

# Third-party instrument control with Chromeleon Chromatography Data System Software

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LC, IC, GC, driver development kit  
(DDK)

## Executive summary

Over the last few decades chromatographic instrumentation and separations have become mainstream techniques for most laboratories. The main techniques are Gas Chromatography (GC) and High Performance Liquid Chromatography (HPLC). All these chromatographic instruments are operated using software called a Chromatography Data System (CDS), for instrument control and data handling, which has developed significantly over the last three decades. Thermo Scientific™ Chromeleon™ Chromatography Data System software was a pioneer of third-party instrument control and has continued to be the market leader with multivendor control.

## Instrument control in Chromatography Data Systems

The history of instrument control in chromatography data systems can be traced back to the development of the personal computer (PC) in the early 1980s, which led to the introduction of PC based CDS. Operation was similar to the microprocessor-based integrators introduced in the 1970s, but data files from all injections of a run were now available for reprocessing. At this time data collection from any instrument was only possible through conversion of the instrument data from the analogue output signal to a digital signal that could be read by the CDS (A/D conversion). This A/D conversion only allowed the recording of a single data channel from the instrument and did not cover instrument control at all.

As higher-performance PCs became more affordable, manufacturers were able to add instrument control in addition to their existing data processing and reporting tools. Even so, for the next decade, CDS were only capable of full digital control of instruments that were supplied by the same manufacturer as the CDS so it was common for one vendor to supply both the CDS and the chromatographic equipment with the majority having a connection of only a single chromatograph per PC. As CDS were further developed, the ability to control multiple instruments from one PC appeared albeit with the same 'single manufacturer' restriction. This type of installation can be described as a "workstation CDS."

Commonly, laboratories have always had a variety of chromatographic instruments from different manufacturers. With the single manufacturer workstation CDS approach, this led to the installation of several different CDS in the laboratory with inherent efficiency, data handling, training, validation and regulatory complications. The only way to reduce the number of CDS was to use A/D conversion to create a digital signal that could be read and imported by the chosen CDS(s), and relinquish control of the instruments, with the fundamental problems of over-ranging or 'flat-topping' of peaks, excess noise, and a complete lack of traceability.

Through the 1990s advances in PCs combined with improved networking standards allowed for CDS to become networked. When networked, data handling becomes more efficient and instrument utilization can be optimized. In addition, it is easier to meet regulatory guidelines because it allows the physical decoupling of data handling from data storage, thus increasing security of the acquired data. These networked CDS, with decoupled data handling and storage, are often referred to as "enterprise" or "client/server" systems.

With one method, all data from instruments in the same format, and one common report for results, regardless of the instrument that was used to generate them, the efficiency gains and productivity increases from using a scalable, enterprise CDS were huge.

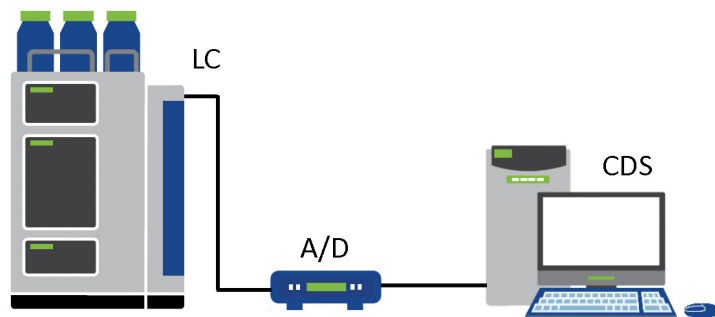


Figure 1: Early CDS – data collection with no control

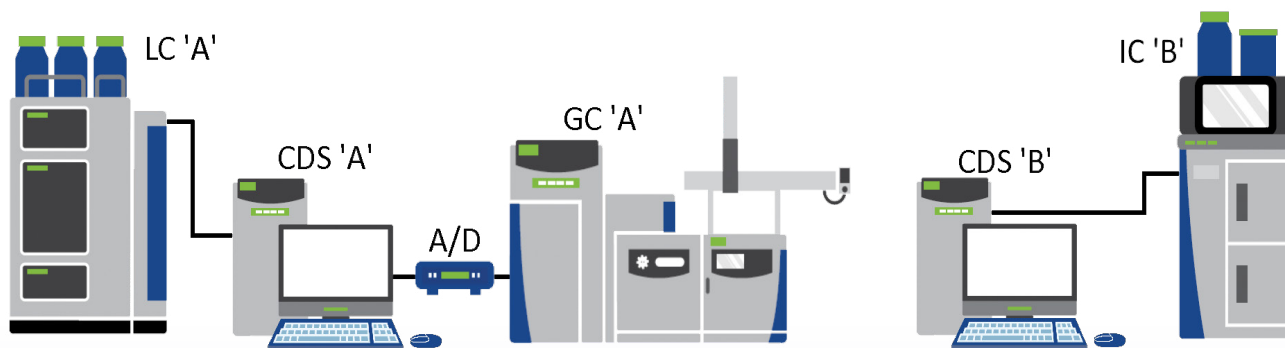


Figure 2: Workstation CDS for a variety of chromatographic instruments

## Establishing demand for multi-vendor instrument control

With the increasing adoption of enterprise CDS configurations, the de facto linking of the instrument and CDS manufacturer started to erode. Some suppliers started to focus on the development of CDS solutions while others emphasized instrument development. Chromatographic instrument suppliers with a smaller market share, and/or with no interest in developing their own CDS, started to look for non-competing, software-only suppliers of CDS, and supported them in achieving control for their instruments in the data system. Conversely, as CDS suppliers saw their products become more and more important to the efficient operation of chromatographic laboratories, the control of instruments from other major suppliers (third-party instruments) became an attractive market opportunity. Thus, the desire for control of third-party instruments (multi-vendor control) arose in CDS.

While, at first, the benefits of central data management and storage initially outweighed the inherent limitations in A/D conversion of data from third-party instruments, the mandate from the United States Food and Drug Administration (FDA) in 1997 for electronic records and electronic signatures (21 CFR Part 11) clearly identified such instrument control (or lack of it) as not in line with compliance guidelines.

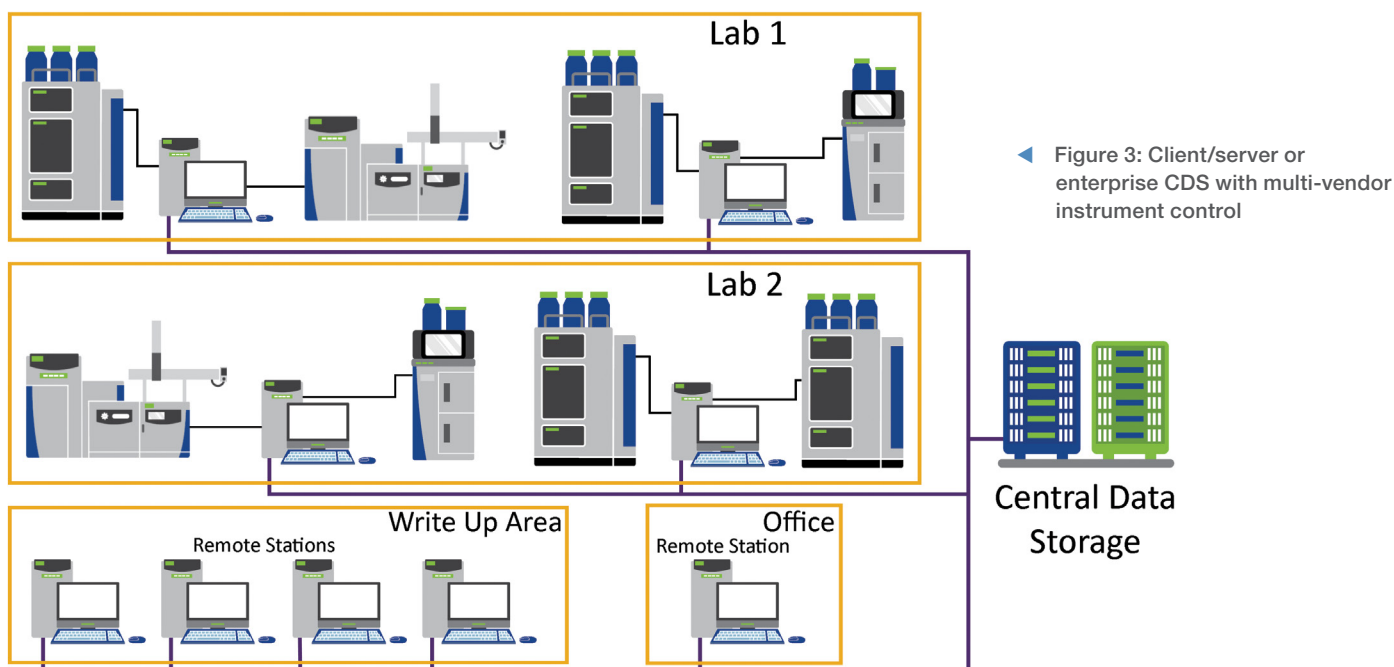
This mandate established a need for third-party instrument control in CDS, and the demand for fully-digital control of proprietary and third-party instruments became pressing. The market need for data systems that supported compliance with 21 CFR Part 11 with fully-digital

instrument control also led to a sharp consolidation in the market place, resulting in only three global CDS suppliers having a significant share (>10% installed base and annual license sales) in the market. Given that there are many more instrument suppliers with a relevant market share (>5%) than suppliers of enterprise CDS, the necessity for third-party instrument control becomes obvious.

1993 saw the introduction of the world's first commercially available chromatography data system – Thermo Scientific Chromeleon CDS (at that time still under the brand name of Gynkosoft). This was the first CDS solution providing full digital control of instruments from leading third-party suppliers.

By the late 1990s it was still rare for a CDS to have significant third-party control, but it was common for it to control its own manufacturers instruments, be able to set up methods and analytical run information, acquire, process, report and save the data, and even transmit it to other laboratory systems, such as a Laboratory Information Management System (LIMS). At this time, Chromeleon CDS already provided support for over 60 third-party instruments, with more instruments being added.

With feasibility for digital third-party instrument control proven, the interest in CDS with multi-vendor instrument control grew rapidly. Chromeleon CDS established itself as the market leader in multi-vendor instrument control, capable of controlling over 525 proprietary and third-party modules from 22 different manufacturers, ensuring that nowadays, multivendor instrument control is a standard 'must have' function for any CDS.



## From early adopters to mainstream market – overcoming the challenges

While some laboratories quickly adopted third-party instrument control with CDS, a number of challenges had to be overcome before third-party control was mature enough to really become accepted broadly.

The first challenge was that the earliest third-party controls were developed by CDS companies based on limited information, and mainly focused on covering only the general commands for controlling the third-party instruments. This also required the programmers to write a driver for an instrument without a deeper knowledge of the general operation of the instrument. For Chromeleon CDS, the initial development of third-party instrument control was carried out by analyzing the control protocols of the instrument, and then writing an instrument control “driver” in a Chromeleon CDS compatible control language – a “native driver”.

Even when cooperation was established between the parties, communication between the CDS group writing the instrument control and the third-party supplying the control codes was often slow and tedious. This was because most of the CDS suppliers were also direct competitors as instrument manufacturers. Furthermore, it would often be the same CDS group developing drivers for both their own in-house instruments and third-party instruments from competing suppliers, which could lead to priority conflicts and delayed availability of the control codes for the third-party instrumentation.

The second challenge was the increasing complexity and growing number of instrument configurations. With each introduction of a new instrument came new technology and features along with the market demand to be able to control these instruments and new features from their chosen CDS. This increased the complexity, and hence, the effort required for programming third-party instrument control.

In the mid-2000s, with the introduction of UHPLC (Ultra High Performance Liquid Chromatography) as an extension of the traditional HPLC, the demands for instrument control became even more sophisticated. More functionality, such as method translation from traditional HPLC to UHPLC methods, moved into the instrument controlling driver. Recreating this complex functionality was time and resource consuming, and could lead to significant delays between instrument release from the third-party hardware manufacturer and

availability of control of these instruments in the CDS. In parallel the number of third-party instruments to be controlled grew substantially – some large manufacturers having more than one hundred (HPLC and UHPLC) modules in active distribution.

## Third-party instrument “printer driver” concept – from native instrument drivers to plugin instrument drivers

Addressing these challenges triggered a change in the concept of third-party instrument control. The key instrument suppliers started to explore ways to provide their instruments with a la carte drivers to easily and quickly plug into a third-party CDS. A “printer driver” concept for control of chromatographic instruments could provide the instrument control drivers directly from the instrument suppliers, and would deliver them in a fashion that allowed easy integration to third-party CDS.

This provided the obvious benefits of a more efficient development process – instead of each CDS company writing a driver for the same third-party instrument, now only one driver had to be written (by the instrument manufacturer) for all CDS, thus expediting control of new instruments in third-party data systems. To make this approach work it was required that the instrument supplier developed and maintained driver architecture that not only provided the actual instrument control, but also a standardized framework that provided the plugin and necessary adaptations to be used in a third-party data system.

However, not all instrument suppliers can or want to provide such an infrastructure. Smaller, or hardware-focused suppliers, quite often just need a simple way to bring digital control of their instruments into a third-party CDS.



## The Chromeleon CDS provides the ultimate third-party driver solution

Chromeleon CDS provides the ultimate solution for third-party instrument control with both the “printer driver” plugin concept and a Driver Development Kit (DDK) approach to address the needs of the smaller, or more hardware-focused, manufacturers.

Integrated within Chromeleon CDS are the wrapped driver plugin solutions provided by leading instrument manufacturers, including the Agilent Instrument Control Framework (ICF) and the Waters Instrument Control Software (ICS). This ensures fast, comprehensive support for all drivers and functions released to these plugins.

The Chromeleon DDK provides driver developers and instrument vendors with a straightforward approach to implementing instrument driver, configuration, and editor plugins for Chromeleon CDS. All new drivers implemented by Thermo Fisher Scientific use the DDK. It is designed for cross-version compatibility – write one driver and it can usually be used with all newer versions of Chromeleon CDS without the need for further development. There is very little ‘must have’ code to be included, so it is very quick and easy to learn how to implement instrument drivers – the basic driver framework can be created in a matter of hours, rather than the days or weeks it would take for a native driver. This considerably speeds up driver development.

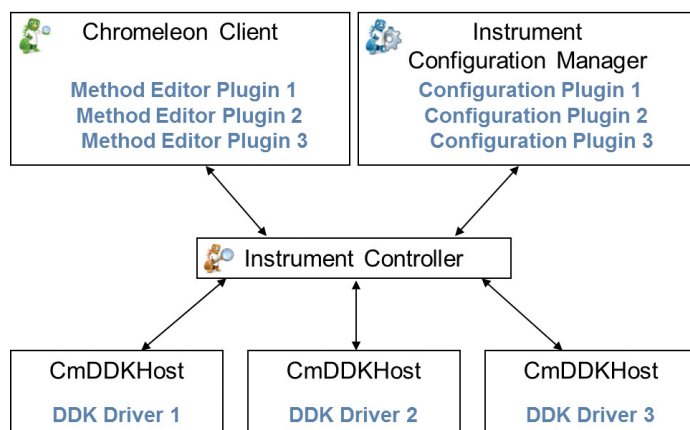


Figure 4: Chromeleon DDK plugins simplify driver creation

The quality of all drivers is assured by certification and validation procedures. All new drivers must meet the requirements of the certification process and pass a series of validation tests before acceptance for inclusion in Chromeleon CDS.

The DDK in Chromeleon is actively supported with a comprehensive set of documents (including a driver ‘cook book’ with example code and the certification process), programmer training courses, and support with programming to enable third-party companies to develop drivers directly in a Chromeleon software-compatible format. For suppliers who do not wish to create their own drivers, there are certified Chromeleon DDK development partners to quickly develop Chromeleon DDK drivers.

Recently, Thermo Fisher and Agilent have collaborated to enable Agilent to utilize the DDK to create the ‘Agilent Drivers for Chromeleon 7’ kit, which allows Chromeleon CDS versions 7.2 SR5, and above to have advanced control of their LC hardware. This advanced control allows Chromeleon CDS-specific features to be utilized with the Agilent hardware, something that was not possible while using ICF. By using the Chromeleon DDK to develop these drivers, Agilent was also able to include a Software Verification Tool (SVT) to verify the correct installation of the software components. Though developed by Agilent using the DDK, the drivers are tested and certified by Thermo Fisher before inclusion in a Chromeleon software release.

## What else is needed to make third-party instrument control successful?

In order to maintain high quality drivers that are released in a timely manner, especially for new instruments, it is important that the instrument vendor and CDS vendor establish regular meetings to share technical knowledge, roadmaps for upcoming releases, and to discuss and resolve technical issues. This requires commitment from both parties for regular, on-going maintenance and improvements of the wrapped driver package and its integration into the CDS, alongside maintenance and improvements, in the case of Chromeleon CDS, of the DDK.

Control of Mass Spectrometer (MS) equipment is the newest challenge for third-party instrument control. As MS data evaluation starts to become common in CDS software, some CDS vendors are able to control, and collect data from, their own MS equipment, but are not able to do this with third-party equipment. The situation is similar to where the industry was with chromatography instruments in the late 1990s where driver and code sharing was not common. With vendors having already worked together to provide a driver solution for their chromatography instruments, it would make sense that third-party control for MS equipment will not be far behind.

## Summary

Chromeleon CDS pioneered third-party instrument control, and has continued to be the market leader to a point where Chromeleon software is now synonymous with multi-vendor control, and has made this a 'must have' feature of any CDS. With over 25 years of development experience, Chromeleon software offers all the tools to instrument suppliers who may be interested in third-party instrument control. Chromeleon CDS is the most future-proofed, enterprise-ready, multi-vendor CDS on the market.



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