Chromeleon 7.2 CDS
The Easiest Way to Boost Your IC Productivity

Mississauga, ON, 10/13/15
Carl Fisher, Ph.D, Application Scientist
40th Anniversary of Ion Chromatography

Congratulations!
Agenda

• Introduction
  • Thermo Scientific™ Dionex™ Chromeleon Chromatography Data System (CDS) software at a Glance
• Chromeleon CDS – A Closer Look
• eWorkflows
  • IC Chromatography at its simplest and most powerful
• Intelligent Run Control
• Virtual Column
  • A Simple and Effective Tool for Method Development
• AppsLab
  • An Invaluable Resource for IC Applications
The Quickest Way from Samples To Results

eWorkflows automate all chromatography

Future proof architecture

For all instruments

Dynamic data processing

Unmatched reporting

Built for Compliance
• Streamline your laboratory – use one CDS to control all chromatography instruments and process and report all data:

• Reduced training effort for the laboratory staff – one single software package instead of several

• All your chromatographic instruments, including MS in one software

• Highest laboratory uptime and prevention of data loss through Operational Security and secure XVault infrastructure

• Lower operating cost with centralized management of one single software

• Interface with LIMS, SDMS or ELN for seamless workflows
• Chromeleon CDS provides the ultimate solution for third party instrument control providing:
  • “Printer driver” plugin concept
  • Integration of wrapped driver plugin solutions from leading instrument manufacturers
    • Agilent Instrument Control Framework (ICF)
    • Waters Instrument Control Software (ICS)
  • Driver Development Kit (DDK)
    • Used by Thermo Fisher Scientific for all internal driver development
    • Available to other suppliers for driver development

• Chromeleon CDS supports over 400 different modules from 18 different manufacturers
Chromeleon is Built for Compliance

Chromeleon CDS meets all of your regulatory compliance needs with:

- Multi-tiered security for controlling access with comprehensive user management tools
- Comprehensive tracking of all actions without hindering workflow
- History views of objects track changes and easily revert to prior versions
- Complete record management with direct access to meta-data and full electronic signature support
- Powerful built-in, automated qualification tools for all aspects of system operation
Network Capabilities - Client/Server Architecture

Chromeleon Domain

Stand-Alone Workstation
Remote Client or TS Client
File/Database Server
Chromeleon Domain Controller (CDC)
Citrix / WTS Server
Mobile Client
Internet
VPN
Firewall

Laboratory Workstation
IC
Laboratory Workstation
LC/MS
Instrument Controller

VPN
Some of the ~ 10,000 Chromeleon Accounts
Chromeleon CDS – A Closer Look
The Chromeleon CDS User Interface consists of two major parts:

- **Chromeleon Console**
  - Designed to provide easy navigation through your data

- **Chromatography Studio**
  - Used for all data evaluation
Familiarity – Similar to Microsoft® Outlook®

Test e-mail #10
van Cann, Barbara on behalf of software.softrotnsupport

Sent: Mon 07-Oct-13 14:16
To: van Cann, Barbara

This is a test e-mail to show the similarity of the Chromelon Console and Microsoft® Outlook®.
Chromeleon CDS Console

Navigation Pane

Category Bars
Integrated Sequence Editor

Direct modification of Injection List
MiniPlots – Quick Access to Data

See if chromatogram ran properly

Presence/absence of peaks

Quality of separation
### Result Formula Columns – Quick Access to Results

- **View results without opening sequence data**
- **Immediate SST result check**
Category Bars – Easy Access

Control your instruments via intuitive ePanels
Comprehensive Instrument Control - ePanels

• All controls available on device ePanels

Select device ePanel
Access Audit Trail and Queue

ePanel tabset
All controls available
Chromatography Studio

Ribbon

Navigation Pane

Category Bars

All details of an experiment
Familiarity – Spreadsheet Based Reporting
Work with multiple objects at the same time
Easier Processing Method Setup
Creating your component table can be time consuming and error prone
• Setting correct integration parameters can be a laborious trial and error process
• Setting up calibration levels can be an unintuitive, complex procedure
• Updating component retention times as peaks drift is often a lengthy, manual activity, especially when many peaks are present.

Chromeleon CDS offers a suite of functionality to simplify and speed up processing method creation including:
• A component table wizard
• Cobra™ peak detection algorithm and wizard
• SmartPeaks™ Integration Assistant
• Fast, intuitive calibration level creation
• One-click retention time updating
Unique tool for easily reaching your integration goals for unresolved peaks

Requires no training

Great example of Operational Simplicity

- Process is clear and understandable
- Requires only a few steps
- Correctly integrates all unresolved peaks in seconds
1. Activate SmartPeaks Wizard

2. Select Area of Interest

3. Select the Integration You Want
Peak Detection – SmartPeaks Integration Assistant

- Parameters added to component table
- Changes apply to ALL chromatograms in sequence

Your integration is done!
eWorkflows
How do you ensure that your sequence is created and structured correctly? How do you know you have the right methods and report?

- **eWorkflows** for fast, easy, accurate sequence creation. They contain:
  - Instruments on which the analysis can be run
  - **All** associated files:
    - Instrument methods
    - Processing methods
    - Reports
    - Spectral libraries
    - External documents (e.g., SOP)
  - Template for sequence name and storage location
  - Custom variables
  - Rules for sequence layout
eWorkflows - Controlled Sequence Creation

- eWorkflows make it easy for anyone to run analyses

Select eWorkflow, instrument and launch

Set no. of samples and start position

Rack and sequence preview
eWorkflows - Controlled Sequence Creation

- eWorkflows are the fastest way from sample to results with minimal effort and training

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With a few mouse clicks sequence is created and is ready to run

All required files are included
eWorkflows – From Samples to Final Report

- Including automatic creation of final report
Can you react to changing conditions during the sequence? What if your RTs drift or the %RSD is out of spec? Can you re-inject a bad injection?

Usually left to analyst to decide – subjective and often too late.

Conditional system suitability tests (SST) with Intelligent Run Control (IRC)

Allows decisions to be made during run:
- Insert Injections
- Re-inject
- Perform arithmetic processes
- Extract Channels or optimum integration from a PDA 3D field

Can be performed Conditionally or Unconditionally

Includes error handling
Run-time Sequence Control – IRC

• Any measurable parameter can be monitored and reacted to using built-in SSTs
• Can also check results against specifications
Run-time Sequence Control – IRC

- Configure pass and/or fail actions – multiple actions are possible

Select required action
Specify multiple actions
Set pass and/or fail actions
Built in error handling
Run-time Sequence Control – IRC

- Example: Autodilute if peak amount falls outside of calibration range

- SST and IRC ensure you get more right first time analyses
Virtual Column Separation Simulator
IC Method Development

• Wide range of analytes, for which to identify the best:
  • Column
  • Eluent
  • Separation Conditions

• This is Consuming
  • Time – Preparing and Running Instruments
  • Material – Columns, Eluent, Samples, Instrument Wear
  • Analysis Time – Occupying Instrument Time

• Difficult to find true optimum
Virtual Column Separation Simulator

- Determine the best column and separation conditions
  - Takes just a few minutes
  - No need to turn on your instrument
- Virtual Column models behavior of IC separations
- Simply choose:
  - Analytes to separate
  - Column
  - Eluent type
- Virtual Column displays:
  - Expected chromatogram
  - Resolution map - Indicating eluent condition producing best separations
Thermo Scientific™ AppsLab™ Library of Analytical Applications:

- … is an on-line search engine for Thermo Scientific applications
- … provides comprehensive application information and ready-to-run analytical methods (‘one click workflows’).
- … is a central repository for Thermo Scientific chromatography and MS application information

- [www.thermoscientific.com/appslab](http://www.thermoscientific.com/appslab)
- Google Type Search to find analysis parameters
- Filter results to narrow down the list of applications
- View and download all application details
- Run the application immediately
Summary
Summary

• Chromeleon CDS provides a familiar environment
  • Minimize training time and lower costs
• Easier method setup and results analysis
  • Chromeleon CDS offers a suite of functionality to simplify and speed up everything from method generation to final analysis of chromatographic results
• eWorkflows
  • Ensure fast, easy sequence creation with correct structure, methods and reports
• Virtual Column
  • Eliminate the risks, hassles and costs in optimizing IC separations
• AppsLab
  • Quickly find applications of interest; download and start running immediately
• Chromeleon’s unparalleled ease of use and scalable architecture makes lab work easier and more enjoyable with one CDS for the entire lab