

How to upgrade your chromatography data system

Preparation, planning and straightforward software implementation

Takeda Ltd, a pharmaceutical company with a presence in 80 countries, delivers innovative medicines to people around the world. The Takeda Oranienburg pharmaceutical production site in Germany employs a variety of different chromatography techniques during the manufacture of its 40 products, which include tablets, pellets and capsules. Using high performance liquid chromatography (HPLC) methods for determination of identity, content uniformity, purity and bulk dissolution tests, and gas chromatography (GC) methods for detecting residual solvents, the site employs the Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) to support its HPLC and GC systems.

Recently, the team at Takeda Oranienburg migrated all of its 40 chromatography (HPLC and GC) instruments to the latest version of Chromeleon 7 CDS. In this case study, we offer key considerations for successfully installing and migrating the CDS software to the latest version to take advantage of its enhanced capabilities, while minimizing disturbance to routine chromatography runs.

Why upgrade? Reasons for moving from Chromeleon CDS, version 6 to version 7

Transferring from Chromeleon software version 6 to version 7 brought numerous benefits for a better functioning system. Firstly, it promised continued support for all chromatography analyses as Chromeleon 6 CDS would soon be out of support. Secondly, the new version provided the highest degree of data integrity and traceability, ensuring compliance with the latest regulatory requirements. For instance, its enhanced administrative functions are particularly useful for audits

and troubleshooting in a good manufacturing practice (GMP) environment. Further, from a user perspective, the upgrade provided compatibility with Microsoft® Windows® 10 and other third-party software allowing the continued use of preferred and familiar systems. Finally, the powerful new tools in Chromeleon 7 CDS, such as eWorkflow™ procedures and smart peak detection algorithms, made data processing easier and faster, improving laboratory productivity and enabling automation in routine chromatography analyses.



Planning the upgrade: What resources will you need?

Any software upgrade requires meticulous planning to ensure a smooth transition. As a result, it is often helpful to appoint a project manager who can oversee and monitor the entire upgrade process. Below, we list the steps that the Takeda Oranienburg team successfully followed ahead of the upgrade to Chromeleon 7 CDS:

- **IT considerations**

It is important to ensure that as many existing analytical instruments as possible, and any future planned instruments, are compatible with the new software. Full control of the instrumentation enhances data integrity and quality. You should also ensure the necessary IT infrastructure, such as servers, terminal servers and databases, are available for both a test environment and the final installation. Receiving continuous IT support during different phases of the project facilitates a successful software upgrade. “You also have to pay attention to the necessary hardware interfaces and drivers, especially for third-party instruments,” says Thomas Pietsch, the Chromeleon CDS administrator at the Takeda Oranienburg site who oversaw the whole installation process. To ensure a stable system with good performance, estimate how many users will interface with the new software and define the system size, i.e., the number of instruments and clients that will be used.

- **User Requirement Specification**

Identify the required and desired software functions, typically in the form of a ‘User Requirement Specification’. If needed, Thermo Fisher Scientific can offer support to ensure full functionality of the software for its intended use with supporting documentation.

- **Define key users**

Gather a group of technically experienced lab users familiar with the chromatography protocols to test the implementation of the software, generate necessary reports and assist other users.

- **Design validation and project plans**

Working with the quality management department, design a validation plan to perform functional testing and determine user acceptance of the new software. Create a project plan with expected timelines, resource allocation and goals for each phase of the software upgrade.

“After the order confirmation, a kick-off meeting with all stakeholders on site of the customer is necessary to set the schedule for the project,” advises Thomas Guenther,

project manager for Chromeleon enterprise installation at Thermo Fisher Scientific. “To avoid unexpected issues in an upgrade project, it makes sense to hold regular *jour fixe* meetings to provide updates on the current status and, if necessary, re-establish the timelines. Any recurring issues arising in these meetings can be solved quickly and safely.”

- **(Key) User Training and Software Implementation**

To ensure a seamless transition, the Chromeleon support team provided training workshops to address any questions or concerns by the lab members who will use the new software. The team also offers any assistance required with the transfer of current methods to minimize downtime and resume routine analysis, as soon as possible. The Thermo Fisher services team facilitates the final rollout of the new software, connecting all instruments to Chromeleon 7 CDS.

From old to new: The installation process at the Takeda Oranienburg site

The entire installation process to upgrade all 40 HPLC and GC instruments at the Takeda Oranienburg site was divided into multiple steps. The first step was a simple *test environment*, which assessed the new version on a smaller scale, next, the *production environment* tested the validation plan and finally the *phased integration* connected all instruments for the site-wide upgrade.

The test environment: Here, one HPLC system was integrated with the new Chromeleon 7 software. Setting up the necessary infrastructure of servers, installing a database and meeting other system requirements to enable pre-testing under “real” conditions.

The production environment: After successful tests and setting up the required infrastructure, two different HPLC instruments were integrated to run the validation plan.

Step-by-step integration of additional instruments:

Working with clusters of four instruments, Chromeleon 7 CDS was gradually rolled out across all of the 40 instruments, adhering to instrument, operational and performance quality. “Today, all of our instruments are successfully migrated to the new system,” says Thomas Pietsch, reflecting on the completed site-wide upgrade at Takeda Oranienburg. “With the finished project, we now have a validated, stable and up-to-date system.”

Frequently asked questions about the site-wide Chromeleon 7 CDS upgrade

Offering insights from his experience, Thomas Pietsch answers some frequently asked questions regarding the installation process.

How long did it take to upgrade all 40 functioning chromatography instruments?

The installation of the test environment, production environment and successful integration of 40 instruments was completed in approximately one year.

What's your advice for converting files like instrument methods, processing methods and report templates from Chromeleon 6 to 7 CDS?

From a technical perspective, it may seem like converting methods and templates requires little time investment, but in our experience, the process can take much longer than anticipated. What you should pay attention to are instrument methods on third-party systems because some functions and syntax can change after the conversion when newer drivers are utilized. We got a recommendation from Thermo Fisher to re-write these programs, which added more time to the process.

In case of report templates and processing methods, the conversion of files was again straightforward but depended on the complexity of the report functions. Where we used complex report functions, we decided to re-create them. In every case, you should carefully test your converted files to assess the functionality. The testing basically takes more time than the pure conversion process.

After the installation, do you still need to access data from previous versions of the software?

Yes, we needed to access data from Chromeleon 6.8 CDS for audits and future reviews. Upon realizing this, we worked towards integrating and mounting Chromeleon 6.8 datasources directly into the Chromeleon 7 software in "read-only" mode. This was successfully validated in our test environment. There were some challenges in database configuration, but we resolved it through good communication with Thermo Fisher, our local IT support and an external database specialist partner. So, the very last step of our upgrade was the integration of the old data into our production environment.

Did you implement eWorkflow procedures for all your methods? If yes, does it make the process easier?

We use eWorkflow procedures for our routine methods where we work in a highly standardized way. We don't use it for new methods in the implementation phase or for validation, due to variability during these stages.

Upon completing the implementation of new products, we create eWorkflow templates when these methods are transferred to routine analytics. Notably, with Chromeleon 7 CDS and after creating templates, we saw a reduction of lab errors. Using one tool, it is now easier to administer different sequences, such as the instrument methods, processing methods and report templates. We also received positive feedback from the lab as the eWorkflow feature is well-structured and easy to handle.

Changes in interfaces can be challenging for users. What did the end users think of the new software?

All in all, we got a lot of positive feedback. Before the installation project, of course, there were doubts from some users who felt uncertain about using the new software, but we managed this with comprehensive training. Now all the people in our lab are trained and are confident to use the software in the right way to ensure stable lab processes.



A change for the better: Added benefits from upgrading to Chromeleon CDS, Version 7

The Chromeleon 7 software promises to bring operational simplicity to its users. Below are some of the user benefits from the upgrade brought about by the new features designed into Chromeleon 7 CDS:

Extensive administrations tools with an improved user interface

Chromeleon 7 CDS provides centralized administration to enable a clear, structured overview of the entire chromatography set up. Users can view information about licenses, scheduler services, policies and instrument configuration in a single access-controlled location. The Chromeleon Console utilizes category bars to enable quick access to connected instruments, saved eWorkflow procedures and sample data. With the better structured report functions, users can perform periodic system reviews, allowing transparency towards regulatory authorities. The 'Chromatography Studio,' used primarily for data evaluation, provides access to methods, templates, libraries and injection lists from its interface.

Automated chromatogram integration

The Cobra Peak Detection Algorithm available in Chromeleon 7 CDS allows even inexperienced users to obtain accurate chromatogram integration, delivering substantial time savings, while minimizing manual processes. With the SmartPeaks™ Integration Assistant function, users can consistently integrate all unresolved peaks in as little as 3 clicks. These two new tools, equipped within Chromeleon 7 software, eliminate the need for training and simplify data processing for users.

Standardized workflows and faster results

The eWorkflow function offers the possibility of creating template sequences, allowing users to standardize workflows and minimize errors without the need for

extensive training. From a single user interface, it controls all aspects of the chromatography run starting from the instruments involved, the associated files, such as methods or reports, the stored templates for the sequence, the necessary rules for the sequence layout, and any variables associated with the runs. With the click of a button, the eWorkflow procedures runs the analysis, processes the data and calculates the results, thereby automating the entire process for users.

Increased controllability of third-party systems

The new upgrade enables access to all connected PCs inside the network, facilitating remote troubleshooting. With formal code agreements with major manufacturers, Chromeleon 7 CDS can control third-party instruments for LC, GC, ion chromatography and routine mass spectrometry applications from the same interface, streamlining workflows and simplifying operations.

Conclusion

A successful upgrade to Chromeleon 7 CDS involves detailed preparation and planning. Once implemented, the new software offers an array of added capabilities, accelerating chromatography analyses and making laboratories more productive. "The Chromeleon software upgrade is not an out-of-the-box installation. It requires meaningful planning and implementation," notes Thomas Guenther. "A project plan with milestones and resource allocation is inevitable." By upgrading to the new Chromeleon 7 software, laboratories benefit from having a fully functional, validated chromatography data system that controls the entire operation from one application, meets regulatory standards and receives industry-leading support.

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