Software Solution for Standard and Highly Sophisticated GPC Systems

Today's analytical laboratories require universal, flexible and open software solutions to cope with the ever changing needs. This report illustrates how these requirements for chromatographic data processing software can be met in different types of laboratories.

Acquisition and Processing of Chromatography Data

In former times an analytical chemist spent most of the time with the analysis itself. Today acquisition and processing of the analytical data are the most time consuming processes. Very often new instruments come with their own external software, which has to be learned, validated and integrated into the processes of the laboratory. This produces high permanent costs for software training and management and the integration of different data formats into your system. Such a waste of resources is no longer adequate due to the central role automated data processing and application software play in our laboratories today.

Instead universal, flexible and open software solutions are needed which follow established software engineering standards and comply national and international standards like ISO 13885 and ASTM D5296-97. A modern chromatography software package communicates with a variety of laboratory devices and data systems from different manufacturers and allows the acquisition and combined processing of all the data. An example which meets these requirements is the PSS WinGPC Unity, a Macromolecular Chromatography Data System (MCDS).

Evaluation of the Laboratory Software Requirements

The implementation of software requirements for different size laboratories will be discussed by presenting four examples. Those illustrate how the general requirements for chromatography software can be met in various environments. Stable and reliable data acquisition is the most important concern. Additionally, software solutions should be available for stand-alone workstations and networks alike. Another important aspect is the flexibility (supported computer and operating systems) and adaptability of the data system to laboratory conditions (mainly requirements of instruments and the associated methods). The adaptability of the software allows the processing of data from different detectors without tedious data import or export procedures. The modular structure minimizes the training period for users. The user interface only provides the functions which are needed for the actual task. Another advantage of a modular setup is the seamless integration of new functionality whenever needed.

Independent from the size of the data system used, experience shows that the validation of a software package is often one of the biggest problems for end users. Therefore not only users working in regulated and controlled laboratories expect software which is easy to validate. The compliance with all national and international regulations for data acquisition and processing (ISO, ASTM, DIN, Pharmacopoeia, etc.) is also of great importance. These requirements are much easier to meet with an integrated chromatography software solution than with several different packages. The comprehensive validation of PSS WinGPC Unity offers not only solutions for standard systems and methods but also for highly sophisticated systems with special detectors like light scattering and on-line viscosimetry. The validation of data

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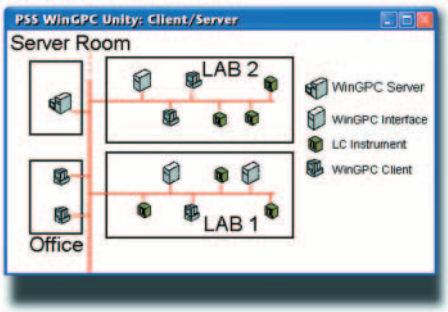
systems can be easily checked on-site any time in any laboratory using WinGPC's AutoVal tool.

Case Studies

Four live case scenarios from everyday identify decision-making scenarios faced by scientists and companies. In each case, the specific needs will be satisfied with the same MCDS, but in a different configuration.

Case 1: Client/Server GPC Solution for Distributed Work Processes

A manufacturer of pharmaceutical products needs fully validated GPC software in different working areas, using the existing infrastructure. The software must be compatible with methods at other sites. GPC measurements have to be carried out and controlled from various departments. The analytical staff from different labs and offices, corporate-wide, must have on-line access to the data initially processed at the measurement site. The comprehensive analysis of the measurement is done in specialist departments; this should be possible even without having the equipment to execute GPC measurements on their own (Fig. 1).



Selection Criteria

The customer needs a software which

- Is compliant with all national and international GPC standards (e.g. ISO, EN, ASTM, DIN, JS), making it easier and faster to put the products on the market
- Offers comprehensive software validation easy to verify in audits
- Has a central database with straightforward data management and search routines
- Integrates all GPC data in the existing worldwide LIMS system
- Offers high level data security and central access control using existing authentication mechanisms (e.g. a domain server)
- Guarantees accessibility and support world wide
- Handles all current and future tasks, minimizing training and support costs
- Allows a comprehensive and fast data exchange between labs in different countries
- Offers in client/server mode business-wide control over analytical jobs, no matter where they have to be done ("data follow people" technology)
- Permits data acquisition via LAN, allowing a flexible, friendly use of the existing infrastructure
- Facilitates the creation and publication of results and reports in the intranet, or via e-mail

Solution

After a comprehensive test phase, the company chooses the PSS WinGPC Unity Client/Server GPC solution for distributed working

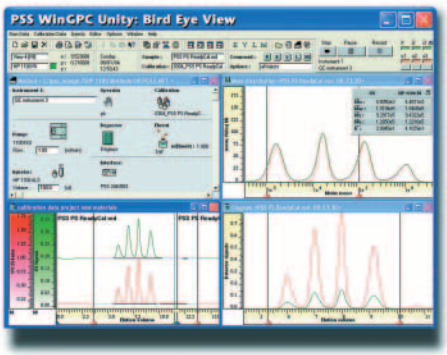
Case 2: Easy and Flexible Software Solution for Stand-alone Systems

A research lab needs a GPC system to build up a new working direction. The conceptual formulation demands further processing of the primary GPC data with in house software. An older HPLC instrument and a computer with MS Win 95 need to be integrated in the new setup (Fig. 2).

Selection criteria

The software has to meet following requirements:

- It allows the integration of the HPLC instrument and further use of the old personal computer



- The data export function facilitates further processing of GPC data
- The easy to learn user interface minimizes learning curve time requirement
- It provides straightforward integration of results into research reports

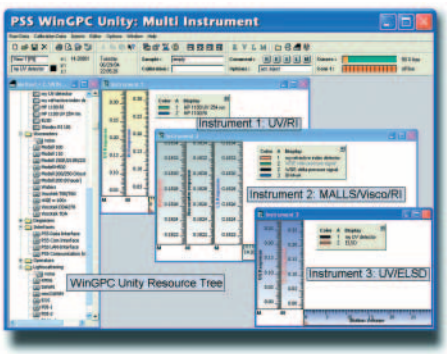
Solution

One Simple WinGPC Unity setup for a single instrument system

Case 3: Modular Multi Instrument System in a Heterogeneous Laboratory Environment

A central analytical laboratory that operates a (heterogeneous) chromatography infrastructure has to upgrade the equipment in order to meet customer requirements. The upgrade includes the purchase of new special detectors and the development of new analytical and data processing methods. Special requirement emphasis is placed on flexibility for all staff members to use the complete equipment (Fig. 3).

Selection criteria



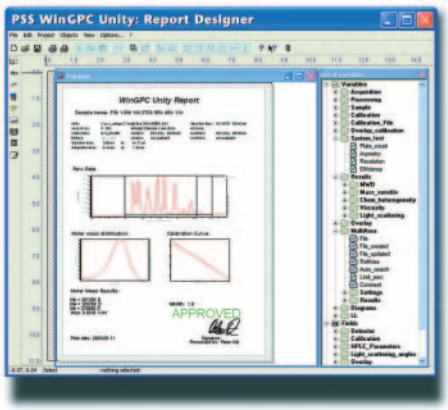
The customer chooses the MCDS package because it

- Is compatible with existing equipment
- Integrates new instruments independent of the manufacturer
- Supports not only evaluation of conventional GPC data, but also a lot of special methods/tasks and is modular
- Meets the requirements of all national and international standards
- Is fully validated and easily satisfies the needs of internal and external auditors
- Uses the same user interface and data structure for all possible tasks
- Has a safe and consistent database structure, guaranteeing maximum data security
- Allows a flexible distribution and assignment of the existing resources
- Data evaluation licenses are free of charge
- Creates task and customer specific result reports
- Supports the results distribution by e-mail, fax and internet

Solution

PSS WinGPC Unity with network support (Multi system/multi instrument setup) for data acquisition and processing department-wide

Case 4: Robust and Easy to Use Quality Control System



A production lab needs a complete GPC system for quality control to meet the demanding requirements of the customers (Fig. 4).

Selection Criteria

The software requirements are:

- Data acquisition and processing can be fully automated
- High availability and stability
- Customer specific result reports
- The possibility to automate the acceptance criteria of products with specific, targeted reports
- The measurement results can easily be merged into the existing LIMS

In addition, there are many advantages to buy the complete solution from the same company which

- Has broad experience in quality control
- Develops customer specific analytical methods and applications
- Offers complete solutions with modern analytical hard- and software, columns, polymer standards and training courses
- Sells only certified products which are developed, produced, distributed and supported under ISO 9001

Solution

PSS Columns, Standards and WinGPC Unity for robust and easy to use GPC systems for quality control

Conclusion

From the decision-making presentation above it is possible to generalize some of the features that are important to users in the marketplace, such as stability and reliability for data acquisition, flexibility to support various computer and operating systems as well as adaptability of the data system to the laboratory conditions and ease of implementation and integration into the lab.

All users have their own specific needs and demands, easy to validate, whether or not they work in regulated laboratories. Independent from the size of the data system used, experience shows that the validation of a software package is often one of the biggest problems for the end user. The comprehensive validation of WinGPC Unity offers not only solutions for standard systems and methods but also for highly sophisticated systems with special detectors.

The compliance with all national and international regulations for data acquisition and processing (ISO, ASTM, DIN, Pharmacopoeias etc.) is also of great importance. With an integrated chromatography software solution, these requirements are much easier to meet than with several different packages.

No longer will an analytical chemist have to spend most of the time learning multiple software products, or validating and integrating multiple processes and data formats into the data flow. Using WinGPC Unity will result in lower overhead costs and a better use of your human resources.

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