Streamline your laboratory workflow with Thermo Scientific Chromeleon CDS

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• Industry Challenges
• How can Chromeleon help you?
• Chromeleon and SampleManager LIMS
• Deploying and Administering Enterprise Chromeleon
• Where are we going?
• **Industry Challenges**
• How can Chromeleon help you?
• Chromeleon and SampleManager
• Deploying and Administering Enterprise Chromeleon
• Where are we going?
Industry Challenges

- Demands from your **business** to do more
- **Staff reductions** and **decreasing skills** of your workforce
- Increasing rate of **technology** changes
- Requirement for **data management** and disaster planning
- **Integrating** disparate software systems
Business factors

• Global business trends:
  • Production costs increasing
  • Savings expected in all areas, including software and analysis
  • Increase throughput
  • Faster methods
• Demand to increase speed, flexibility, quality and cost controls
• Efficiency – do more with less
  • Automation and speed to results
• Cloud-based capabilities gaining momentum in analytical industries
  • Driven by big data, computing elasticity, & data security
• IT budgets squeezed, making software update projects harder and more time-consuming
• Global personnel trends:
  • Reduction in numbers of analysts
  • Analyst roles become deskilled
  • Fewer experienced analysts
  • Lower understanding of how to optimize chromatography methods, what choices to make about equipment, what to do if results don’t meet expectations

• Increasing emphasis on simplicity and ease-of-use
  • Reduced training cost/time
  • More streamlined operation

• Driving towards “push button” systems that answer a particular question
• Require simpler integration, more automation, simpler reporting, and minimal ‘human’ review
Global environmental trends:
- Changing source materials, move towards shale gas / oil
- Depleting Helium reserves
  - Requires method translation away from He
- Stricter environmental testing
  - EPA (US) / EEA (Europe) regulations
  - Increased environmental awareness and testing in emerging regions
  - Need for improvement in identifying contaminants
- Greater implementation of continuous production techniques
- Compliance standards and regulations, as will environmental threats, continue to evolve
  - Year-by-year, country-to-country
Data issues

• Data trends:
  • Accuracy
  • Security / integrity
  • Data storage and access
  • Disaster recovery
• What do I do with all this data?
• How do I make it available to users?
• What can I learn from it?
• How can it help me?
Equipment and instrumentation

- Multi-site standardization of equipment and software
- How can I make the most out of my existing instruments?
- How can I ensure that my expensive new instruments will work with my existing system and methods?
- How do I bring new instruments on-line without retraining my analysts?
- High-speed / Fast GC
- Trend towards GC-MS as a more routine tool
  - Q, QqQ, HRAM is becoming robust, reliable and easy enough to use in routine settings
  - Instrumentation cost coming down - need for fast answers going up
  - Growing need for reliability and confidence in the results
What we hear from our CDS customers. . .

- "I need my CDS as simple as can be - the ideal software has a single start button."
- "My lab technicians spent 90% of their time reviewing and double-checking data!"
- "Automation of routine tasks eliminates user errors and improves my result quality"
- "I can't afford my QC being down for hours because of a network problem at 2 AM"
- “I need a CDS that controls all of my instruments”
- "I need simple, intuitive software for my quantitative Mass Spec analysis."
- "I need a future-proofed, cost-effective CDS, but it is a huge undertaking to upgrade and validate a new solution."
- “My boss wants results like they get on TV cop shows”
Industry Challenges

How can Chromeleon help you?

Chromeleon and SampleManager LIMS

Deploying and Administering Enterprise Chromeleon

Where are we going?
Our goal for Enterprise Chromeleon CDS...

To provide you with the software tools to make your life easier

**Reduce** the **effort** required to administer your Enterprise CDS

**Simplify** the **routine tasks** your users have to perform in order to analyse samples

Make it **easier** to achieve fast **results** with minimal user interaction
Single Software Platform

- One software platform for the entire lab
  - Direct control of over 450 modules from 17 different vendors including:
    - Thermo Scientific (LC, IC, GC, MS, Sample Prep)
    - Agilent (LC, GC)
    - Shimadzu (LC, GC)
    - Varian (LC, GC)
    - PerkinElmer (LC, GC)
    - CTC PAL (Sample Prep)

- One location for all your data
- One system to manage
- One reporting tool
  - Reduced training
  - Reduced administration
  - Reduced infrastructure
Automation of routine tasks: Auto-reporting

- Report results immediately a sequence/injection finishes acquiring
- Create and save a report
- Print a report to specified location
- Export results to specified location
- Transfer results to LIMS
- Enforce per instrument
- No manual action required
Automation of routine tasks: Intelligent Run Control

- Intelligent Run Control checks your chromatography and automatically acts upon its findings

- Set up pre-defined tests:
  - Check standard quality
  - Check column performance
  - Spot contaminants / carry-over
  - Out-of-spec components
  - Inconsistent replicates

- Overnight sequences can be automatically managed by Chromeleon – no user action needed

Choose action(s) to be performed, based on the pass/fail result of each test
Automation of routine tasks: Sequence notifications

- Checking for results from multiple instruments is time-consuming
- Un-observed errors reduce productivity
- Automatic notifications inform you when a Sequence has stopped
  - Normal completion
  - Error/abort by instrument
  - Cancelled by user
- Set up different recipients for each type
- Spend less time checking statues
- Let Chromeleon keep you informed
• Industry Challenges
• How can Chromeleon help you?

**Chromeleon and SampleManager LIMS**
• Deploying and Administering Enterprise Chromeleon
• Where are we going?
Chromeleon and SampleManager LIMS link - Introduction

• Bi-directional interface between SampleManager LIMS and Chromeleon CDS
  • Define tests in SampleManager and link with eWorkflows in Chromeleon
  • Creation Chromeleon sequences in SampleManager
  • Check instrument status
  • Acquire, analyse, and review in Chromeleon, approve results and automatically send to SampleManager
  • Acquire, analyse and report results without ever opening Chromeleon
  • Automatically notify the decision-maker and provide them with the report/data they require

• SampleManager LIMS compatibility
  • SampleManager 10.0 SP2 onwards

• Chromeleon Compatibility
  • Add-in Extension to Chromeleon 7.2 SR4 onwards
Chromeleon and SampleManager LIMS link - Overview

Dedicated Explorer Cabinet to see all Chromeleon Link related data and options

Chromeleon Link options are also available from the top menu
Sequences are created in SampleManager and grouped by Instrument, Analysis and Status

Initial sequence status is Uploaded to Chromeleon (V) and the terminal states are Authorized (A) or Cancelled (X)

Authorized
Results Downloaded
In Progress
Uploaded to Chromeleon
Cancelled
Create Sequence from Samples, Tests, Batches or LES

Samples can be selected from dedicated explorer folders to generate a sequence.

The analysis/instrument needs to be selected when using samples.
Chromeleon and SampleManager link - Create Sequence from Samples

The sequence can be reviewed and updated prior to creation in Chromeleon CDS

Create and acquire in SampleManager, without running Chromeleon
Chromeleon and SampleManager link - Creating a Sequence via eWorkflow

Chromeleon eWorkflow™ includes sequence definition capabilities, and can also default sequence names, injection names, volumes etc.

SampleManager data can be slotted into the unknown slots within those eWorkflow sequences.
Chromeleon and SampleManager link – Pull Available Samples into eWorkflow

The link adds a Select Batch/Tests button to eWorkflow wizard, which pulls available samples, standards, blanks from SampleManager directly into Chromeleon.

Create and acquire in Chromeleon, without running SampleManager.
Preparation values captured during an LES execution can be passed into the sequence configured in the Chromeleon mapping.
Chromeleon and SampleManager link – Passing injection preparation parameters

Test parameters created by LES are automatically transferred into the Chromeleon Sequence.
Chromeleon and SampleManager link – Acquiring

Chromeleon adds Sequences to instrument queue and manages the acquisition
Chromeleon client doesn’t need to be opened for this to take place
After the sequence has been run, processed results for each sample are obtained ready to be sent back to SampleManager.
Mapping results can be done in SampleManager - on a per component basis, on everything found, or on everything identified

<table>
<thead>
<tr>
<th>Component Name</th>
<th>Chromleon Name</th>
<th>Expression</th>
<th>Signal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Coliform Positive</td>
<td>Chrom Component A</td>
<td>peak.retention_time</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>peak.retention_time</td>
<td></td>
</tr>
</tbody>
</table>

The expression is a Chromeleon expression and it’s evaluated for each peak and stored in the corresponding result.
Chromeleon and SampleManager link – Report Values

Chromeleon’s Excel-like reports can include complex post-analysis calculations.

SampleManager can also pull values from cells in these reports rather than specifying the expression in LIMS.
Chromeleon and SampleManager link – Report Values

Report templates can be specified in the mapping.

Sheet coordinates may be specified along with any Chromeleon Expression.
After the sequence has been run, processed results can be automatically sent to SampleManager, at a pre-determined stage in the Sequence lifecycle.
SampleManager results are generally for a specific attribute of an identified peak. Mapping options provide control over which attributes map to which components.

Results may be retrieved manually for a sequence.

Result retrieval can be automated via a Watch Dog Timer entry.
Options are available to review and authorise results by sequence.
Chromeleon and SampleManager link - Instrument Status

Dashboard shows all mapped instruments and their current status

Chromeleon property sheet also shows all known Chromeleon Instruments (even if they are not mapped to a SampleManager Instrument)
Chromeleon and SampleManager link – Ready Check

Ready check is performed when a Sequence starts/resumes

User is warned/prevented about:
- Calibration
- Maintenance/service
- Instrument training
- Method/application training

Results of all checks are recorded for every Sequence
Chromeleon and SampleManager link - Benefits

• Sequence Creation, Result Transfer, Sequence management and Instrument status information is provided in both Chromeleon or SampleManager
• Operator can work in either SampleManager LIMS or Chromeleon CDS, whichever they are more familiar with
• Extensive configuration options exist to support both simple sequences and eWorkflows
• Automatic sample parameter and result transfer reduces manual actions and decreases likelihood of manual transcription errors
• Integrating SampleManager’s asset tracking, instrument maintenance schedules, user training records, and sample preparation functionality improves stock management, reduces waste, prevents production delays and facilitates cost savings
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Comprehensive Enterprise software Offering

Chromeleon

CDS
Chromatography & Mass Spectroscopy
Designed for 24/7 operation
Advanced automation for better quality results
Multi-vendor, multi-technique
Support MS for development & QA/QC workflows

Chromeleon XTR
Launched Q1/18

LMS
Chromeleon + Basic Lab and Data Management
Basic sample management and tracking
Analyses can only be performed by authorized, trained individuals on calibrated instruments
Long-term data storage and archival of data regardless of instrument type

Chromeleon & SampleManager

Chromeleon XTR + Complete Laboratory Management
Comprehensive sample, test & result management
Management of lab personnel & resources
Specification management and ERP integration
Configurable to meet your end to end business process

Chromeleon XTR + Basic Lab & Data Management
Basic sample management and tracking
Analyses can only be performed by authorized, trained individuals on calibrated instruments
Long-term data storage and archival of data regardless of instrument type

ThermoFisher Scientific
Chromeleon 7.2 SR5 – Targeted at the Enterprise

Comprehensive Support for Large-Scale Rollout

- Optimized for Large-Scale Installation
  - Windows 10, Oracle 12, MS SQL Server 2016, Citrix 7.15
  - Pre-configure via Command Line Options
  - Built-in Maintenance Window
  - Keeps Track of Running Analysis

Administration Simplicity & Efficiency

- Manage thousands of users and instruments
  - Filter, Group and Report
  - Retire Users
  - Email Notification
  - Resources Overview
  - Consolidated Audit Trail
  - System Health Audit Trail

Meet Increased Compliance Requirements

- Compliance & Data Integrity
  - Latest Connection Security
  - Time Zone Info Everywhere
  - Standardized Comments and Privileged Actions
  - Global Policies and Instrument Configuration Audit Trails
  - Direct Import of Chromeleon 6
  - E-Signatures and CMB

Targeted at the Enterprise
Data Integrity

• Secure Data Vault structure
  • Chromeleon Data Vaults are configured so that they can’t be accessed by non-Chromeleon means

• Detect Manipulations on Raw Files
  • Chromeleon automatically detects if raw files have been manipulated

• Data Transport Security
  • Communication is secured by latest standards using SHA-256 and TLS 1.2

• Emerging Standard Requiring User Logoff and Tracking Network related Events
  • Chromeleon captures user events, including logon/logoff in the user management audit trail
  • Permanently stores network interruptions, run abortions etc in new „station“ audit-trail
Simple Administration – Chromeleon Domain Resources

Detailed overview of your entire system - Instruments, Data Vaults, Computers, Consoles, All Resources

Easily see how many Chromeleon sessions are currently open
Filter, Group and Report
Context menus for additional actions
Simple Administration: System Printers

• Chromeleon’s System Printers ensure that printers are:
• Available to all users / clients
• Configured correctly
• Don’t require drivers to be installed on every client

Identify a Chromeleon server to act as a Chromeleon System Printer Server
Define one or more of its printers as System Printers
Chromeleon automatically makes these available to clients

If you move or replace the printer, simply edit the System Printer
One action
All Clients, Report Templates, Sequences are automatically updated

Users can run Chromeleon from any client and still be able to access their printer(s)
Keeping productivity high – Performance Testing

- Thoroughly tested up to the limits of our test network
- Test Network for Data Acquisition
  - 125 IPCs with 4 simulated instruments each (LC incl. DAD, GC, MS)
  - Simultaneous run / acquisition of 500 instruments acquiring data to one DataVault (without load balancing) succeeded
- Tested stress cases, e.g. power cycle of Data Vault Server
- Targeted usability testing
- Test Network for Domain Controller
  - 8 VMs simulating 600 clients / IPCs, running test harnesses for licensing, user management with 1600 users and discovery
Keeping productivity high – Maintenance Windows

• Maintenance Windows ensure that:
  • Administrator can define a time for scheduled maintenance
    • Windows Updates
    • Chromeleon Updates
    • Instrument Maintenance / Calibration
  • During the window, connected instrument(s) will not be acquiring

Define a Start and End time/date and notification period
Deploying software in the cloud can provide many benefits:
- Flexibility, disaster recovery, maintenance, cost, expandability

Chromeleon now supports deployment of server-side components on cloud-based servers:
- Chromeleon Domain Controller
- Chromeleon Data Vault Server
- Chromeleon Clients (similar to Terminal Server installation)

Supported from Chromeleon 7.2.9 and Chromeleon 7.2 SR5 MUg

* Warning: requires a suitable, reliable network connection

* This slide contains forward-looking statements based on current expectations and assumptions which involve risks and uncertainties that could cause actual results to vary materially from those stated or implied.
Flexible Deployment – 247 Instrument Controller

- Large disparate Enterprise systems
  - Instruments widely distributed (across buildings, sites, countries)
  - Servers housed in Data Center or Cloud
  - Users accessing via a range of clients

- Instruments still require a physical connection into Chromeleon domain
  - Secure
  - Low maintenance
  - Centrally managed
  - Inaccessible to users
What is the 247 instrument controller?

Secure network device for connecting instruments into a Chromeleon domain
Dedicated to one purpose - handling communication to/from Chromeleon instruments

- Communicates with instruments
- Downloads instrument methods
- Updates clients with live status
- Buffers acquiring data
- Transfers data to Data Vault and Chromeleon Clients
So it's just an IPC, right?

Think again… the 247 IC has a number of unique features which make it very different from an IPC

- Secure
- Compact, fits anywhere, saves bench space
- Low management
- Reliable
- Designed and validated exclusively for our software
I’m interested….what else?

Unlike a PC, the 247 IC has been designed specifically for controlling laboratory instruments in an Enterprise CDS:

- Custom-built operating system
- Inaccessible to users – no chance of user ‘meddling’
- TCP/IP hardened – open only for Chromeleon
- Low maintenance
- Large data buffer – collects data if network down
- High mean time to failure
  - Solid-state drive
  - Off-board power
  - 10 year old devices in daily use
- Connections for all GC, LC and IC instruments
- Fully validated by Thermo Fisher Scientific
What about Virtual and Cloud?

The 247 Instrument Controller handles all instrument communication, allowing Enterprise Chromeleon Clients to be distributed via traditional desktop PCs, virtualised platforms, Cloud, or mobile devices.
What about updating with new versions of Chromeleon?

Our technology is always developing to make deployment and management of your Enterprise Chromeleon system even easier

- Manage 247 Instrument Controllers from Admin Console
  - Check installed Chromeleon version
  - Select 247s to update
  - Select Maintenance Window time and date
  - Automated Background Download of Setup kit
  - Automatic update of Chromeleon*
  - Managed by Windows Service
  - No interactive Administrator logon required
Flexible Deployment – Automated roll-out of software updates

Define maintenance window and select an available Chromeleon version

Choose the 247 Instrument Controllers to update

Monitor download progress
Disaster recovery – Read-Only Data Vault

• Use Cloud services to create a read-only shadow copy of the Data Vault
  • Automatically copy all changes to the database into a cloud hosted database instance
  • Automatically copy all changes to raw files into the cloud

• Technically this is done independently of Chromeleon
  • The cloud hosted instance of the database and files can be mounted as a read-only Data Vault

• In case of an on-site disaster, all data (including methods, templates, etc) can be recovered from the Cloud-based Data Vault

• A case study is in progress. This will be used as a basis for documenting how this can be done
Simplifying the installation process

- Chromeleon Installation and Qualification Services
  - Global team of experts to guide you through an installation / upgrade
  - Services Engineer time (on-site or remote) available at every stage of deployment
  - Range of document templates covering every stage of a CDS implementation
  - Purchase templates singly or as a complete Installation and Qualification kit
  - At each stage, choose the level of input required by our services team to:
    - Prepare documents
    - Perform installation steps
    - Perform qualification testing

- Let our trained installation engineers help you from initial planning to final sign-off
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- Where are we going?
• Connect Chromeleon to InstrumentConnect in a generic way so that all instruments connected to Chromeleon become accessible via Thermo Fisher Cloud

• Allow users to monitor their instrument remotely via web browser and from their phone using the Instrument Connect App

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Some of our customers want to utilize a hosted version of Chromeleon in a similar fashion like we use Office 365.

The goal is to create a comprehensive cloud offering of Chromeleon.

Making Chromeleon securely accessible from anywhere.

Without the effort of managing physical server assets.

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Summary

- Need for professional installation services
- Demand to do more with less
- Fast pace of technology change
- More emphasis on data management and disaster planning
- Need for more automation and connectivity between software tools
- New deployment models becoming standard
- Connecting distributed instruments with the 247 Instrument Controller
- New tools for managing your Chromeleon domain

Chromeleon CDS has the tools and services to streamline your workflow, save you time, and improve your productivity
Thank You – Any Questions?

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