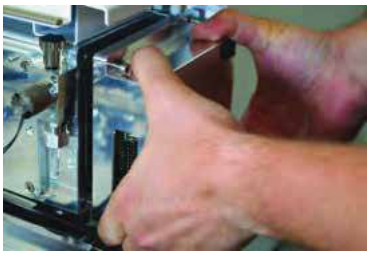
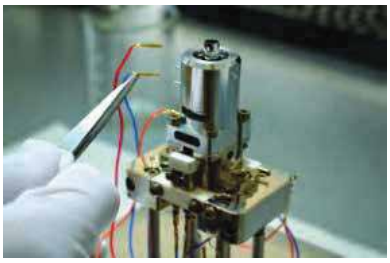
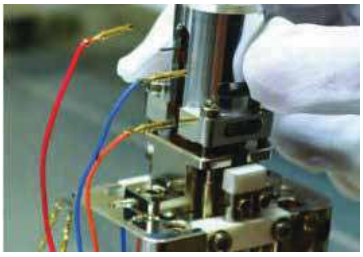
Using hydrogen as a carrier gas, made it possible to successfully separate more than 75 pesticide compounds in less than 8 minutes, with the sensitivity of the method at 5 ppb

Easy operationa and easy maintenance

The MS-detector user maintenance involves cleaning the ion source, replacing the filaments, and replacing the electron multiplier. All procedures are illustrated in detail in the "user Guide", as well as in video tutorials.

• The ion source is accessed from the front side of the system, no need to swing open the entire analytical flange for ion source maintenance.

Only 3 wires!

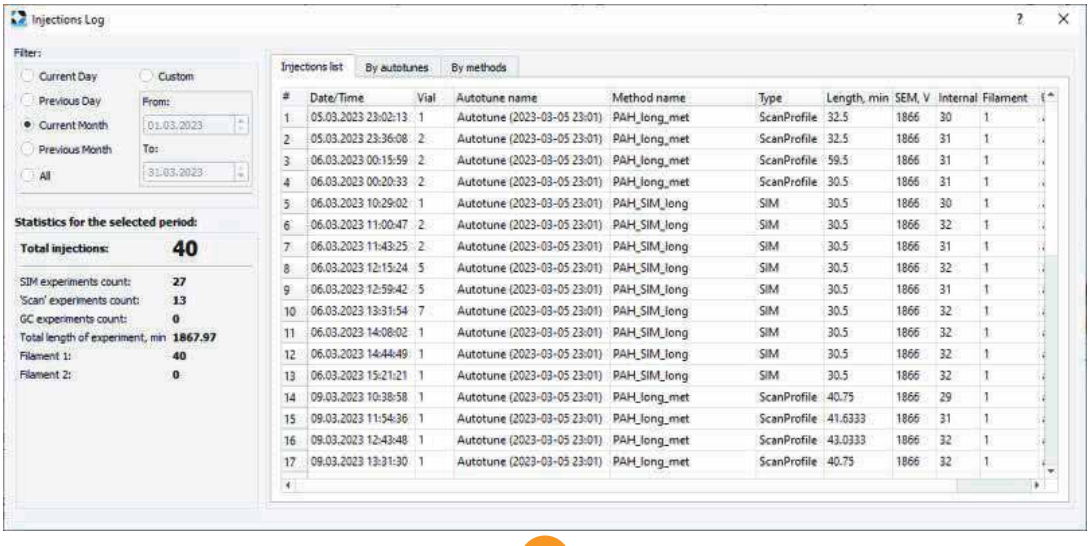
Software has a number of built-in remote and self diagnostics features, designed to autonomously maintain system operation at maximum performance level or to restore system performance at low cost. They make a requirement for extensive training of supporting personnel redundant.

Software keeps logging of operator actions and system parameters during each run.

Monitored parameters includes:

- Number of injections through septa;
- Number and total duration of runs;
- Working time of each filament;
- The value of the vacuum in the fore-vacuum line and others.

As soon as any threshold value of the monitored parameters is reached, the system displays a warning message.



#	Date/Time	Vial	Autotune name	Method name	Type	Length, min	SEM, V	Internal	Filament
1	05.03.2023 23:02:13	1	Autotune (2023-03-05 23:01)	PAH_long_met	ScanProfile	32.5	1866	30	1
2	05.03.2023 23:36:08	2	Autotune (2023-03-05 23:01)	PAH_long_met	ScanProfile	32.5	1866	31	1
3	06.03.2023 00:15:59	2	Autotune (2023-03-05 23:01)	PAH_long_met	ScanProfile	59.5	1866	31	1
4	06.03.2023 00:20:33	2	Autotune (2023-03-05 23:01)	PAH_long_met	ScanProfile	30.5	1866	31	1
5	06.03.2023 10:29:02	1	Autotune (2023-03-05 23:01)	PAH_SIM_long	SIM	30.5	1866	30	1
6	06.03.2023 11:00:47	2	Autotune (2023-03-05 23:01)	PAH_SIM_long	SIM	30.5	1866	32	1
7	06.03.2023 11:43:25	2	Autotune (2023-03-05 23:01)	PAH_SIM_long	SIM	30.5	1866	31	1
8	06.03.2023 12:15:24	5	Autotune (2023-03-05 23:01)	PAH_SIM_long	SIM	30.5	1866	32	1
9	06.03.2023 12:59:42	5	Autotune (2023-03-05 23:01)	PAH_SIM_long	SIM	30.5	1866	31	1
10	06.03.2023 13:31:54	7	Autotune (2023-03-05 23:01)	PAH_SIM_long	SIM	30.5	1866	32	1
11	06.03.2023 14:08:02	1	Autotune (2023-03-05 23:01)	PAH_SIM_long	SIM	30.5	1866	32	1
12	06.03.2023 14:44:49	1	Autotune (2023-03-05 23:01)	PAH_SIM_long	SIM	30.5	1866	32	1
13	06.03.2023 15:21:21	1	Autotune (2023-03-05 23:01)	PAH_SIM_long	SIM	30.5	1866	32	1
14	09.03.2023 10:38:58	1	Autotune (2023-03-05 23:01)	PAH_long_met	ScanProfile	40.75	1866	29	1
15	09.03.2023 11:54:36	1	Autotune (2023-03-05 23:01)	PAH_long_met	ScanProfile	41.6333	1866	31	1
16	09.03.2023 12:43:48	1	Autotune (2023-03-05 23:01)	PAH_long_met	ScanProfile	43.0333	1866	32	1
17	09.03.2023 13:31:30	1	Autotune (2023-03-05 23:01)	PAH_long_met	ScanProfile	40.75	1866	32	1

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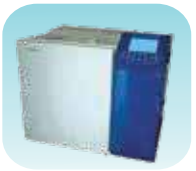

Optima Gas Chromatograph 2979 Plus

Flash Chromatograph

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Liquid Partical Counter

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DSC/TGA

Semi Auto Bio Chemistry Analyzer

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