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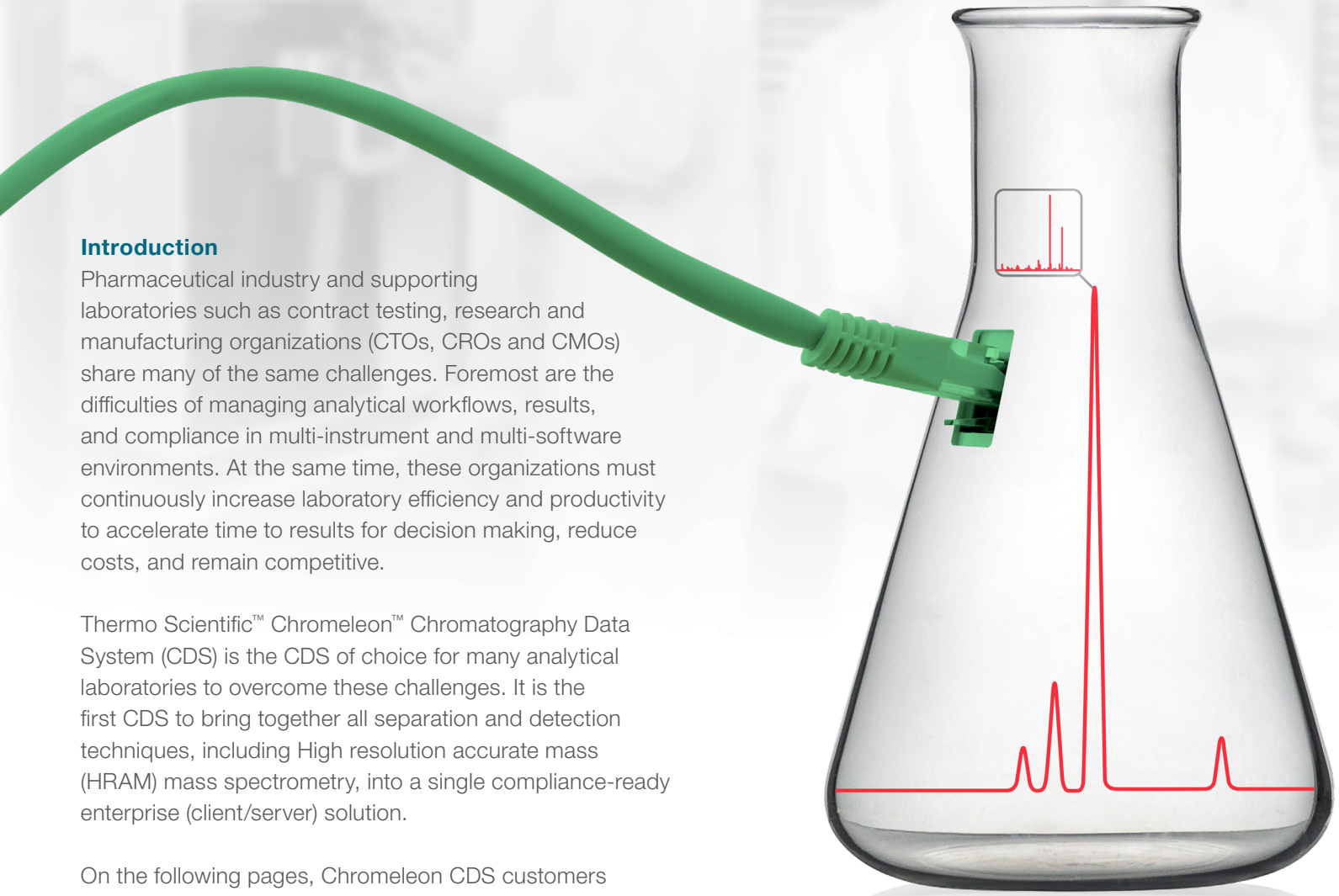
CASE STUDY 000109

Compliance-ready MS Chromeleon CDS: customer perspectives



Introduction

Pharmaceutical industry and supporting laboratories such as contract testing, research and manufacturing organizations (CTOs, CROs and CMOs) share many of the same challenges. Foremost are the difficulties of managing analytical workflows, results, and compliance in multi-instrument and multi-software environments. At the same time, these organizations must continuously increase laboratory efficiency and productivity to accelerate time to results for decision making, reduce costs, and remain competitive.

Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) is the CDS of choice for many analytical laboratories to overcome these challenges. It is the first CDS to bring together all separation and detection techniques, including High resolution accurate mass (HRAM) mass spectrometry, into a single compliance-ready enterprise (client/server) solution.

On the following pages, Chromeleon CDS customers provide their perspectives about how the software enhances the efficiency of their chromatography and MS workflows, while providing comprehensive compliance capabilities.

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"Chromeleon CDS allows us to audit trail everything that we need to, making it easier when we are audited. The user management system and centralized resourcing means that data access and backup is easily managed, ensuring data integrity."

– Adam Neaves, Quality and Compliance Specialist, Broughton Laboratories

Built for compliance without compromise

Efficiently meeting compliance requirements is a concern when methods and data are spread among many different data systems. Chromeleon CDS brings methods and data for numerous analytical techniques together in secure centralized storage where access can be controlled, shared, and monitored. In fact, the software provides industry-leading multi-vendor control, with support for over 540 instrument modules from over 20 manufacturers, including Thermo Scientific™ chromatography systems and single or triple quadrupole and Orbitrap™ mass spectrometers.

Chromeleon CDS provides all of the necessary functionality and more to reduce the effort needed to achieve and demonstrate GxP and 21 CFR Part 11 compliance:

- Audit trails of all actions in the software
- Version control for methods and data
- Secure controlled access to methods and data with permissions for more than 160 user privileges
- Compliant eSignatures
- Automated System Suitability Testing (SST)

Sterling Pharma Solutions

Centrally secures information for data integrity and compliance

SAFC Madison, a Sigma-Aldrich CMO that provides development and scale-up manufacturing of Active Pharmaceutical Ingredients (APIs), deployed Chromeleon CDS to solve the challenges of maintaining audit trails in their multi-vendor instrument environment. According to Michael Faley, Analytical Supervisor, "Among other issues with our historical data systems, the lack of a full data audit trail was a big concern. We needed to be able to trace who did what, where, and when to chromatographic data. That meant having a networked solution with centralized data storage."

Broughton Laboratories, a global analytical services business likewise chose Chromeleon CDS to maintain data integrity and compliance for their HPLC and triple quadrupole MS workflows. Their centralized storage deployment allows automated backups and prevents data loss via the secure XVault™ infrastructure. Adam Neaves, Quality and Compliance Specialist said, "The centralized resourcing of the system allows us to easily access and maintain centralized database systems as well so we can maintain backup and data integrity."

With facilities in the UK and US, Sterling Pharma Solutions provides contract development and manufacturing services for advanced drug intermediates and APIs. The need for improved data integrity and compliance to meet regulatory standards was one of the drivers behind Sterling's decision to adopt a single CDS to support all of the GC and HPLC systems used across their QC and R&D laboratories.

"Chromeleon CDS has really improved our data integrity and ticks all of the boxes for compliance with 21 CFR Part 11 and the MHRA GMP data integrity definitions and guidance for industry. Overall, I would say that Chromeleon CDS is a very powerful tool for QA review and compliance."

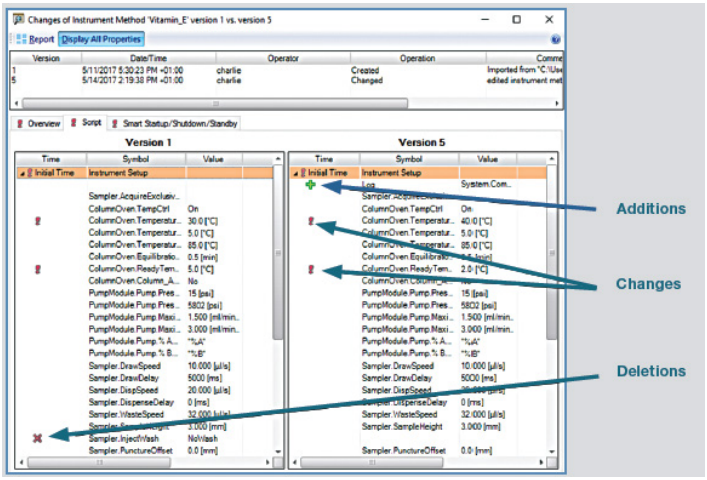
– Brian Alliston, Data Integrity Expert and CDS Specialist, Sterling Pharma Solutions

Explaining the choice, Brian Alliston, Data Integrity Expert and CDS Specialist, Sterling Pharma Solutions said, "We chose Chromeleon CDS for several reasons, the main one being the centralized data storage. Also the fact that both separate parts of the site could operate the same system, the high level of cGMP compliance and data integrity, the ability to create bespoke product-specific report templates, and the fact we could continue to use our existing instruments."

Provides easy-to-review audit trails

Audit trails are a regulatory requirement proven effective for detecting data integrity issues. Chromeleon CDS provides a simple, clear way of reviewing data, along with in-depth audit trails and versioning history to ensure that the process of who did what, when, and why can be easily viewed for any changes made within the system.

According to Alliston, "The audit trails in Chromeleon CDS are very comprehensive and track everything that the user and system does. Our users regularly review the audit trails for each sequence, and with the audit trails easily accessible on-screen and the ability to group, filter and search for events, it is very quick and easy for users to review and allows them to ensure that the correct versions of instrument methods and report templates are used for each analysis. The version comparison tool is also very useful; allowing us to easily demonstrate what changed between different versions, and all changes are very clearly identified."



Changes between versions are easily identified using the version comparison tool.

Explaining the software's audit trail capabilities, Broughton's Neaves said, "Chromeleon CDS allows us to audit trail everything that we need to, making it easier when we are audited." Neaves continued, "The Chromeleon system allows us to audit trail pretty much anything on the network. We can provide that to the inspectors if and when they want to look at it."

"Each Regis Chromeleon Data Vault has distinct privileges provided to the users and has been validated for use in a 21 CFR environment."

– Maurice Andrew (Andy) Hippleheuser,
Director of Quality Control, Regis Technologies, Inc.

Ensures 21 CFR Part 11 compliant eSignatures

Chromeleon CDS fully supports 21 CFR Part 11, allowing records to be electronically signed with two levels of protection: controlled pre-submission preview of final results (the Electronic Report) for structured review and Electronic Signatures where the Electronic Report and entire sequence are locked and protected from further changes. Andy Hippleheuser, Director of Quality Control, Regis Technologies, a CMO that provides synthesis and separations services to pharmaceutical and biotechnology companies, set up Chromeleon CDS to meet the needs of Regis' various laboratories. According to Hippleheuser, "Each Regis Chromeleon Data Vault has distinct privileges provided to the users and has been validated for use in a 21 CFR environment. Being a CMO, we conduct methods with a lot of variation. Chromeleon CDS lets me create and 'lock' individual templates for each method, process, and report." He continued, "We have now moved to Electronic Signatures and this allows us to save time and paper. Only the final approved report is printed and goes into the individual batch record."

Automates System Suitability Testing

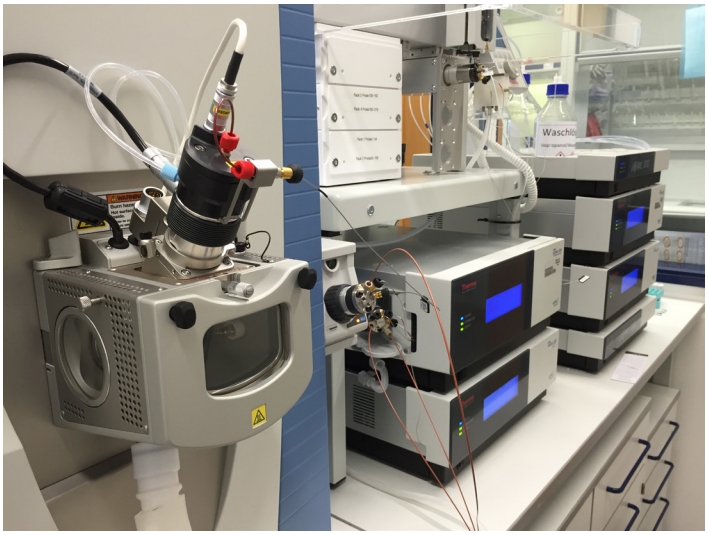
In regulated laboratories, SST is required to ensure that a chromatography system (instrument, reagents, columns, etc.) is suitable for the intended application. The goal is to monitor results to ensure chromatographic suitability and consistent system performance. Chromeleon software can automatically perform SSTs on any parameter, such as injection repeatability, capacity factor, peak-tailing factors, relative retention time, area %, peak width, concentration, and many more.

According to Regis' Hippleheuser, automated SST substantially increases productivity. "The largest saving is in the use of Chromeleon software's SST feature in the processing method. Since Regis runs a two-shift operation, there was always an 8-hour period per day when analyses would run but could not be monitored. This meant running finals at risk since you could not physically view system suitability criteria. Now SST data allows me to build the criteria into the run and the software can decide to continue or abort any run. Now I can make use of a whole extra shift."

SAFC's Analytical Group works closely with its Process Development team to create a complete information package with SST results that can be transitioned to GMP production and quality control. Prior to deploying Chromeleon CDS, data was stored on individual chromatography systems without central access, making gathering SST data and generating reports time-consuming. Faley explained, "Previously for a residual solvent analysis of seven to eight solvents, we would transfer all the SST, calibration, and concentration data into controlled Excel spreadsheets for calculations. This could take up to an hour per sequence. Now, Chromeleon CDS pulls the information directly into the report and all we have to do is review and print it. By avoiding the process of taking the data and putting it into Excel, we are saving mountains of time and reducing opportunities for errors."

"With the fully automated workflow provided by Chromeleon, we are now able to run analyses over lunch, evenings, and weekends, so we can analyze more samples with the same number of technicians."

– Rene Spang, Head of Laboratory Mass Spectrometry Service, Bayer Pharma AG



Laboratory instrumentation at Bayer Pharma AG

Streamlines workflows, boosts laboratory efficiency with one CDS

In addition to compliance, streamlining laboratory operations using one centrally implemented CDS for both chromatography and MS workflows enables access to all resource, data, and results from any location. A single CDS also provides considerable efficiency gains through time reductions in training and validation. Chromeleon CDS provides a single platform that integrates chromatography and MS, from instrument control with compliant tuning to reporting. Designed with the user in mind, its smart tools simplify tasks, eliminate manual steps, and reduce errors. Specific capabilities that increase productivity include:

- Fully integrated chromatography and MS workflows in one intuitive solution, reducing the need for staff to be proficient in multiple software packages
- eWorkflow™ procedures, customizable methods, and built-in SST with intelligent run control (IRC)
- Automated chromatography and MS data processing tools for rapid, consistent, high-quality results including Cobra™ Wizard and SmartPeaks™ Integration Assistant, Tentatively Identified Peaks, and Intact Mass Deconvolution capabilities
- Fast, flexible, and integrated data review with MiniPlot™ thumbnails and SmartLink panes to simplify data visualization
- An advanced, spreadsheet-based Report Designer to consolidate data streams from multiple instruments and data types, including MS data, and eliminate calculations outside the CDS

The Cobra peak detection algorithm simplifies integration by providing consistent and reliable peak detection, while the SmartPeaks Integration Assistant guides the chromatographer to correctly integrate rider peaks and other unresolved peaks. Explaining how these tools improve laboratory efficiency at Sterling, Alliston said, "Use of the Cobra Wizard allows for quick setup of optimum integration parameters giving us consistent integration much faster than either of our previous CDS. Before, we were probably a little 'heavy' on manual integration. Chromeleon CDS and the Cobra Wizard have readdressed this balance with manual integration becoming the exception and not the norm."

Said Regis' Hippleheuser, "The MiniPlot data visualization tool in Chromeleon CDS is one of our customers' favorite features. It presents large amounts of data graphically, simultaneously, and clearly. For example, MiniPlots instantly display detailed miniature thumbnail images of chromatograms corresponding to each injection in a list – you can rapidly scan through dozens of injections and immediately compare and identify gross differences. This new tool is a fast and convenient way to keep up with today's deluge of data that demands faster analysis of larger data sets."

"Chromeleon CDS is a very efficient platform for acquiring, processing, and reviewing data. Despite having a large number of samples, we can quickly review results comparing the theoretical masses with the measured masses of our lead candidates. It's very easy to visually process a lot of samples in a very short time."

– Dr. Dan Bach Kristensen, Principal Scientist, Symphogen

Integrates chromatography and MS

Symphogen, an antibody oncology-focused company, selected Chromeleon CDS as an easy-to-use, unified platform to streamline its operations, including processing, reviewing, and reporting of LC-MS data. Symphogen typically analyzes 400 samples per study by native SEC-MS, generating huge amounts of data that must be efficiently processed and reviewed for confirmation. Chromeleon software enables the screening and characterization of intact proteins through the intact protein deconvolution (IPD) tool.

"To process so many samples, it's really nice to have a solid unified platform for acquiring, processing, and reviewing data, which we have with Chromeleon CDS," said Dr. Dan Bach Kristensen, Principal Scientist at Symphogen, "When we do our lead selection studies, the first thing is to determine if our candidate molecules are aggregating and their identities. We can do that in a single experiment with native SEC-UV-MS and Chromeleon software, and it's a matter of seconds screening through the results." Chromeleon CDS provides a single software workflow to view and report identity confirmation and aggregation. Once data are acquired, the software automatically compares the theoretical mass with the experimentally determined mass and presents the results in an easy-to-visualize format making it very easy to review numerous samples in a matter of seconds.

The MS service laboratory of Bayer HealthCare AG also uses Chromeleon CDS to analyze thousands of samples per day using GC, LC, and MS. Describing the reasons for selecting Chromeleon CDS, Rene Spang, Head of Laboratory Mass Spectrometry Service said, "Another big factor in our purchase was the control of both the LC and MS from the same software and the ability to combine the UV and MS data in one report, so I would not have to switch between different software packages for chromatography and mass spectrometry information. We have used the system now for five months and it works very well."

Spang continued, "We have worked with Thermo Fisher Scientific technicians to produce a report that combines the UV and MS data and presents everything my customer needs to see. Chromeleon checks both the positive and negative MS traces for the target mass and will label the peak if a match is found. So now my customers get all the information they need on their sample in just one three-page report. Chromeleon automatically exports these pages to a single PDF report after each analysis."

Built-in methods to complete downloadable workflows

eWorkflow procedures provide a template for creating a complete, correct sequence, ensuring that procedural rules and guidelines are followed. The templates minimize training and can be used with any instrument controlled by Chromeleon CDS, streamlining laboratory workflows. With as little as two mouse clicks, any user can run an eWorkflow procedure to set up and run analyses.

Broughton Laboratories uses eWorkflow procedures to ensure that operators build sequences correctly and use the correct methods and reports. Said Kerry Malone, Team Leader, "Setting up sequences on the LC-MS is really simple and guided through the use of eWorkflows; analysts can come in and select the relevant workflow which contains all the relevant methods which are locked down and validated, only needing to add the samples to the LC as the system automatically brackets samples."

"After a brief familiarization it felt like you could just walk up to the system and accomplish what needed be done without jumping through an excessive number of hoops. You can tell that the software was built for the user's ease. It has a familiar layout with the list of chromatography instruments on the left side."

– Michael Faley, Analytical Supervisor, SAFC, Inc.

Spang described how Bayer HealthCare AG uses a customized eWorkflow procedure: "We have developed an eWorkflow to allow us to quickly create the daily sequence with the correct methods and injection list. We use the sequence start delay function to enable the system to automatically start up each morning at 6:30 am and run a series of injections to ensure everything is running OK before the technicians arrive. We also use advanced programming to automatically shut the system down at the end of the day, or if there is a problem with the system or a QC standard."

Produces various reports without time consuming, error prone transcription

Reporting is easy, fast, and flexible using the built-in, spreadsheet-based Chromeleon Report Designer. Microsoft-Excel-like functionality means that calculations can be easily copied and pasted into the report, simplifying the learning and reporting process. In addition, data remain in a secure environment, eliminating the possibility of transcription errors.

With the previous CDS at Sterling, data was commonly transcribed into spreadsheets to perform calculations. This was inefficient, since all the transcriptions took time and needed to be checked. Alliston explained, "As the Chromeleon CDS report template is basically a spreadsheet, product-specific templates can be set up reporting the exact data needed for each product, removing the need for transcribing and checking data. As you can imagine this saves a lot of time and effort."

Regis' Hippleheuser added, "Even larger is the gain in efficiency from the use of the Report Designer feature for creating reports that can be locked down so that entry of data such as area counts etc. is handled automatically by the system. This has taken what was a two- to three-hour job to less than one hour in most cases. Now all the results come from the Report Designer and Electronic Report features in the Chromeleon software. Everything is in one report, which can be converted to several viewing stills with the click of a mouse."

Provides exceptional usability

Designed with scientists and technicians in mind, Chromeleon CDS minimizes the steps and time needed to perform tasks while making the tasks easy to understand and use. This intuitiveness and speed significantly reduces training requirements and saves huge amounts of time. Describing his first impressions of the software SAFC's Faley said, "After a brief familiarization it felt like you could just walk up to the system and accomplish what needed be done without jumping through an excessive number of hoops. You can tell that the software was built for the user's ease. It has a familiar layout with the list of chromatography instruments on the left side."

Sterling related a similar experience: "Having previously used several 'older' CDS systems, Chromeleon CDS proved to be a very intuitive system. It has a 'familiar feel' which means it's easy to learn. The user interface is simple and clear and everything is where you would expect it to be. Chromeleon CDS is much quicker in all activities.'

Conclusion

Built for compliance and multi-instrument workflow productivity, Chromeleon CDS is meeting the needs of the pharmaceutical industry and supporting CTO, CRO and CMO customers. The software offers proven significant gains in laboratory efficiencies, while delivering everything needed to make it easier to meet evolving regulatory compliance and data integrity requirements. As the first CDS that combines all separation and detection techniques, including MS, into a single compliance-ready and scalable solution, Chromeleon CDS streamlines your chromatography and MS quantitation workflows in one application, enabling you to use your MS like any other routine detector.

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Related case studies

1. Case Study 72207, Sterling Pharma Solutions, Chromeleon CDS delivers efficiency gains and compliance and data integrity improvements to UK CRO/CMO
2. Case Study 80086, Broughton Laboratories, Delivering client success through unique and pre-emptive service – A global analytical GMP business perspective
3. Case Study 70754, Regis Technologies gains significant efficiencies in pharma/biopharma manufacturing
4. Case Study 70797, SAFC Madison, Sigma-Aldrich CMO helps customers comply with 21 CFR Part 11 using Chromeleon CDS software
5. Case Study 73994, Symphogen, Boosting productivity of monoclonal antibody development using Chromeleon CDS
6. Case Study 71783, Bayer Pharma AG implements a fully automated interpretation workflow for finding target masses

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