



ThermoFisher
S C I E N T I F I C

Welches Chromatographie-Datensystem ist das Richtige für mich?

Matthias Hrobarsch
Chromleon Support Specialist
Thermo Fisher Scientific, Dreieich

The world leader in serving science

- Innovative Benutzeroberfläche
- Universelle Instrumentensteuerung
- Erfolgreiches Starten von Analysen
- Datenbearbeitung – schnell und zuverlässig
- Arbeiten im regulierten Umfeld



- **Innovative Benutzeroberfläche**
- Universelle Instrumentensteuerung
- Erfolgreiches Starten von Analysen
- Datenbearbeitung – schnell und zuverlässig
- Arbeiten im regulierten Umfeld



Thermo Scientific™ Dionex™ Chromeleon™ 7.2 SR4 Chromatography Data System (CDS) Software

- „**Operational Simplicity**“ by Design
 - Reduzierung der Anzahl an Schritten, um etwas Bestimmtes zu erreichen
 - Alle Schritte sind leicht zu verstehen und zu bedienen
 - Schnell zu einem Ergebnis
- Drei Hauptmerkmale von **Operational Simplicity**:
 - Intuitives Aussehen und „Gefühl“
 - Peak Erkennung mit Cobra- und Smart Peaks Assistent
 - eWorkflows™ (automatischer Arbeitsablauf)

Schnell und einfach von der Probe zum Ergebnis

Chromeleon Chromatography Studio- alle Informationen im Blick

The screenshot displays the Chromeleon Chromatography Studio interface for a '20130311 Water Analysis' sequence. The main window shows a chromatogram with seven peaks labeled 1 through 7. The x-axis represents time in minutes (0.0 to 12.5), and the y-axis represents signal intensity in μS (-5.0 to 25.0). The peaks are identified as: 1 - Fluoride (2.063 min), 2 - Chloride (3.277 min), 3 - Nitrite (3.963 min), 4 - Bromide (5.853 min), 5 - Nitrate (6.807 min), 6 - Phosphate (9.297 min), and 7 - Sulfate (11.523 min).

Below the chromatogram is a data table with the following columns: Peak No., Peak Name, Ret. Time (min), Amount (mg/L), Rel. Area (%), Area ($\mu\text{S} \cdot \text{min}$), Height (μS), Type, Width (50%) (min), Asym. EP, Resol. EP, and Plates EP.

Peak No.	Peak Name	Ret. Time (min)	Amount (mg/L)	Rel. Area (%)	Area ($\mu\text{S} \cdot \text{min}$)	Height (μS)	Type	Width (50%) (min)	Asym. EP	Resol. EP	Plates EP
4	1 Fluoride	2.063	4.0258	7.22	0.6232	7.54	BMB	0.071	1.31	8.74	4674
5	2 Chloride	3.277	19.6986	26.17	2.2599	21.71	BMB	0.093	1.08	3.85	6910
6	3 Nitrite	3.963	19.7425	14.61	1.2612	9.66	BM	0.118	1.11	7.78	6285
7	4 Bromide	5.853	19.8716	9.86	0.8512	4.61	M	0.169	1.12	3.01	8659
8	5 Nitrate	6.807	19.8562	12.37	1.0680	4.73	M	0.205	1.23	5.84	6090
9	6 Phosphate	9.297	39.7254	13.15	1.1358	3.50	BM	0.298	1.14	4.03	5389
10	7 Sulfate	11.523	19.6236	16.63	1.4360	3.75	MB	0.354	1.07	n.a.	5876
11	Maximum		39.7254	26.17	2.2599	21.71		0.354	1.31	8.74	6910
12	Minimum		4.0258	7.22	0.6232	3.50		0.071	1.07	3.01	4674
13	Sum		142.5437	100.00	8.6353	55.49					

The interface also includes a 'Data Processing' sidebar with options for Injections, Channels, and Components. The 'Injection List' shows 10 injections, including 'Seven Anion Standard II' and 'Drinking Water'. The 'Instrument Method' is 'ECD_1'. The 'Data Processing' section is currently active, showing a 'Data Processing Home' view with various tool icons for Chromatogram, Calibration Plot, and Interactive Results.

Chromeleon Chromatography Studio- alle Informationen im Blick

Multifunktionsleiste

The screenshot displays the Chromeleon Chromatography Studio interface for a '20130311 Water Analysis' sequence. The main window shows a chromatogram with seven peaks labeled 1 through 7, corresponding to Fluoride, Chloride, Nitrite, Bromide, Nitrate, Phosphate, and Sulfate. The x-axis represents time in minutes (0.0 to 12.5), and the y-axis represents signal in μS (-5.0 to 25.0). A multifunction toolbar at the top provides access to various tools like Injection, Results, Calibration, and Chromatogram. On the right, several calibration plots are visible, showing the relationship between concentration (mg/L) and signal ($\mu\text{S}/\text{min}$) for each ion.

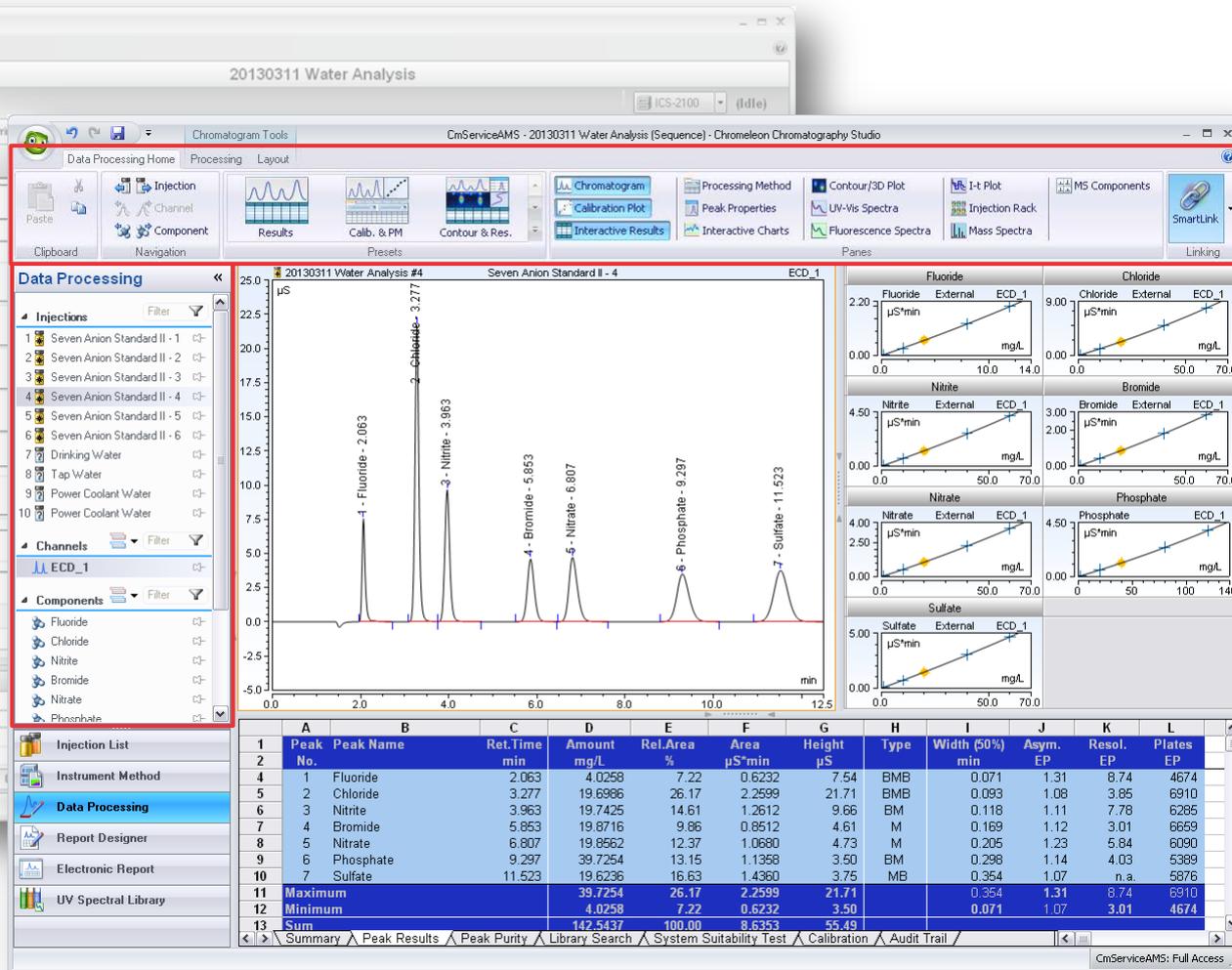
Below the chromatogram is a detailed results table:

Peak No.	Peak Name	Ret.Time min	Amount mg/L	Rel.Area %	Area $\mu\text{S} \cdot \text{min}$	Height μS	Type	Width (50%) min	Asym. EP	Resol. EP	Plates EP
1	Fluoride	2.063	4.0258	7.22	0.6232	7.54	BMB	0.071	1.31	8.74	4674
2	Chloride	3.277	19.6986	26.17	2.2599	21.71	BMB	0.093	1.08	3.85	6910
3	Nitrite	3.963	19.7425	14.61	1.2612	9.66	BM	0.118	1.11	7.78	6285
4	Bromide	5.853	19.8716	9.86	0.8512	4.61	M	0.169	1.12	3.01	8659
5	Nitrate	6.807	19.8562	12.37	1.0680	4.73	M	0.205	1.23	5.84	6090
6	Phosphate	9.297	39.7254	13.15	1.1358	3.50	BM	0.298	1.14	4.03	5389
7	Sulfate	11.523	19.6236	16.63	1.4360	3.75	MB	0.354	1.07	n.a.	5876
11	Maximum		39.7254	26.17	2.2599	21.71		0.354	1.31	8.74	6910
12	Minimum		4.0258	7.22	0.6232	3.50		0.071	1.07	3.01	4674
13	Sum		142.5437	100.00	8.6353	55.49					

Chromeleon Chromatography Studio- alle Informationen im Blick

Multifunktionsleiste

Navigationsleiste

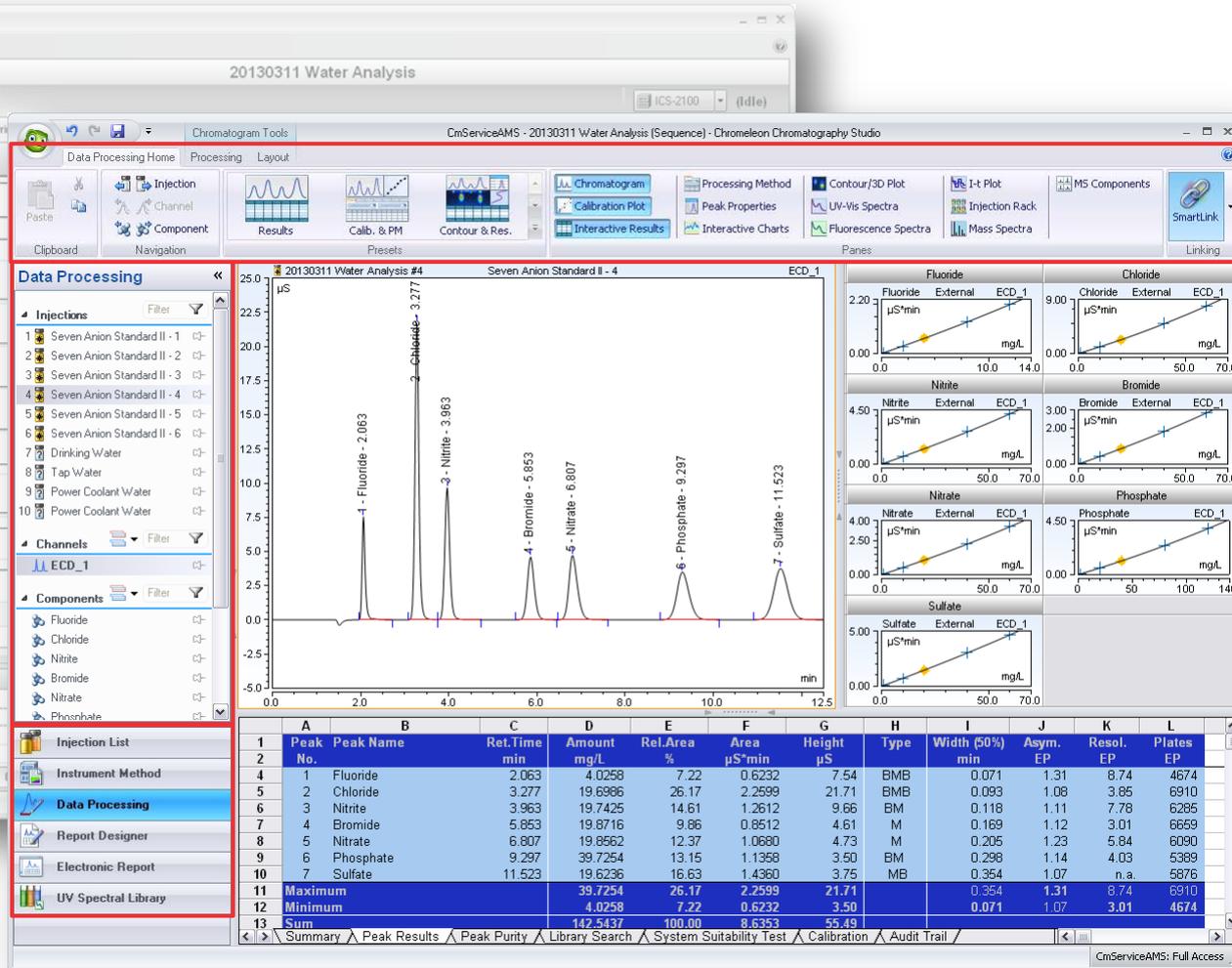


Chromeleon Chromatography Studio- alle Informationen im Blick

Multifunktionsleiste

Navigationsleiste

Kategorie-Schaltflächen

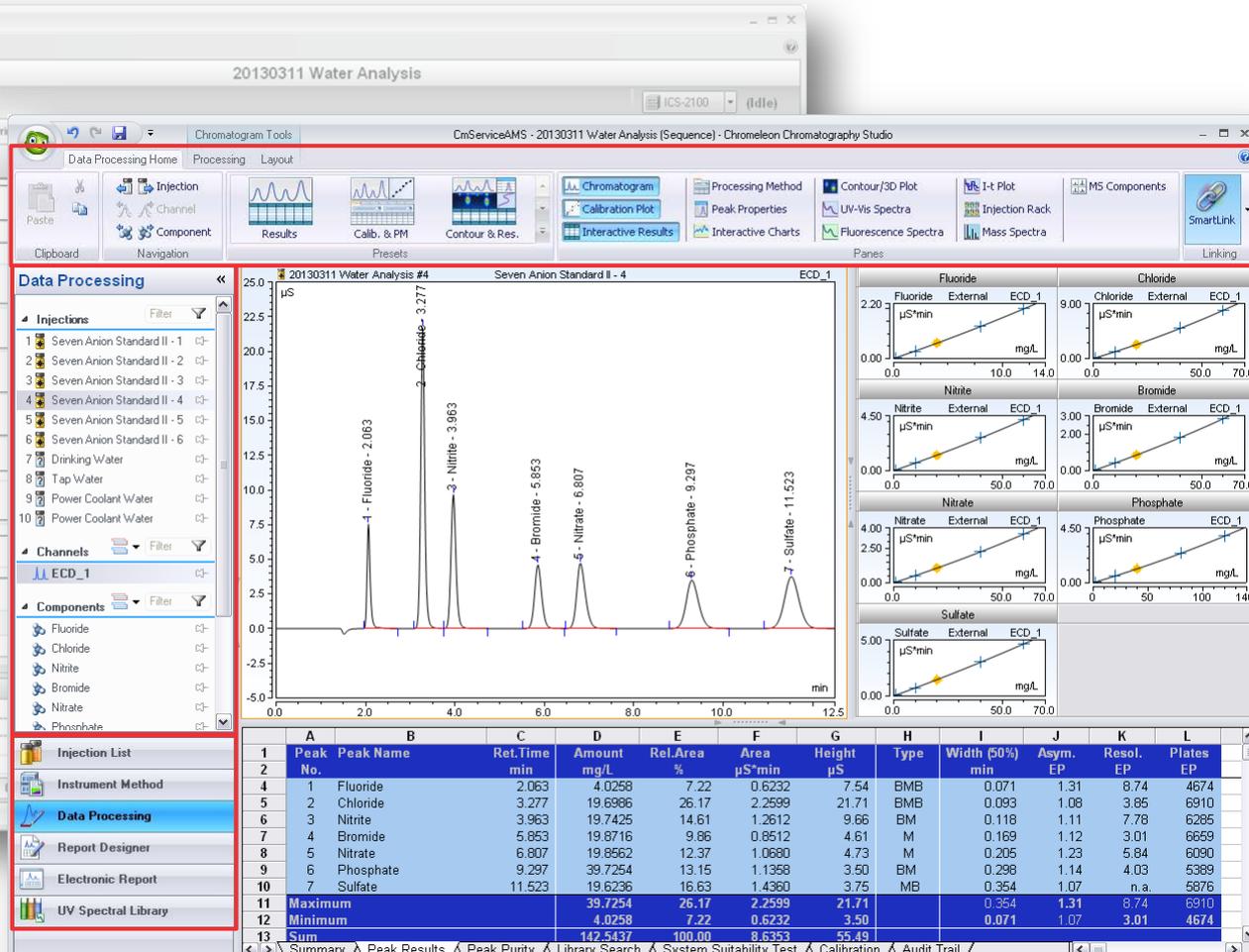


Chromeleon Chromatography Studio- alle Informationen im Blick

Multifunktionsleiste

Navigationsleiste

Kategorie-Schaltflächen



Alle Details Ihrer Daten

Ergebnisspalten – Schneller Zugriff auf Ergebnisse

20130311 Water Analysis

Run Finished ICS-2100 (Idle)

Save Studio Print Up Insert Row Fill Down Lock Filtering Grouping Custom Columns Find Next

#	ECD_1	Name	Type	Level	Position	Volume [μl]	#Amount [mg/L] Chloride [ECD_1]	#Chloride Amount Test [ECD_1]	Processing Me
1		Seven Anion Standard II - 1	Calibration Standard	01	RA1	25.0	0.141	Not Executed	AS12A Anions
2		Seven Anion Standard II - 2	Calibration Standard	02	RA2	25.0	0.858	Not Executed	AS12A Anions
3		Seven Anion Standard II - 3	Calibration Standard	03	RA3	25.0	9.330	Not Executed	AS12A Anions
4		Seven Anion Standard II - 4	Calibration Standard	04	RA4	25.0	19.699	Not Executed	AS12A Anions
5		Seven Anion Standard II - 5	Calibration Standard	05	RA5	25.0	40.610	Not Executed	AS12A Anions
6		Seven Anion Standard II - 6	Calibration Standard	06	RB1	25.0	59.798	Not Executed	AS12A Anions
7		Drinking Water	Unknown		RB2	25.0	3.269	Passed	AS12A Anions
8		Tap Water	Unknown		RB3	25.0	12.887	Failed	AS12A Anions
9		Power Coolant Water	Unknown		RB4	25.0	n.a.	NA -> Passed	AS12A Anions
10		Power Coolant Water	Unknown		RB4	25.0	0.018	Passed	AS12A Anions

Click here to add a new injection

Injection Peak View

Ergebnisse anzeigen
ohne Öffnen der Probe

Sofortige Kontrolle
des Systemtests

Darstellung – Reporting mittels Rechenblatt

CmServiceAMS - 20130311 Water Analysis (Sequence) - Chromeleon Chromatography Studio

Home Insert Page Layout

Paste Injection Channel Component

Clipboard Navigation

Font Arial 10

Alignment

Number % 000

Cells & Sheets

Editing

Protection

Ext. References

Formulas

Linking

Show Formulas

Check for Errors

SmartLink

Report Designer

Injections

- Seven Anion Standard II - 1
- Seven Anion Standard II - 2
- Seven Anion Standard II - 3
- Seven Anion Standard II - 4
- Seven Anion Standard II - 5
- Seven Anion Standard II - 6
- Drinking Water
- Tap Water
- Power Coolant Water
- Power Coolant Water

Channels

ECD_1

Components

- Fluoride
- Chloride
- Nitrite
- Bromide
- Nitrate
- Phosphate
- Sulfate

Injection List

Instrument Method

Data Processing

Report Designer

Electronic Report

UV Spectral Library

C80

Chromatogram and Results

Injection Details

Injection Name:	Seven Anion Standard II - 4	Run Time (min):	12.50
Vial Number:	RA4	Injection Volume:	25.00
Injection Type:	Calibration Standard	Channel:	ECD_1
Calibration Level:	04	Wavelength:	n.a.
Instrument Method:		Bandwidth:	n.a.
Processing Method:	AS12A Anions in Water	Dilution Factor:	1.0000
Injection Date/Time:	02-May-02 13:20	Sample Weight:	1.0000

Chromatogram

20130311 Water Analysis #4 Seven Anion Standard II - 4 ECD_1

Integration Results

No.	Peak Name	Retention Time min	Area $\mu\text{S}^*\text{min}$	Height μS	Relative Area %	Relative Height %	Amount mg/L
1	Fluoride	2.063	0.623	7.544	7.22	13.59	1.0258
2	Chloride	3.277	2.260	21.709	26.17		
3	Nitrite	3.963	1.261	9.661	14.61		
4	Bromide	5.853	0.851	4.606	9.86		
5	Nitrate	6.807	1.068	4.728	12.37		
6	Phosphate	9.297	1.136	3.497	13.15		
7	Sulfate	11.523	1.436	3.748	16.63		

Overview Integration Calibration Peak Analysis SST Summary Audit Trail Chrom

Vertraute Ansicht und Funktionalität

- Innovative Benutzeroberfläche
- **Universelle Instrumentensteuerung**
- Erfolgreiches Starten von Analysen
- Datenbearbeitung – schnell und zuverlässig
- Arbeiten im regulierten Umfeld



- Chromeleon verwendet ein Druckertreiber Plug-In Konzept zur eigenen Gerätesteuerung und der von Drittanbietern
- Standardisierte Gerätesteuerung für Thermo Scientific und 3rd Party Instrumenten über das Chromeleon Driver Development Kit (DDK)
 - Von Thermo Fisher Scientific für alle internen Treiberentwicklungen verwendet
 - Für andere Hersteller zur Treiberentwicklung verfügbar
 - Integration von Treiber Plug-In Lösungen führender Gerätehersteller
 - Agilent Instrument Control Framework (ICF)
 - Waters Instrument Control Software (ICS)
- Chromeleon unterstützt über 400 unterschiedliche Module von 18 verschiedenen Herstellern

Chromeleon für die Massenspektroskopie



Thermo Scientific™
ISQ™ Series GC-MS



Thermo Scientific™ Q
Exactive™ MS

- Client-Server Architektur
- Einmalige Bedienerfreundlichkeit
- Fremdgerätesteuerung
- Umfangreiche Compliance Tools



- über 30 Jahre MS Erfahrung
- Spitzentechnik im MS Portfolio
- Hohe MS Applikationsexpertise
- Integrierte MS Gerätetreiber



Das CDS mit integrierter MS-Funktion für den Routinealltag!

- Innovative Benutzeroberfläche
- Universelle Instrumentensteuerung
- Erfolgreiches Starten von Analysen**
- Datenbearbeitung – schnell und zuverlässig
- Arbeiten im regulierten Umfeld



Mehr “Right First Time” Analysen

- Workflow Automatisierung mittels eWorkflows
 - Erstellen und automatisches Starten von Analysen nach eigenen SOP´s mit wenigen Mausklicks
- Sequence Ready Check
 - Statuskontrolle der Sequenzen gewährleistet korrekten Start
- Sicherstellen der Messbereitschaft
 - Instrument Smart Startup sichert kontrollierte Bedingungen vor der Datenaufnahme
- Entscheidungen während der Datenaufnahme
 - Integrierte System Suitability Tests mit Intelligent Run Control übernehmen automatisch innerhalb der Sequenz Aktionen, basierend auf den aktuellen chromatographischen Ergebnissen



- eWorkflows automatisieren / vereinfachen
 - alle chromatographischen Prozesse
 - LC / IC / GC / MS
 - Routine & Methodenentwicklung
- In wenigen Schritten von der Probe zum Ergebnis
- **Operational Simplicity™** - Design

- eWorkflows stellen sicher, dass die SOP befolgt wird
- Verringert Fehler
- Produziert schneller zuverlässige Ergebnisse
- Wird auf die Applikation angepasst
 - QA/QC
 - Methodenentwicklung
 - Research & Development
- Minimaler Aufwand an Training durch hohe Automatisierung

- Definition der eWorkflows
 - Auswahl des Instruments
 - Alle notwendigen Dateien vorhanden
 - Instrumentenmethode, Auswertemethode
 - Reports, Spektrenbibliotheken
 - Zusätzliche Anhänge, wie z.B. PDFs, Excel-Dateien, etc.
 - Sequenzname und Speicherort können vorgegeben werden
 - Custom Variables, Benutzerdefinierte Variablen (Custom Variables)
 - Sequenzlayout festlegen

eWorkflows – Erfolgreiches Starten von Analysen

cmadmin - Chromeleon Console

Back Create File Edit View Tools Help

eWorkflows

Filter

ChromeleonLocal

- CUT Templates Stage 1 (10 units)
- CUT Templates Stage 2 (+20 units)
- Demo_eWorkflow
- Dissolution Templates
- GPC Templates
- ICH Accuracy
- ICH Intermediate Precision
- ICH Linearity
- ICH Linearity-2
- ICH LOD LOQ (Blank SD)
- ICH LOD LOQ (Curve)
- ICH LOD LOQ (SN)
- ICH Repeatability
- ICH Robustness
- ICH Specificity (PP)
- ICH Specificity (RS)

Instruments

Data

eWorkflows

CUT Templates Stage 1 (10 units)

Description: This eWorkflow contains all files required for performing Content Uniformity calculations FOR THE FIRST 10 INJECTIONS. Please refer to attached user manual for more information.

Type: HPLC

Status: Approved for Use

CUT Demo Data.cmbx CUT Templates - User Manual.pdf

Launch < Run 'CUT Templates Stage 1 (10 units)' using instrument 'UltiMate3000' > Edit

#	Instrument Name	Instrument Status	Sequence Status	Queue Status
1	01_ICS-5000+	Monitoring Baseline	Manual (Injection: 1 of 1)	
2	02_ICS-5000_Dual_1	Idle		
3	03_ICS-5000_Dual_2	Idle		
4	UltiMate3000	Idle		
5	UltiMate3000_RS	Idle		Pending sequences: 1

eWorkflow 'CUT Templates Stage 1 (10 units)' selected

cmadmin: Full Access

eWorkflows – Erfolgreiches Starten von Analysen

1. eWorkflow auswählen

CUT Templates Stage 1 (10 units)

Description: This eWorkflow contains all files required for performing Uniformity calculations FOR THE FIRST 10 INJECTIONS. Please refer to the user manual for more information.

CUT Demo Data.cmbx | CUT Templates - User Manual.pdf

Launch < Run 'CUT Templates Stage 1 (10 units)' using instrument 'UltiMate3000' > Edit

#	Instrument Name	Instrument Status	Sequence Status	Queue Status
1	01_ICS-5000+	Monitoring Baseline	Manual (Injection: 1 of 1)	
2	02_ICS-5000_Dual_1	Idle		
3	03_ICS-5000_Dual_2	Idle		
4	UltiMate3000	Idle		
5	UltiMate3000_RS	Idle		Pending sequences: 1

eWorkflow 'CUT Templates Stage 1 (10 units)' selected | cmadmin: Full Access

eWorkflows – Erfolgreiches Starten von Analysen

The screenshot displays the Chromeleon Console interface. On the left, the 'eWorkflows' tree is expanded to 'ChromeleonLocal', showing a list of workflows including 'CUT Templates Stage 1 (10 units)'. The main panel shows the details for 'CUT Templates Stage 1', including a description and a 'Launch' button. Below the launch button is a table of instrument sequences.

#	Instrument Name	Instrument Status	Sequence Status
1	01_ICS-5000+	Monitoring Baseline	Manual (Injection: 1 of 1)
2	02_ICS-5000_Dual_1	Idle	
3	03_ICS-5000_Dual_2	Idle	
5	UltiMate3000_RS	Idle	Pending sequences: 1

Two yellow callout boxes are overlaid on the interface:

- 1. eWorkflow auswählen
- 2. Instrument wählen

A white callout box highlights the 'UltiMate3000' instrument name in the table.

At the bottom of the console, the status bar shows 'eWorkflow 'CUT Templates Stage 1 (10 units)' selected' and 'cmadmin: Full Access'.

eWorkflows – Erfolgreiches Starten von Analysen

1. eWorkflow auswählen

2. Instrument wählen

3. Launch anklicken

#	instrument name	Instrument Status	Sequence Status
1	01_ICS-5000+	Monitoring Baseline	Manual (Injection: 1 of 1)
2	02_ICS-5000_Dual_1	Idle	
3	03_ICS-5000_Dual_2	Idle	
4	UltiMate3000	Idle	
5	UltiMate3000_RS	Idle	

Pending sequences: 1

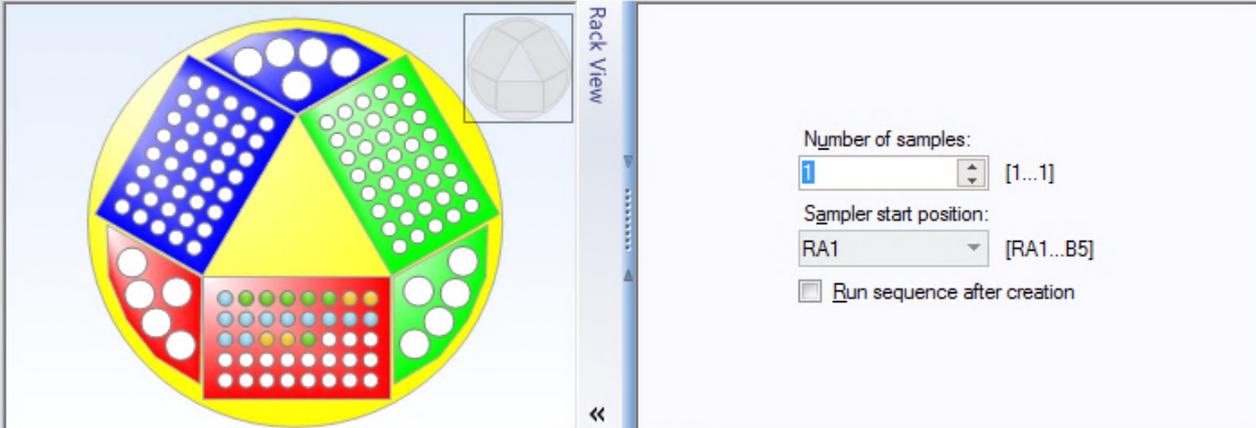
eWorkflow 'CUT Templates Stage 1 (10 units)' selected

cmadmin: Full Access

eWorkflows – Erfolgreiches Starten von Analysen

eWorkflow Wizard

Sample
Define the desired number of samples and the corresponding start position



Number of samples: 1 [1...1]
Sampler start position: RA1 [RA1...B5]
 Run sequence after creation

Sequence Preview

#	Chromatog	Name	Type	Level	Replicate ID	Position	Volume [µL]	Instrument
1	None	Blank	Unknown			R41	10.0000	
2	None	SST Standard 1	Check Standard			R42	10.0000	
3	None	SST Standard 2	Check Standard			R43	10.0000	
4	None	SST Standard 3	Check Standard			R44	10.0000	
5	None	SST Standard 4	Check Standard			R45	10.0000	

Cancel Finish

4. Anzahl der Proben

Number of samples: 1

Sampler start position: RA1 [RA1...B5]

Run sequence after creation

#	Chromatog	Name	Type	Level	Replicate ID	Position	Volume [μL]	Instrument
1	None	Blank	Unknown			R41	10.0000	
2	None	SST Standard 1	Check Standard			R42	10.0000	
3	None	SST Standard 2	Check Standard			R43	10.0000	
4	None	SST Standard 3	Check Standard			R44	10.0000	
5	None	SST Standard 4	Check Standard			R45	10.0000	

Cancel Finish

4. Anzahl der Proben

5. Vialposition festlegen

Number of samples: 1 [1...1]

Sample location: R41

Run sequence after creation

#	Chromatog	Name	Type	Level	Replicate ID	Position	Volume [µL]	Instrument
1	None	Blank	Unknown			R41	10.0000	
2	None	SST Standard 1	Check Standard			R42	10.0000	
3	None	SST Standard 2	Check Standard			R43	10.0000	
4	None	SST Standard 3	Check Standard			R44	10.0000	
5	None	SST Standard 4	Check Standard			R45	10.0000	

Cancel Finish

4. Anzahl der Proben

5. Vialposition festlegen

Number of samples: 1 [1...1]

Sampler start position: RA1 [RA1...B5]

Run sequence after creation

Optional

#	Chromatog	Name	Type	Level	Replicate ID	Position	Volume [µL]	Instrument
1	None	Blank	Unknown			R41	10.0000	
2	None	SST Standard 1	Check Standard			R42	10.0000	
3	None	SST Standard 2	Check Standard			R43	10.0000	
4	None	SST Standard 3	Check Standard			R44	10.0000	
5	None	SST Standard 4	Check Standard			R45	10.0000	

Cancel Finish

4. Anzahl der Proben

5. Vialposition festlegen

Number of samples: 1 [1...1]

Sampler start position: RA1 [RA1...B5]

Run sequence after creation

Optional

#	Chromatog	Name	Type	Level	Replicate ID	Position	Volume [µL]	Instrument
1	None	Blank	Unknown			R41	10.0000	
2	None	SST Standard 1	Check Standard			R42	10.0000	
3	None	SST Standard 2	Check Standard			R43	10.0000	
4	None	SST Standard 3	Check Standard			R44	10.0000	
5	None	SST Standard 4	Check Standard			R45	10.0000	

Cancel Finish

Sequenz Vorschau

4. Anzahl der Proben

5. Vialposition festlegen

Number of samples: 1 [1...1]

Sampler start position: RA1 [RA1...B5]

Run sequence after creation

	Type	Level	Replicate ID	Position	Volume [µL]	Instrument
1	None	Blank	Unknown	R41	10.0000	
2	None	SST Standard 1	Check Standard	R42	10.0000	
3	None	SST Standard 2	Check Standard	R43	10.0000	
4	None	SST Standard 3	Check Standard	R44	10.0000	
5	None	SST Standard 4	Check Standard	R45	10.0000	

Cancel Finish

Probenteller Ansicht

Optional

Sequenz Vorschau

4. Anzahl der Proben

5. Vialposition festlegen

Number of samples: 1 [1...1]
Sampler start position: RA1 [RA1...B5]
 Run sequence after creation

#	Chromatog	Name	Type	Level	Replicate ID	Position	Volume [μL]	Instrument
1	None	Blank	Unknown			RA1	10.0000	
2	None	SST Standard 1	Check Standard			RA2	10.0000	
3	None	SST Standard 2	Check Standard			RA3	10.0000	
4	None	SST Standard 3	Check Standard			RA4	10.0000	
5	None	SST Standard 4	Check Standard			RA5	10.0000	

Ca Finish

6. Finish anklicken

eWorkflows – Erfolgreiches Starten von Analysen

The screenshot displays the Chromeleon Console interface. The main window shows a sequence titled "Fruehschicht -2016_07_12" with 13 rows of injection data. The table columns are: #, UV_VIS_1, Name, Type, Position, Volume [µl], Instrument Method, Processing Method, Status, and Inje. The status for all rows is "Idle".

#	UV_VIS_1	Name	Type	Position	Volume [µl]	Instrument Method	Processing Method	Status	Inje
1	None	Spülen	Blank	RA1	5.000	Produkt_A	Proben_Produkt_A	Idle	
2	None	Kessel 1_1	Unknown	RA2	5.000	Produkt_A	Proben_Produkt_A	Idle	
3	None	Kessel 1_2	Unknown	RA3	5.000	Produkt_A	Proben_Produkt_A	Idle	
4	None	Spülen	Blank	RA4	5.000	Produkt_A	Proben_Produkt_A	Idle	
5	None	Kessel 1_1	Unknown	RA5	5.000	Produkt_A	Proben_Produkt_A	Idle	
6	None	Kessel 1_2	Unknown	RA6	5.000	Produkt_A	Proben_Produkt_A	Idle	
7	None	Spülen	Blank	RA7	5.000	Produkt_A	Proben_Produkt_A	Idle	
8	None	Kessel 1_1	Unknown	RA8	5.000	Produkt_A	Proben_Produkt_A	Idle	
9	None	Kessel 1_2	Unknown	RB1	5.000	Produkt_A	Proben_Produkt_A	Idle	
10	None	Spülen	Blank	RB2	5.000	Produkt_A	Proben_Produkt_A	Idle	
11	None	Kessel 1_1	Unknown	RB3	5.000	Produkt_A	Proben_Produkt_A	Idle	
12	None	Kessel 1_2	Unknown	RB4	5.000	Produkt_A	Proben_Produkt_A	Idle	
13	None	Spülen	Blank	RB5	5.000	Produkt_A	Proben_Produkt_A	Idle	

Below the main table, there is a section for "Name", "Type", "Date Modified", and "Comment" with the following entries:

Name	Type	Date Modified	Comment
065565 Chromeleon 7.2 C...	Associated File	18.07.2013 12:38:06 +02:...	
Ausdruck_Produkt_A	Report Template	25.04.2014 13:25:26 +02:...	
Bildschirmansicht	View Settings	25.04.2014 13:25:26 +02:...	
Proben_Produkt_A	Processing Met...	25.04.2014 13:25:26 +02:...	
Produkt_A	Instrument Met...	25.04.2014 13:56:42 +02:...	

A yellow callout box at the bottom of the screenshot contains the text: "7. Komplette Sequenz ist mit allen Vorgaben für das vorgesehene Instrument erstellt".

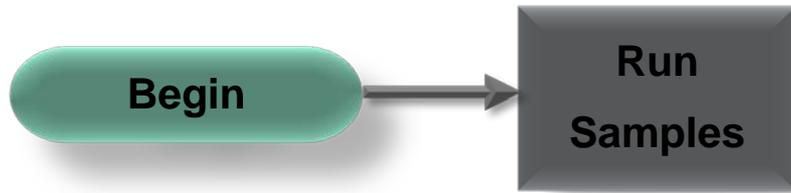
- Innovative Benutzeroberfläche
- Universelle Instrumentensteuerung
- Erfolgreiches Starten von Analysen
- Datenbearbeitung – schnell und zuverlässig**
- Arbeiten im regulierten Umfeld



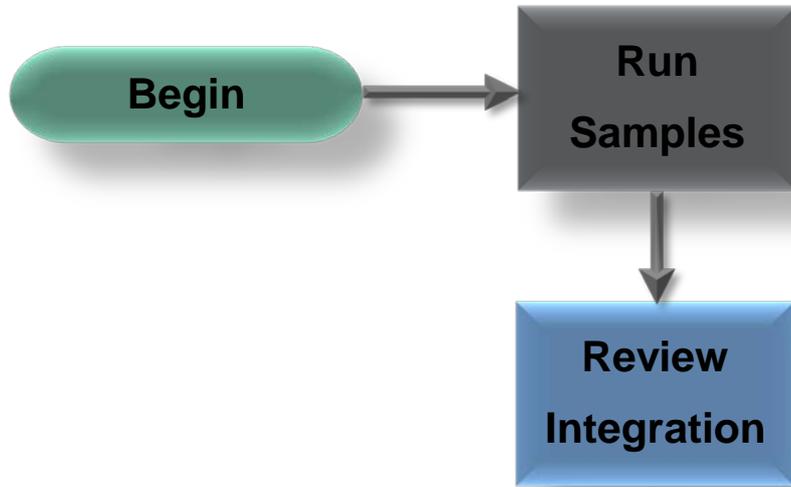
- Das ideale CDS benötigt folgendes:
 - Ein etabliertes Gerät, das zuverlässige Daten (SST) liefert
 - Aufnahme (korrekter) Daten und zuverlässige Integration
 - Etabliertes Kalibrierverfahren
 - Berechnung von Proben und Überprüfung von Qualitätskontrollen mit dem Kalibriermodell
 - Kalkulation von Ergebnissen und Reporterstellung mit Abgleich gegen vorgegebene Spezifikationen

- Nicht alle CDS Systeme können das – oder?
- Und – manche sind deutlich intuitiver als andere!

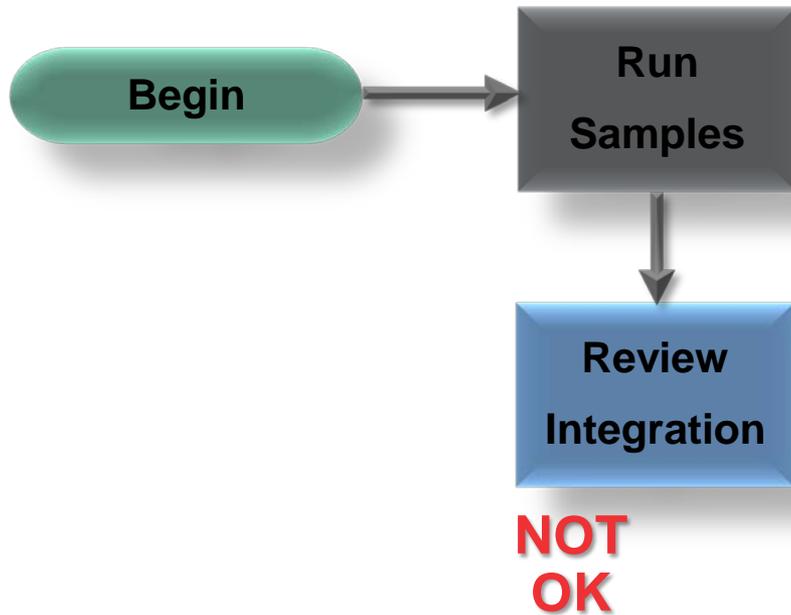
Chromleon CDS Data Processing



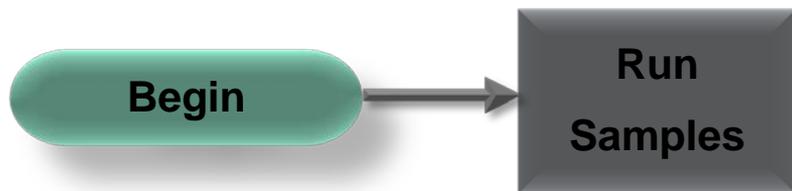
Chromeleon CDS Data Processing



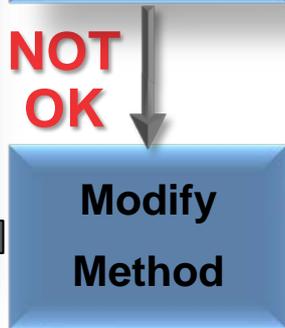
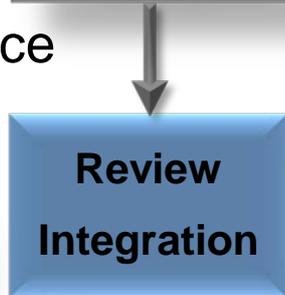
Chromeleon CDS Data Processing



Chromeleon CDS Data Processing



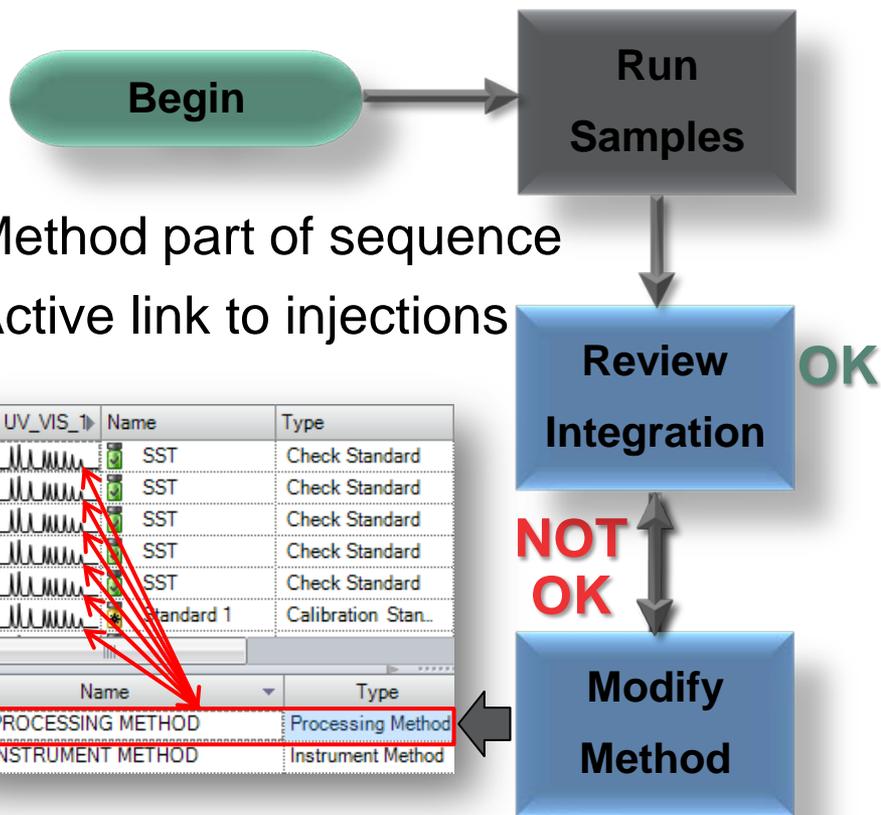
- Method part of sequence



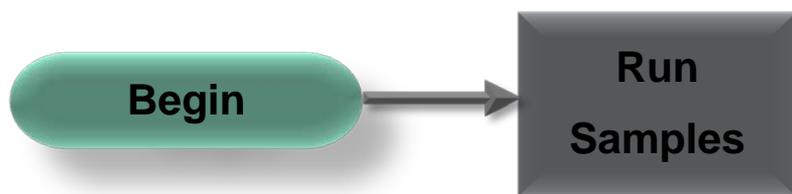
#	UV_VIS_1	Name	Type
1		SST	Check Standard
2		SST	Check Standard
3		SST	Check Standard
4		SST	Check Standard
5		SST	Check Standard
6		Standard 1	Calibration Stan..

Name	Type
PROCESSING METHOD	Processing Method
INSTRUMENT METHOD	Instrument Method

Chromeleon CDS Data Processing



Chromeleon CDS Data Processing



- Method part of sequence
- Active link to injections

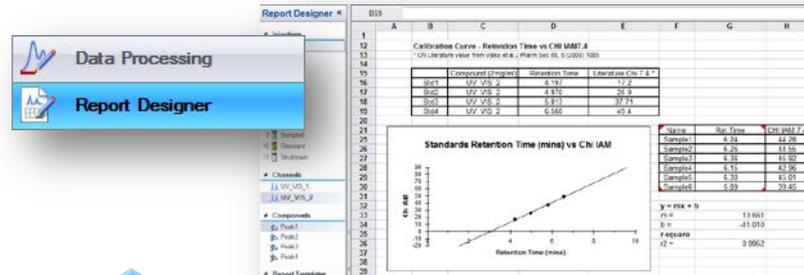


OK

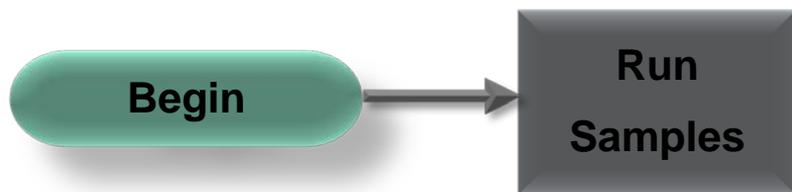


#	UV_VIS_1	Name	Type
1		SST	Check Standard
2		SST	Check Standard
3		SST	Check Standard
4		SST	Check Standard
5		SST	Check Standard
6		Standard 1	Calibration Stan..

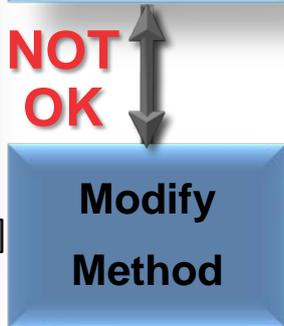
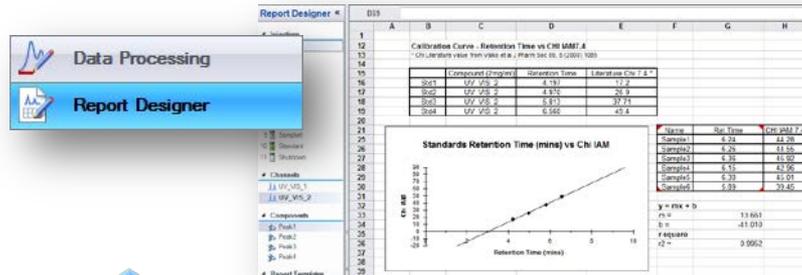
Name	Type
PROCESSING METHOD	Processing Method
INSTRUMENT METHOD	Instrument Method



Chromeleon CDS Data Processing



- Method part of sequence
- Active link to injections

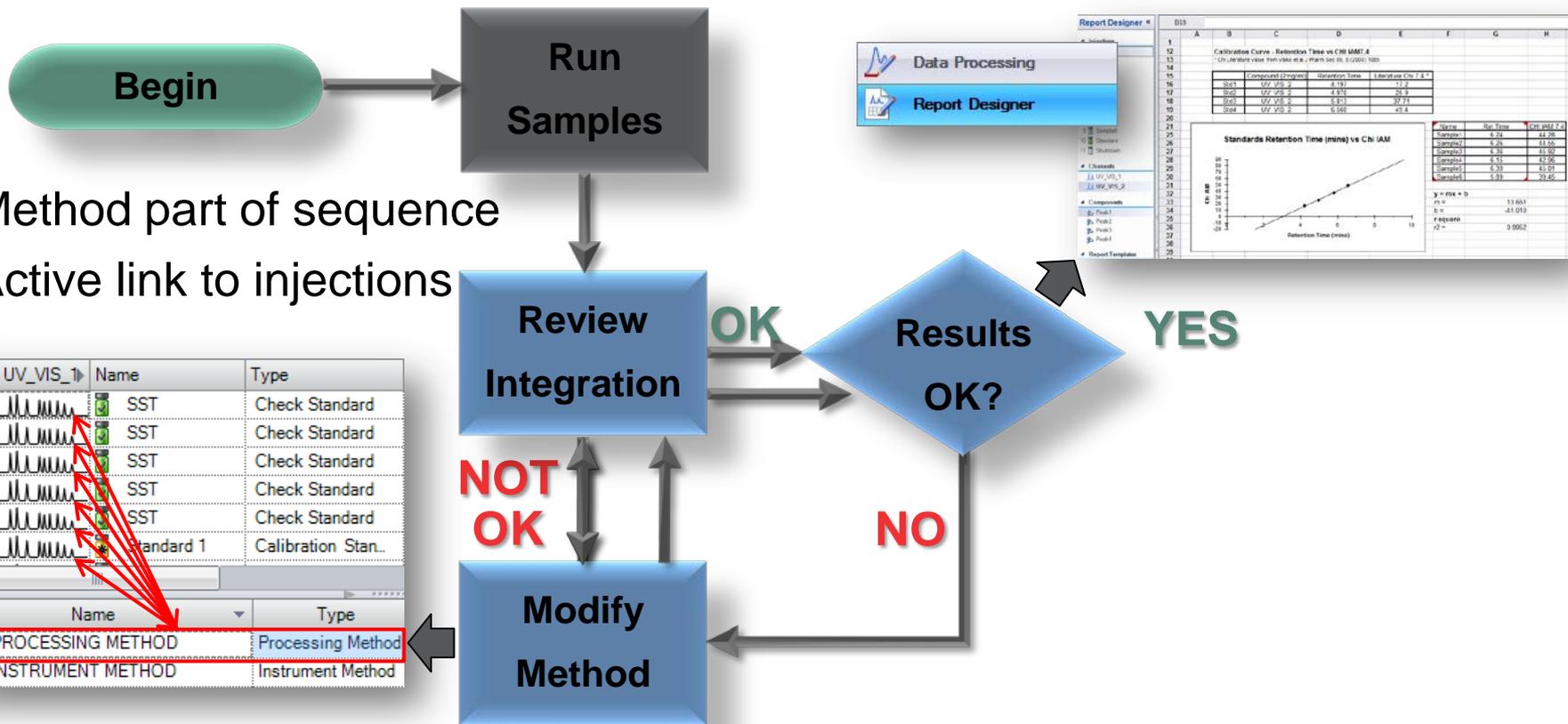


#	UV_VIS_1	Name	Type
1		SST	Check Standard
2		SST	Check Standard
3		SST	Check Standard
4		SST	Check Standard
5		SST	Check Standard
6		Standard 1	Calibration Stan..

Name	Type
PROCESSING METHOD	Processing Method
INSTRUMENT METHOD	Instrument Method

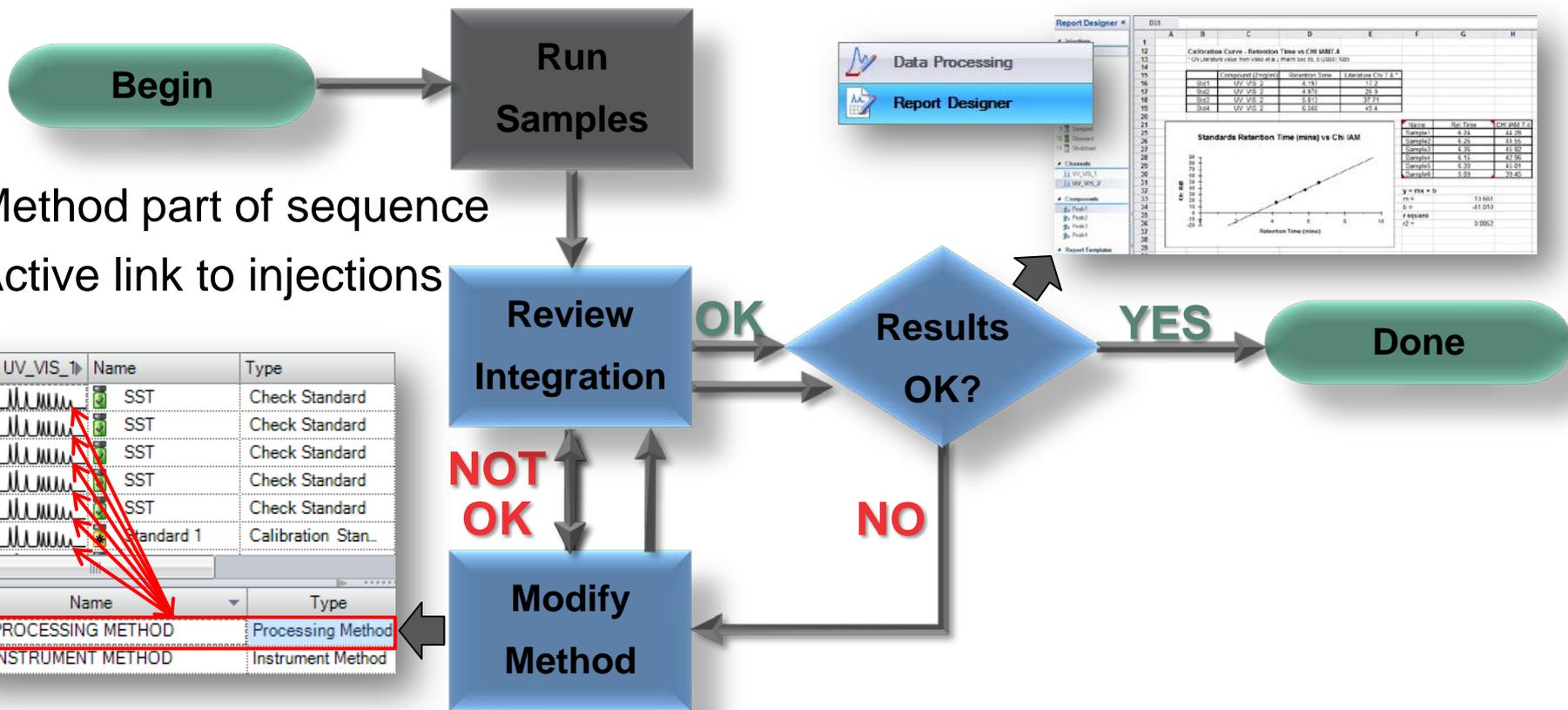


Chromeleon CDS Data Processing

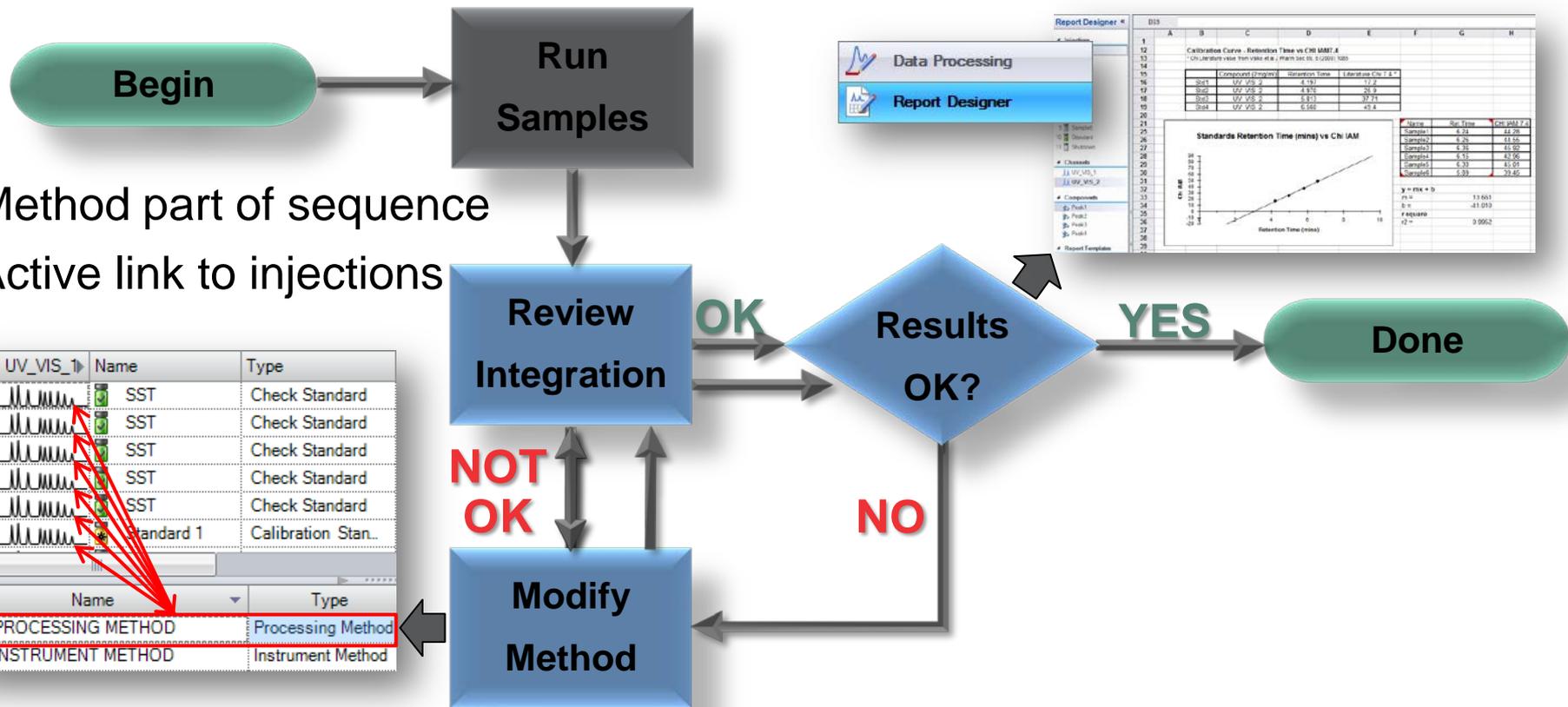


- Method part of sequence
- Active link to injections

Chromleon CDS Data Processing



Chromeleon CDS Data Processing



Operational Efficiency

- Methode dynamisch mit der Injektion verknüpft = sofortige Aktualisierung
- Kein Datenexport notwendig
- Alle Reports und Berechnungen werden im validierten Umfeld erstellt
- Bessere Produktivität – bis zu **98%** Zeitersparnis

- Innovative Benutzeroberfläche
- Universelle Instrumentensteuerung
- Erfolgreiches Starten von Analysen
- Datenbearbeitung – schnell und zuverlässig
- **Arbeiten im regulierten Umfeld**



- Hauptsächlich vorgegeben durch FDA 21 CFR Part 11, August 20, 1997
- Certificate of Software Validation / IQ / OQ / PQ für verwendete Systeme und Methoden
- Digitale Signaturen – eindeutige Definition von Rohdaten und deren Metadaten
- Audit Trail (Instrument und Datenaufnahme / Bearbeitung) – typischerweise mit Zeitstempel und computergeneriert, erfasst alle Änderungen am Objekt und ordnet diese eindeutig einem Anwender zu
- Möglichkeit der elektronischen Unterschrift mit dem Verweis, ob die Ergebnisse überprüft und/oder freigegeben wurden
- Kontrollierter Zugang nur für berechtigte Personen – Zugangsmodell und Sicherheitssystem über klar definierte Privilegien
- IQ / OQ / PQ Prozesse und deren Dokumentation
- Datenintegrität, Archivierung und einfache Wiederherstellbarkeit



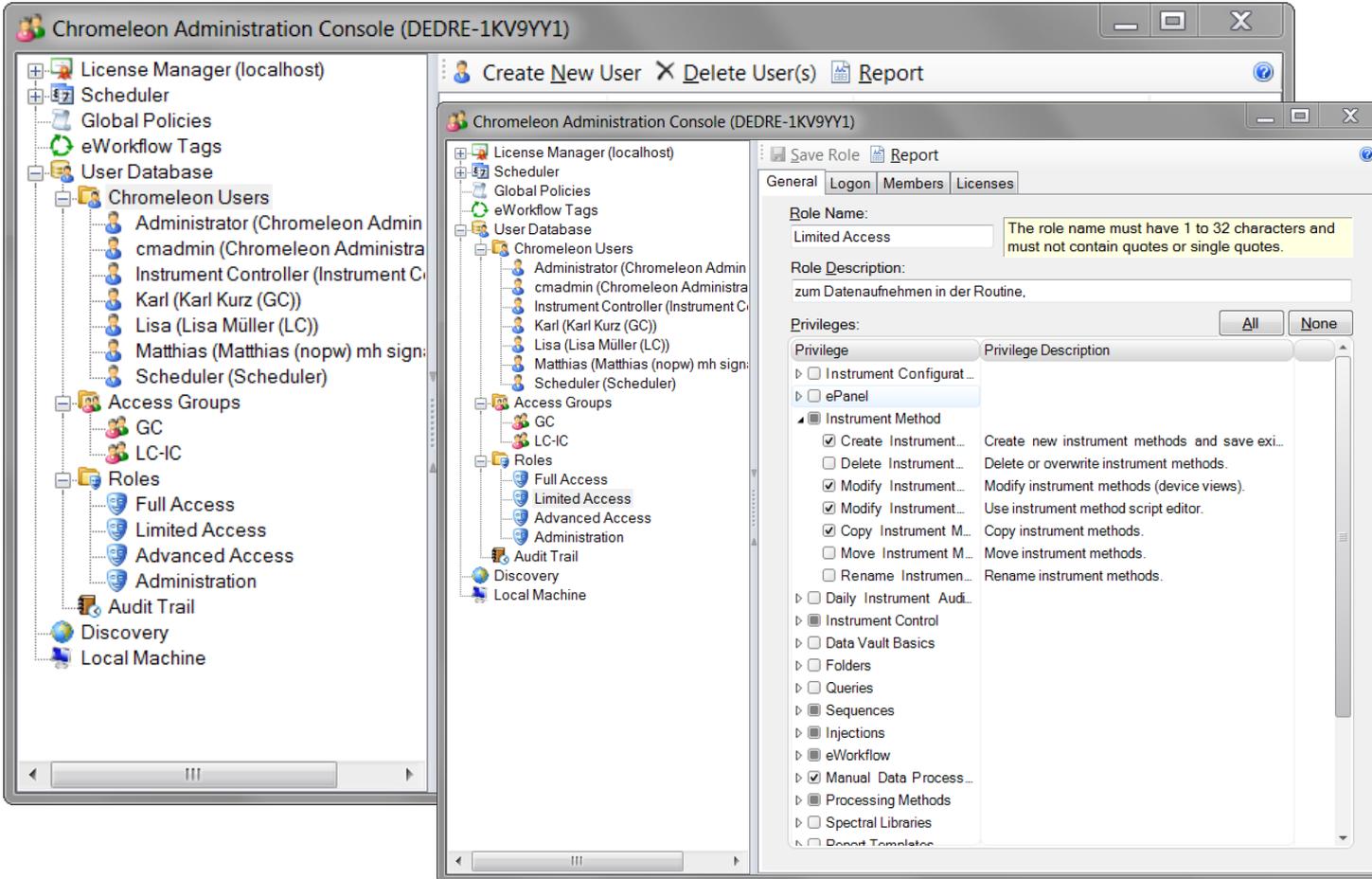
BENUTZER VERWALTUNG

- Erstellen von Users, Roles und Access Groups

The screenshot displays the Chromeleon Administration Console (DEDRE-1KV9YY1) with a tree view on the left and a user list table on the right. The tree view includes categories like License Manager, Scheduler, Global Policies, eWorkflow Tags, User Database, Chromeleon Users, Access Groups, Roles, Audit Trail, Discovery, and Local Machine. The 'Chromeleon Users' folder is expanded, showing a list of users. The right pane shows a table with columns for User Name, Full Name, and Job Title, listing various users such as Administrator, cmadmin, Instrument Contr..., Karl, Lisa, Matthias, and Scheduler.

User Name	Full Name	Job Title
Administrator	Chromeleon Admin (no p...	Administrator
cmadmin	Chromeleon Administrator	Chromeleon Administrator
Instrument Contr...	Instrument Controller	Instrument Controller
Karl	Karl Kurz (GC)	GC Anwender
Lisa	Lisa Müller (LC)	HPLC Anwenderin / IC Urlaubs...
Matthias	Matthias (nopw) mh signa...	CM Admin
Scheduler	Scheduler	Scheduler

- Erstellen von Users, Roles and Access Groups



Zugangskontrolle – Benutzer Verwaltung

- Erstellen von Users, Roles and Access Groups

The image displays three overlapping screenshots of the Chromeleon Administration Console (DEDRE-1KV9YY1) illustrating the process of creating users, roles, and access groups.

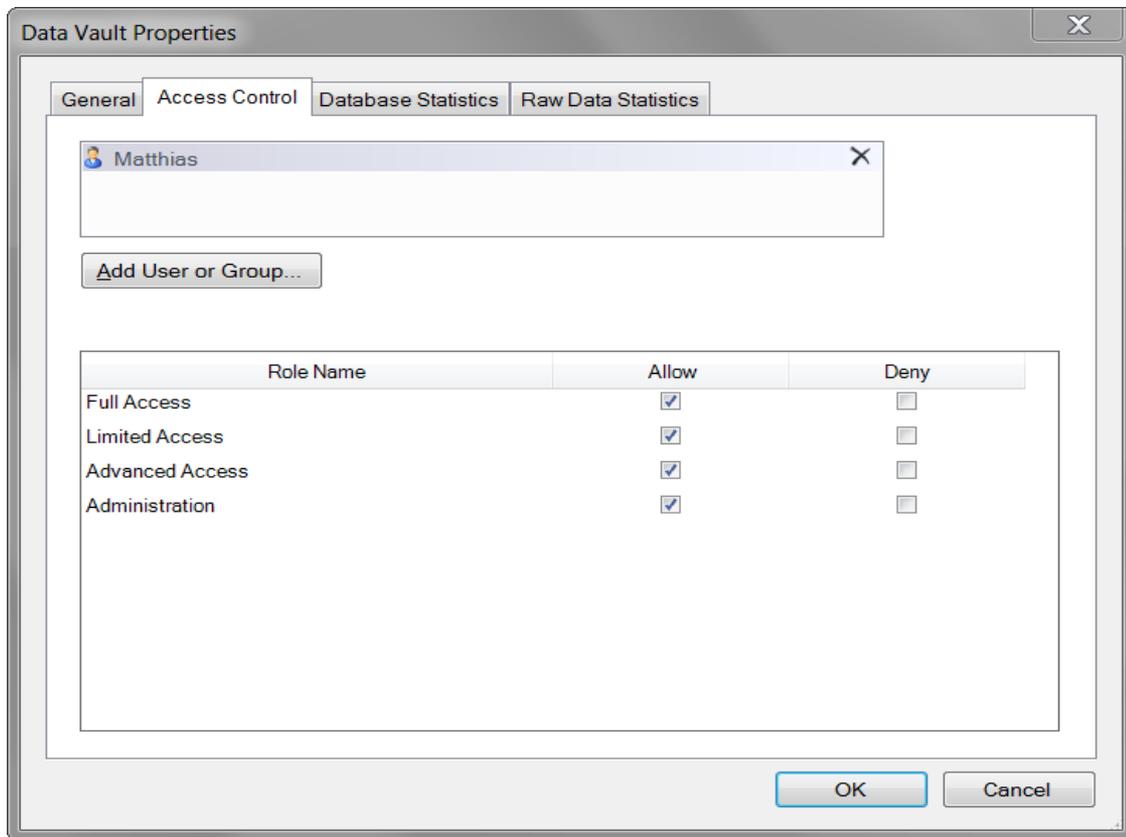
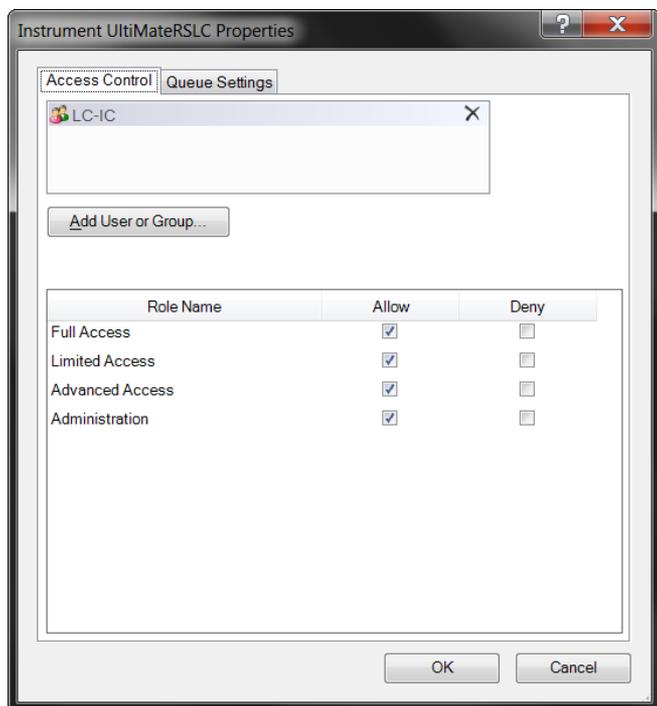
Top Screenshot: Create New User
The 'Create New User' dialog box is open. The left sidebar shows the 'Chromeleon Users' tree with the following users listed: Administrator (Chromeleon Admin), cadmin (Chromeleon Administra), Instrument Controller (Instrument C), Karl (Karl Kurz (GC)), Lisa (Lisa Müller (LC)), Matthias (Matthias (nopw) mh sign), and Scheduler (Scheduler). The 'Roles' section includes Full Access, Limited Access, Advanced Access, and Administration. The 'Access Groups' section includes GC, LC-IC, and Roles.

Middle Screenshot: Save Access Group
The 'Save Access Group' dialog box is open. The 'Members' tab is selected, showing a table of 'Access Group Members':

Name	Full Name
<input checked="" type="checkbox"/>	Administrator Chromeleon Admin (no ...
<input checked="" type="checkbox"/>	cadmin Chromeleon Administra...
<input checked="" type="checkbox"/>	Instrument Co... Instrument Controller
<input type="checkbox"/>	Karl Karl Kurz (GC)
<input checked="" type="checkbox"/>	Lisa Lisa Müller (LC)
<input checked="" type="checkbox"/>	Matthias Matthias (nopw) mh sig...
<input checked="" type="checkbox"/>	Scheduler Scheduler

Bottom Screenshot: General Tab
The 'General' tab of the 'Save Access Group' dialog is visible, showing the 'Access Group Members' table with the same data as the 'Members' tab.

- Zuweisen von Access Gruppen auf Objekte über deren Eigenschaften
- Instruments
- Data Vaults & Folder





AUDIT TRAIL - VERSIONIERUNG

Object Audit Trails – Version Comparison

Compare Instrument Method 'UltiMate3000' version 1 with version 2

Version	Date / Time	Operator	Client Computer
1	02/12/2009 13:02:38	SQuinn	L-GERSQUINN
2	02/12/2009 13:03:44	SQuinn	L-GERSQUINN

Visualization Options
 Complete
 Only Changes

Property Name	Value version 1	Value version 2
Comment	UltiMate3000	UltiMate3000
Instrument Server	L-GERSQUINN	L-GERSQUINN
Instrument	05_UltiMate3000_1	05_UltiMate3000_1

Version 1

Time	Symbol	Value	Comment
Initial Time	Instrument Setup		
	Sampler.InjectMode	Normal	
	Sampler.PumpDevice	"Pump"	
	Sampler.SyncWithPump	On	
	Pump.MaximumFlowRampDown	1.000 [ml/min ²]	
	Pump.MaximumFlowRampUp	1.000 [ml/min ²]	
	Pump.%B.Equate	"Acetonitrile"	
	Pump.%C.Equate	"Methanol"	
	Pump.Pressure.LowerLimit	0 [bar]	
	Pump.Pressure.UpperLimit	400 [bar]	
	UV.UV_VIS_1.Wavelength	254.0 [nm]	
0.00	Inject Preparation		
0.00	Inject		
0.00	Start Run		
	UV.UV_VIS_1.AcqOn		
0.00	Run		
	Pump.Flow	1.000 [ml/min]	
8.00			
	Pump.Flow	1.000 [ml/min]	
8.00	Stop Run		
	UV.UV_VIS_1.AcqOff		

Version 2

Time	Symbol	Value	Comment
Initial Time	Instrument Setup		
	Sampler.InjectMode	Normal	
	Sampler.PumpDevice	"Pump"	
	Sampler.SyncWithPump	On	
	Pump.MaximumFlowRampDown	1.000 [ml/min ²]	
	Pump.MaximumFlowRampUp	1.000 [ml/min ²]	
	Pump.%A.Equate	"0.1M Phosphate Buffer"	
	Pump.Pressure.LowerLimit	0 [bar]	
	Pump.Pressure.UpperLimit	400 [bar]	
	Pump.%B.Equate	"Acetonitrile"	
	UV.UV_VIS_1.Wavelength	280.0 [nm]	
0.00	Inject Preparation		
0.00	Inject		
0.00	Start Run		
	UV.UV_VIS_1.AcqOn		
	Pump.Pump_Pressure.AcqOn		
0.00	Run		
	Pump.Flow	2.000 [ml/min]	
8.00			
	Pump.Flow	2.000 [ml/min]	
8.00	Stop Run		
	UV.UV_VIS_1.AcqOff		
	Pump.Pump_Pressure.AcqOff		

Object Audit Trails – Version Comparison

Compare Instrument Method 'UltiMate3000' version 1 with version 2

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Visualization Options
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 Only Changes

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Instrument Server	L-GERSQUINN	L-GERSQUINN
Instrument	05_UltiMate3000_1	05_UltiMate3000_1

Änderung

Version 1

Time	Symbol	Value	Comment
Initial Time	Instrument Setup		
	Sampler.InjectMode	Normal	
	Sampler.PumpDevice	"Pump"	
	Sampler.SyncWithPump	On	
	Pump.MaximumFlowRampDown	1.000 [ml/min ²]	
	Pump.MaximumFlowRampUp	1.000 [ml/min ²]	
	Pump.%B.Equate		"Acetonitrile"
	Pump.%C.Equate	"Methanol"	
	Pump.Pressure.LowerLimit	0 [bar]	
	Pump.Pressure.UpperLimit	400 [bar]	
	UV.UV_VIS_1.Wavelength	254.0 [nm]	
0.00	Inject Preparation		
0.00	Inject		
0.00	Start Run		
	UV.UV_VIS_1.AcqOn		
0.00	Run		
	Pump.Flow	1.000 [ml/min]	
8.00	Pump.Flow	1.000 [ml/min]	
8.00	Stop Run		
	UV.UV_VIS_1.AcqOff		

Version 2

Time	Symbol	Value	Comment
Initial Time	Instrument Setup		
	Sampler.InjectMode	Normal	
	Sampler.PumpDevice	"Pump"	
	Sampler.SyncWithPump	On	
	Pump.MaximumFlowRampDown	1.000 [ml/min ²]	
	Pump.MaximumFlowRampUp	1.000 [ml/min ²]	
	Pump.%A.Equate		"0.1M Phosphate Buffer"
	Pump.Pressure.LowerLimit	0 [bar]	
	Pump.Pressure.UpperLimit	400 [bar]	
	Pump.%B.Equate	"Acetonitrile"	
	UV.UV_VIS_1.Wavelength	280.0 [nm]	
0.00	Inject Preparation		
0.00	Inject		
0.00	Start Run		
	UV.UV_VIS_1.AcqOn		
	Pump.Pump_Pressure.AcqOn		
0.00	Run		
	Pump.Flow	2.000 [ml/min]	
8.00	Pump.Flow	2.000 [ml/min]	
8.00	Stop Run		
	UV.UV_VIS_1.AcqOff		
	Pump.Pump_Pressure.AcqOff		

Object Audit Trails – Version Comparison

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Visualization Options
 Complete
 Only Changes

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Comment	UltiMate3000	UltiMate3000
Instrument Server	L-GERSQUINN	L-GERSQUINN
Instrument	05_UltiMate3000_1	05_UltiMate3000_1

Änderung

Addition

Version 1

Time	Symbol	Value	Comment
Initial Time	Instrument Setup		
	Sampler.InjectMode	Normal	
	Sampler.PumpDevice	"Pump"	
	Sampler.SyncWithPump	On	
	Pump.MaximumFlowRampDown	1.000 [ml/min ²]	
	Pump.MaximumFlowRampUp	1.000 [ml/min ²]	
	Pump.%B.Equate		"Acetonitrile"
	Pump.%C.Equate	"Methanol"	
	Pump.Pressure.LowerLimit	0 [bar]	
	Pump.Pressure.UpperLimit	400 [bar]	
	UV.UV_VIS_1.Wavelength	254.0 [nm]	
0.00	Inject Preparation		
0.00	Inject		
0.00	Start Run		
	UV.UV_VIS_1.AcqOn		
0.00	Run		
	Pump.Flow	1.000 [ml/min]	
8.00	Pump.Flow	1.000 [ml/min]	
8.00	Stop Run		
	UV.UV_VIS_1.AcqOff		

Version 2

Time	Symbol	Value	Comment
Initial Time	Instrument Setup		
	Sampler.InjectMode	Normal	
	Sampler.PumpDevice	"Pump"	
	Sampler.SyncWithPump	On	
	Pump.MaximumFlowRampDown	1.000 [ml/min ²]	
	Pump.MaximumFlowRampUp	1.000 [ml/min ²]	
	Pump.%A.Equate		"0.1M Phosphate Buffer"
	Pump.Pressure.LowerLimit	0 [bar]	
	Pump.Pressure.UpperLimit	400 [bar]	
	Pump.%B.Equate	"Acetonitrile"	
	UV.UV_VIS_1.Wavelength	280.0 [nm]	
0.00	Inject Preparation		
0.00	Inject		
0.00	Start Run		
	UV.UV_VIS_1.AcqOn		
	Pump.Pump_Pressure.AcqOff		
0.00	Run		
	Pump.Flow	2.000 [ml/min]	
8.00	Pump.Flow	2.000 [ml/min]	
8.00	Stop Run		
	UV.UV_VIS_1.AcqOff		
	Pump.Pump_Pressure.AcqOff		

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Version 1

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	Pump.%B.Equate	"Acetonitrile"	
	Pump.%C.Equate	"Methanol"	
	Pump.Pressure.UpperLimit	400 [bar]	
	UV.UV_VIS_1.Wavelength	280.0 [nm]	
0.00	Inject Preparation		
0.00	Inject		
0.00	Start Run		
0.00	UV.UV_VIS_1.AcqOn		
0.00	Run		
	Pump.Flow	1.000 [ml/min]	
8.00	Pump.Flow	2.000 [ml/min]	
8.00	Stop Run		
8.00	UV.UV_VIS_1.AcqOff		

Entfernen

Version 2

Time	Symbol	Value	Comment
Initial Time	Instrument Setup		
	Sampler.InjectMode	Normal	
	Sampler.PumpDevice	"Pump"	
	Sampler.SyncWithPump	On	
	Pump.MaximumFlowRampDown	1.000 [ml/min ²]	
	Pump.MaximumFlowRampUp	1.000 [ml/min ²]	
	Pump.%A.Equate	"0.1M Phosphate Buffer"	
	Pump.Pressure.LowerLimit	0 [bar]	
	Pump.Pressure.UpperLimit	400 [bar]	
	Pump.%B.Equate	"Acetonitrile"	
	UV.UV_VIS_1.Wavelength	280.0 [nm]	
0.00	Inject Preparation		
0.00	Inject		
0.00	Start Run		
0.00	UV.UV_VIS_1.AcqOn		
0.00	Run		
	Pump.Pump_Pressure.AcqOff		
	Pump.Flow	2.000 [ml/min]	
8.00	Pump.Flow	2.000 [ml/min]	
8.00	Stop Run		
8.00	UV.UV_VIS_1.AcqOff		
	Pump.Pump_Pressure.AcqOff		

Addition

Änderungen der Objekte sind leicht zu identifizieren

Datenaufzeichnung– Elektronische Unterschriften

The screenshot displays the Chromeleon Chromatography software interface. The main window shows an 'Electronic Report' for a sequence named 'Matthias - Fruehschicht -2016_01_28'. The report includes a 'Chromatogram and Results' section with a chromatogram plot showing several peaks. A 'Submit Signature' dialog box is overlaid on the report, prompting the user to enter their Chromeleon User Name and Signature Password. The dialog box also includes a 'Comment' field and 'OK', 'Cancel', and 'Help' buttons.

Chromatogram and Results

Injection Details		
Injection Name:	Kessel_1_1	Run Time (min): 0.21
Vial Number:	RA2	Injection Volume: 5.00
Injection Type:	Unknown	Channel: UV_VIS_1
Calibration Level:		WaveLength: 254.0
Instrument Method:	Produkt_A	ScanWidth: 1
Processing Method:	Proben_Produkt_A	Dilution Factor: 1.0000
Injection Date/Time:	23 Jan 16 16:01	Sample Weight: 1.0000

Chromatogram

Chromatogram showing Absorbance (mAU) vs. Time (min). Peaks are labeled with their retention times and names:

- 1 - Uracil - 0.022
- 2 - Acetanilide - 0.021
- 3 - Acetophenone - 0.044
- 4 - Propiophenone - 0.081
- 5 - Butyrophenone - 0.095
- 6 - Benzophenone - 0.100
- 7 - Valerophenone - 0.102
- 8 - Hexanophenone - 0.146
- 9 - Heptanophenone - 0.164
- 10 - Octanophenone - 0.184

Integration Results

No.	Peak Name
1	Uracil
2	Acetanilide
3	Acetophenone
4	Propiophenone
5	Butyrophenone
6	Benzophenone
7	Valerophenone
8	Hexanophenone
9	Heptanophenone
10	Octanophenone
11	
12	
13	
Total:	

- Drei Hierarchien der Unterschriften
 - Submit, Review, Approve
- Werden im elektronischen Dokument verwendet
- Sequenzen werden über Checksummen geschützt
- Über die Benutzer Privilegien gesteuert

Welches CDS ist denn nun das Richtige für mich?

- Chromeleon 7.2 SR4 Chromatography Data System (CDS) Software
 - die nächste Generation von CDS
- „**Simply Intelligent**“
 - Intelligente Funktionalität – es macht das, was Sie benötigen!
- „**Operational Simplicity™**“
 - alles geht schnell und einfach!
 - Intuitiv - intelligent – leichter zu bedienen
 - Vereinfacht alle chromatographischen Prozesse

Vielen Dank für Ihre Aufmerksamkeit



Benötigen Sie weitere Informationen oder möchten Sie Ihre Demo CD anfordern, dann besuchen Sie uns unter:

www.thermofisher.com/chromeleon

Folgen Sie Charlie Chromeleon auf

facebook.com/CharlieLovesChromatography

Bitte wenden Sie sich mit weiteren Fragen direkt an uns per Email:

analyze.eu@thermofisher.com