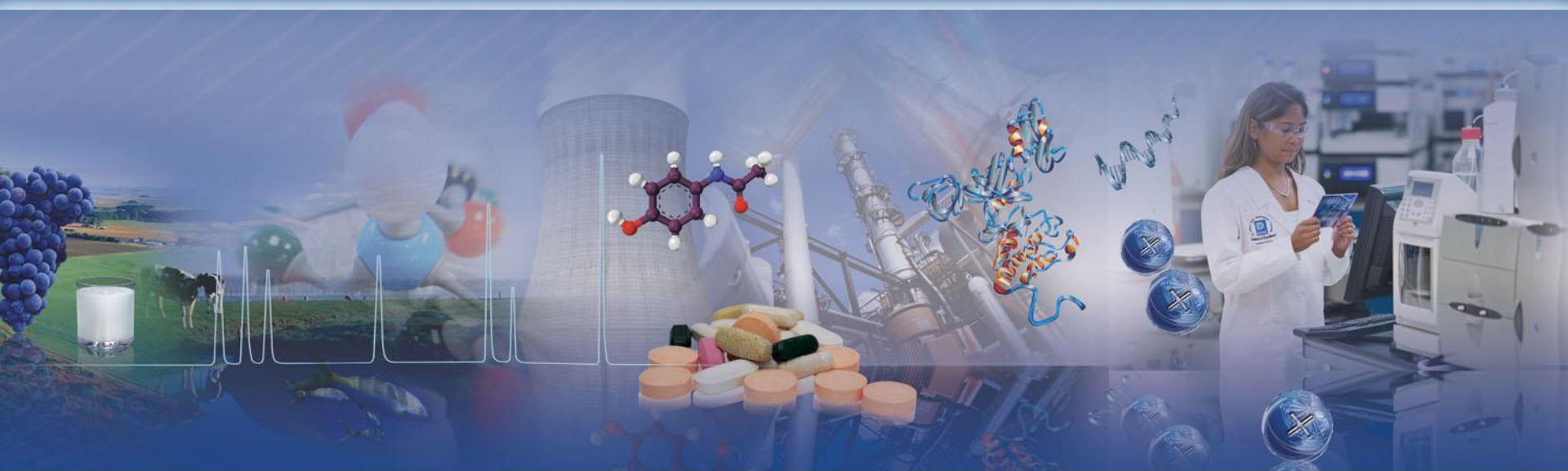


# Getting More Done with Less Effort: Usability Advances in a New Chromatography Data System



Jim Schibler  
Dionex Corporation, Sunnyvale, CA

# Getting More Done with Less Effort

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- The Productivity Challenge
  - What productivity means
  - Key ways to improve productivity in the modern laboratory
- A New Chromatography Data System Designed for Usability
  - User interface and navigation
  - Data review and analysis
  - Workflow management
- Closing Remarks

ISO Slide Number

# What is Productivity?

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Cost per analysis?

Sample turnaround time?

% instrument utilization?

***Some other measure?***

Analyses per labor-hour?

Analyses per week?

Average time per analysis?

# What is Productivity?



## Output Produced per Resources Consumed

- Quantity
- Quality
- Capital equipment
- Consumables
- Utilities
- Labor
- Time

# Key Ways to Improve Laboratory Productivity

- Improve analytical methodology (including sample preparation)
- Increase utilization rate of resources
- Automate to a higher degree
- Improve operator efficiency

***Best opportunities!***

ISO Slide Number

# Software Usability Issues that Limit Operator Efficiency

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- Unclear paths to goals
- Distractions caused by too many options at inappropriate times
- Confusion from poorly chosen or inconsistent logic and terminology
- Unnecessary extra steps in processes
- Unexpected responses of software to user actions
- Failure to trap or prevent operator errors

ISO Slide Number

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# **A New Chromatography Data System Designed for Usability**

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Intelligent Functionality + Operational Simplicity

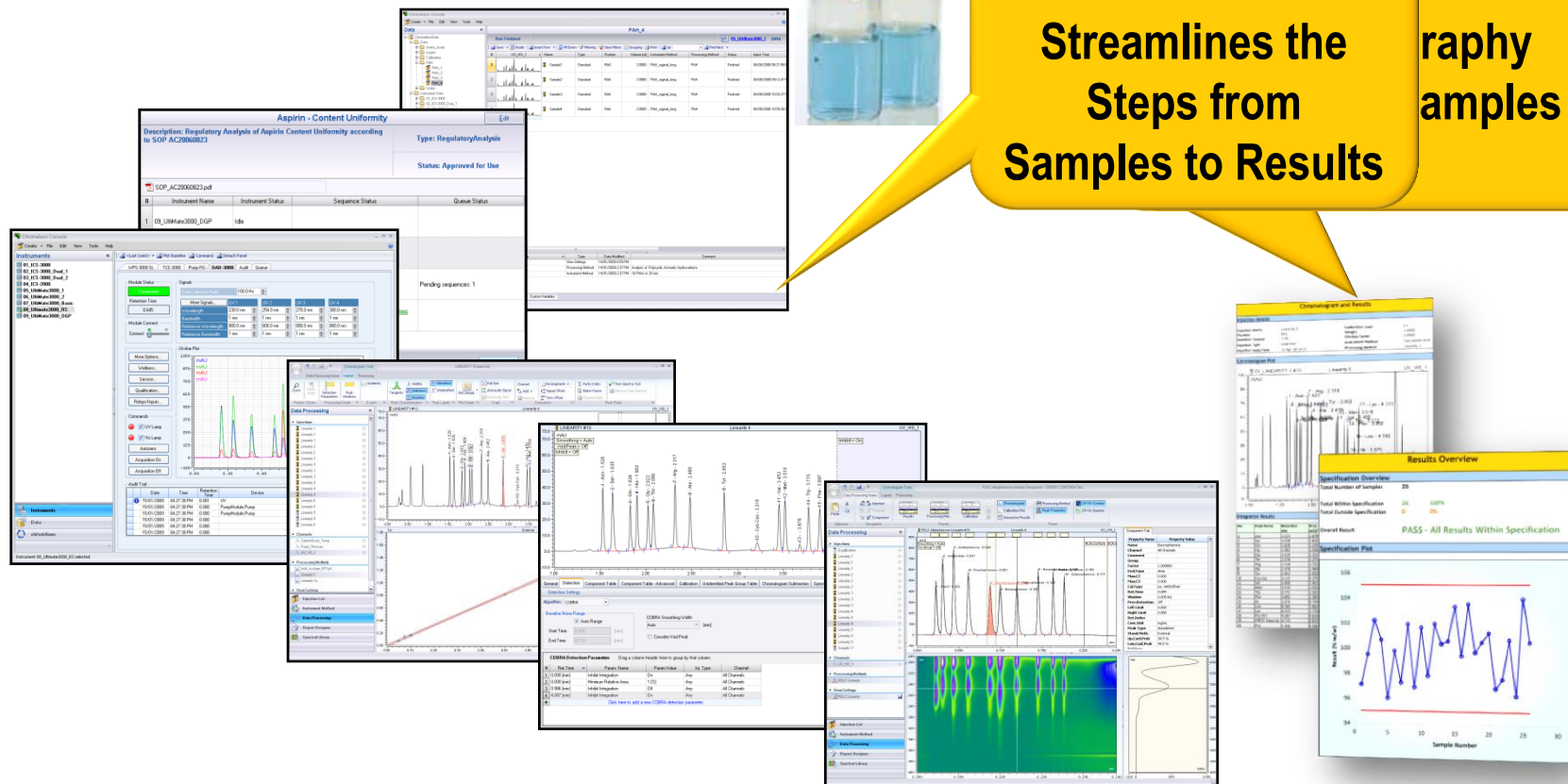
# Chromeleon 7



- Next-generation Chromatography Data System
- **"Simply Intelligent":**
  - Intelligent functionality — everything you need to generate results!
  - Operational Simplicity™ — everything is fast and easy!
- Simplifies all chromatography processes



# raphy amples



# Chromeleon 7—Operational Simplicity

- Operational Simplicity™ was the core design principle
- Major design goals:
  - Minimize number of steps needed to perform any task
  - Make all steps easy to understand and easy to use
  - Minimize time needed to perform any task
- Three major features for **Operational Simplicity**:
  - Modern user interface
  - Peak detection and integration tools
  - eWorkflows

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# Chromeleon 7: User Interface

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# Console: Quick Access to Instruments, Data, eWorkflows

The screenshot displays the Chromeleon Console interface. On the left, the **Data** navigation pane is highlighted with a red box, showing a tree structure of data folders. The main window displays a table titled **AS12A Calibration and Samples** with 10 rows of data. Each row includes a chromatogram plot. A yellow callout points to the **Navigation Pane** on the left. Another yellow callout points to the **Category Bars** at the bottom, which include **Instruments**, **Data**, and **eWorkflows**. A third yellow callout points to the **Associated Items** section at the bottom right.

| #  | ECD_1 | Name                        | Type     | Position | Volume [μl] | Level | Processing Method     |
|----|-------|-----------------------------|----------|----------|-------------|-------|-----------------------|
| 1  |       | Seven Anion Standard II - 1 | Standard | 1        | 25.0000     | 01    | AS12A Anions in Water |
| 2  |       | Seven Anion Standard II - 2 | Standard | 2        |             |       |                       |
| 3  |       | Seven Anion Standard II - 3 | Standard | 3        |             |       |                       |
| 4  |       | Seven Anion Standard II - 4 | Standard | 4        | 25.0000     | 04    | AS12A Anions in Water |
| 5  |       | Seven Anion Standard II - 5 | Standard | 5        | 25.0000     | 05    | AS12A Anions in Water |
| 6  |       | Seven Anion Standard II - 6 | Standard | 6        | 25.0000     | 06    | AS12A Anions in Water |
| 7  |       | Drinking Water              | Unknown  | 7        | 25.0000     |       | AS12A Anions in Water |
| 8  |       | Tap Water                   | Unknown  | 8        | 25.0000     |       | AS12A Anions in Water |
| 9  |       | Power Coolant Water         | Unknown  | 9        |             |       |                       |
| 10 |       | Power Coolant Water         | Unknown  | 10       |             |       |                       |

| Name                               | Type              | Date Modified      | Comment                                           |
|------------------------------------|-------------------|--------------------|---------------------------------------------------|
| Anions in Water                    | Report Definition | 15/01/2009 3:15 PM |                                                   |
| Anions in Water                    | View Settings     | 15/01/2009 3:16 PM |                                                   |
| AS12A Anions in Water              | Instrument Method | 15/01/2009 3:18 PM | Instrument Method Anions in Water on AS12A column |
| AS12A Anions in Water              | Processing Method | 15/01/2009 3:18 PM |                                                   |
| AS12A Production Test Chromatogram | Instrument Method | 14/01/2009 2:37 PM | AS12A Production Test Chromatogram                |
| AS12A Production Test Chromatogram | Processing Method | 14/01/2009 2:37 PM |                                                   |

**Associated Items** Custom Variables (0)

Sequence AS12A Calibration and Samples selected

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# Console: Quick Access to Instruments, Data, eWorkflows

**Chromeleon Console**

**Data**

- ChromeleonData
  - Data
    - Amino\_Acids
    - LINEARITY
    - Aspirin
      - Content Uniformity
        - CU\_Aspirin\_20090119
        - CUT Demo - 1 Peak - n=10
        - CUT Demo - 1 Peak - n=20
      - Dissolution
        - 20090112\_AD\_Lot\_No\_20090110\_13346123
        - 20090112\_AD\_Lot\_No\_20090110\_13346125
        - 20090114\_AD\_Lot\_No\_20090111\_13356984
        - 20090115\_AD\_Lot\_No\_20090111\_13356986
        - 20090117\_AD\_Lot\_No\_20090113\_13357035
    - Calibration
    - PAH
    - System Tests
    - Water
      - Anions
        - AS12A Calibration and Samples
        - AS12A Water Analysis\_20081119\_132906
        - Water Analysis
      - Cations
    - Demo\_Data
    - Instrument Data
    - Template Files
      - Instrument Methods
      - Processing Methods
      - Report Templates
      - View Settings
  - ChromeleonLocal
    - Beta\_Test\_Plan\_Data
    - Data
    - Data\_Processing\_Workshop
    - Demo Data
    - Instrument Data
    - Template Files

**AS12A Calibration and Samples**

Run Finished

Studio | Insert Row | Fill Down | Filtering | Grouping | Print

| #  | ECD_1 | Name                        | Type     | Position |                                  |
|----|-------|-----------------------------|----------|----------|----------------------------------|
| 1  |       | Seven Anion Standard II - 1 | Standard | 1        |                                  |
| 2  |       | Seven Anion Standard II - 2 | Standard | 2        | AS12A Anions in Water            |
| 3  |       | Seven Anion Standard II - 3 | Standard | 3        | 25.0000 03 AS12A Anions in Water |
| 4  |       | Seven Anion Standard II - 4 | Standard | 4        | 25.0000 04 AS12A Anions in Water |
| 5  |       | Seven Anion Standard II - 5 | Standard | 5        | 25.0000 05 AS12A Anions in Water |
| 6  |       | Seven Anion Standard II - 6 | Standard | 6        | 25.0000 06 AS12A Anions in Water |
| 7  |       | Drinking Water              | Unknown  | 7        | 25.0000 AS12A Anions in Water    |
| 8  |       | Tap Water                   | Unknown  | 8        | 25.0000 AS12A Anions in Water    |
| 9  |       | Power Coolant Water         |          | 9        |                                  |
| 10 |       | Power Coolant Water         | Unknown  | 10       |                                  |

Click here to add a new injection

**Associated Items**

| Name                               | Type              | Date Modified      | Comment                                           |
|------------------------------------|-------------------|--------------------|---------------------------------------------------|
| Anions in Water                    | Report Definition | 15/01/2009 3:15 PM |                                                   |
| Anions in Water                    | View Settings     | 15/01/2009 3:16 PM |                                                   |
| AS12A Anions in Water              | Instrument Method | 15/01/2009 3:18 PM | Instrument Method Anions in Water on AS12A column |
| AS12A Anions in Water              | Processing Method | 15/01/2009 3:18 PM |                                                   |
| AS12A Production Test Chromatogram | Instrument Method | 14/01/2009 2:37 PM | AS12A Production Test Chromatogram                |
| AS12A Production Test Chromatogram | Processing Method | 14/01/2009 2:37 PM |                                                   |

Custom Variables (0)

Sequence AS12A Calibration and Samples selected

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**Integrated Sequence Editor**

**"MiniPlots"**

# Console: Access to Instruments via ePanels

The screenshot displays the Chromeleon Console software interface. On the left, the 'Instruments' panel lists various instruments, with '08\_Ultimate3000\_RS' selected. The main window shows the 'Diode Array Detector' configuration, including 'Module Status' (Connected), 'Retention Time' (1.110), and 'Module Connect' (Connect). The 'Signals' section shows four UV channels (UV 1 to UV 4) with their respective Wavelength, Bandwidth, Reference Wavelength, and Reference Bandwidth. The 'On-line Plot' displays a chromatogram with multiple peaks. The 'Audit Trail' table at the bottom provides a log of system events.

|   | Date       | Time        | Retention Time | Device              | Message                                                                          |
|---|------------|-------------|----------------|---------------------|----------------------------------------------------------------------------------|
| i | 17/02/2009 | 11:45:20 AM | 0.003          | UV                  | Reading from demo file C:\Program Files\Agilent\Chromeleon\Software\Demo\Demo1.D |
| i | 17/02/2009 | 11:45:19 AM |                | System              | AcqOn                                                                            |
| i | 17/02/2009 | 11:42:41 AM |                | ColumnOven.Column_A | Chip card detected.                                                              |
| i | 17/02/2009 | 11:42:41 AM |                | ColumnOven          | TCC-3x00 - Serial # Dem                                                          |
| i | 17/02/2009 | 11:42:40 AM |                | UV                  | Connected.                                                                       |
| i | 17/02/2009 | 11:42:40 AM |                | PumpModule          | Connected.                                                                       |
| i | 17/02/2009 | 11:42:40 AM |                | UV                  | DAD-3000(RS) @ USB-12345                                                         |
| i | 17/02/2009 | 11:42:40 AM |                | PumpModule          | Connected to HPG-3200RS @                                                        |
| i | 17/02/2009 | 11:42:40 AM |                | UV                  | VIS Lamp on.                                                                     |
| i | 17/02/2009 | 11:42:40 AM |                | UV                  | UV Lamp on.                                                                      |
| i | 17/02/2009 | 11:42:39 AM |                | PumpModule          | Connecting...                                                                    |
| i | 17/02/2009 | 11:42:39 AM |                | UV                  | Connecting...                                                                    |

Instrument 08\_Ultimate3000\_RS selected

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**Immediate Access to  
Audit Trail and Queue**

**Easy Access to  
All Instruments on  
the Network**

**Direct Control of  
Instrument  
via ePanel Controls**

# Chromatography Studio: All Details of an Experiment

The screenshot displays the Chromatography Studio software interface. The **Navigation Pane** on the left shows a tree view of the project structure, including folders like 'Data', 'Instruments', and 'Data Processing'. The **Ribbon** at the top of the main window contains various toolbars for data processing, including 'Chromatogram Tools', 'Data Processing Home', 'Layout', and 'Processing'. The **Category Bars** on the left side of the main window allow users to switch between different views: 'Injection List', 'Instrument Method', 'Data Processing' (selected), 'Report Designer', and 'Spectral Library'. The main window displays a chromatogram plot of 'AAA\_LINEARITY #13' with peaks labeled by retention time and name. Below the plot is a data table with columns for peak number, name, retention time, area, height, and amount.

**Navigation Pane**

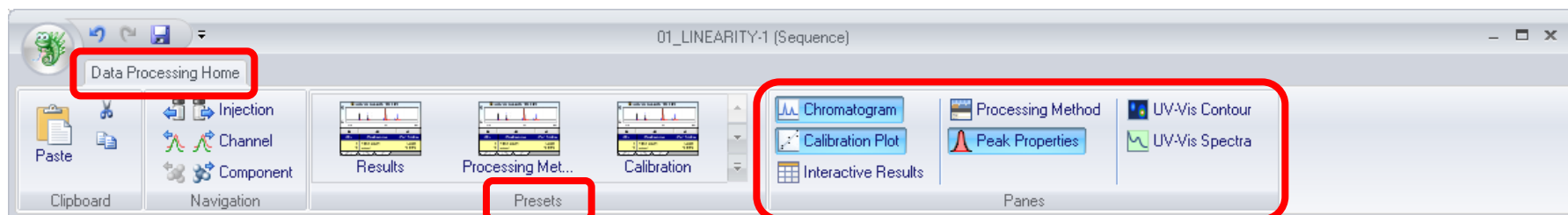
**Ribbon**

**Category Bars**

| No. | Peak Name     | Ret. Time min | Area mAU*min | Height mAU | Amount n.a. |
|-----|---------------|---------------|--------------|------------|-------------|
| 1   | Asn           | 1.52          | 1.6679       | 77.630     | 0.994       |
| 2   | Ser           | 1.63          | 1.8100       | 69.987     | 0.994       |
| 3   | Gln           | 1.83          | 1.2035       | 55.640     | 0.999       |
| 4   | His           | 1.90          | 1.4432       | 66.877     | 0.963       |
| 5   | Gly           | 2.02          | 1.2099       | 55.516     | 1.009       |
| 6   | Thr           | 2.08          | 1.2767       | 53.939     | 1.001       |
| 7   | Arg           | 2.32          | 1.7114       | 78.991     | 0.994       |
| 8   | Ala           | 2.48          | 1.4639       | 62.244     | 0.994       |
| 9   | Tyr           | 2.85          | 1.6052       | 70.724     | 0.997       |
| 10  | Cys-Cys       | 3.22          | 0.3734       | 10.350     | 0.992       |
| 11  | Val           | 3.45          | 1.3500       | 56.153     | 1.002       |
| 12  | Met           | 3.52          | 1.4851       | 60.742     | 1.000       |
| 13  | Trp           | 3.77          | 1.3529       | 54.737     | 0.996       |
| 14  | Phe           | 3.89          | 1.2871       | 51.658     | 0.999       |
| 15  | Ile           | 3.97          | 0.7160       | 28.705     | 1.006       |
| 16  | Leu           | 4.17          | 1.0620       | 40.784     | 0.994       |
| 17  | Lys           | 4.31          | 1.7740       | 68.245     | 0.984       |
| 18  | Pro-OH        | 4.51          | 0.7832       | 12.226     | 1.235       |
| 19  | FMOC Impurity | 4.72          | 0.8151       | 26.856     | 0.975       |

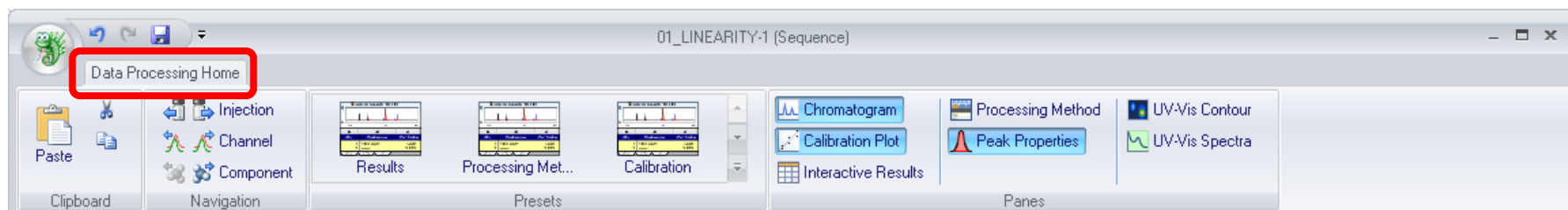
# New Ribbon Interface

- Provides contextual access to commands and options in the Studio
- General options via Home ribbon (always available):



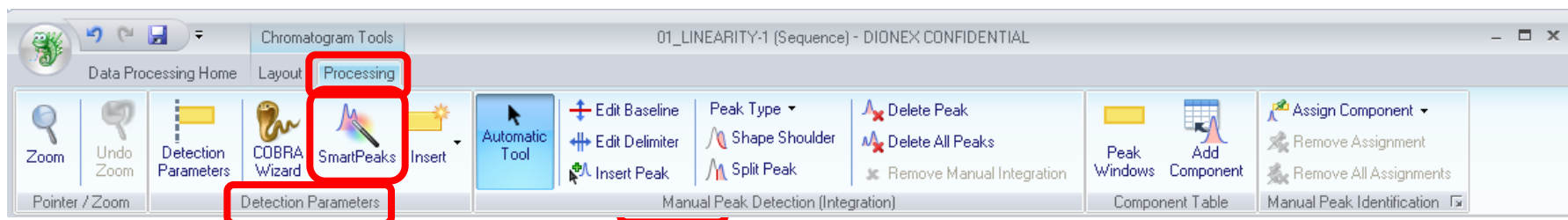
# New Ribbon Interface

- Provides contextual access to commands and options in the Studio
- Minimize the ribbon area by double-clicking any ribbon tab



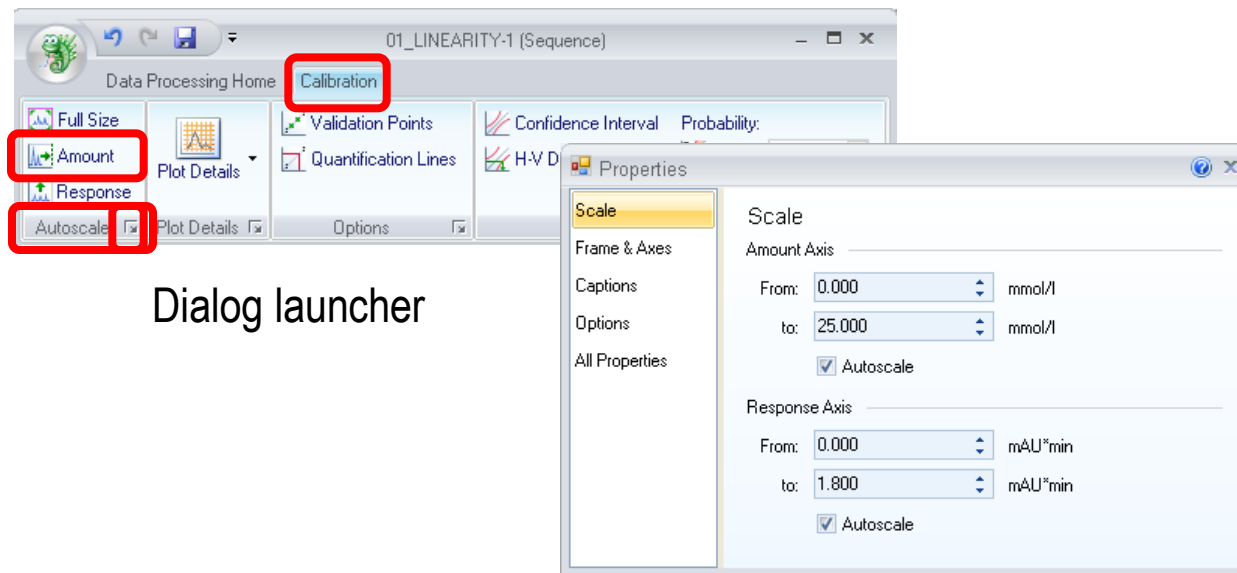
# New Ribbon Interface

- Provides contextual access to commands and options in the Studio
- Chromatogram options via Contextual Ribbons:

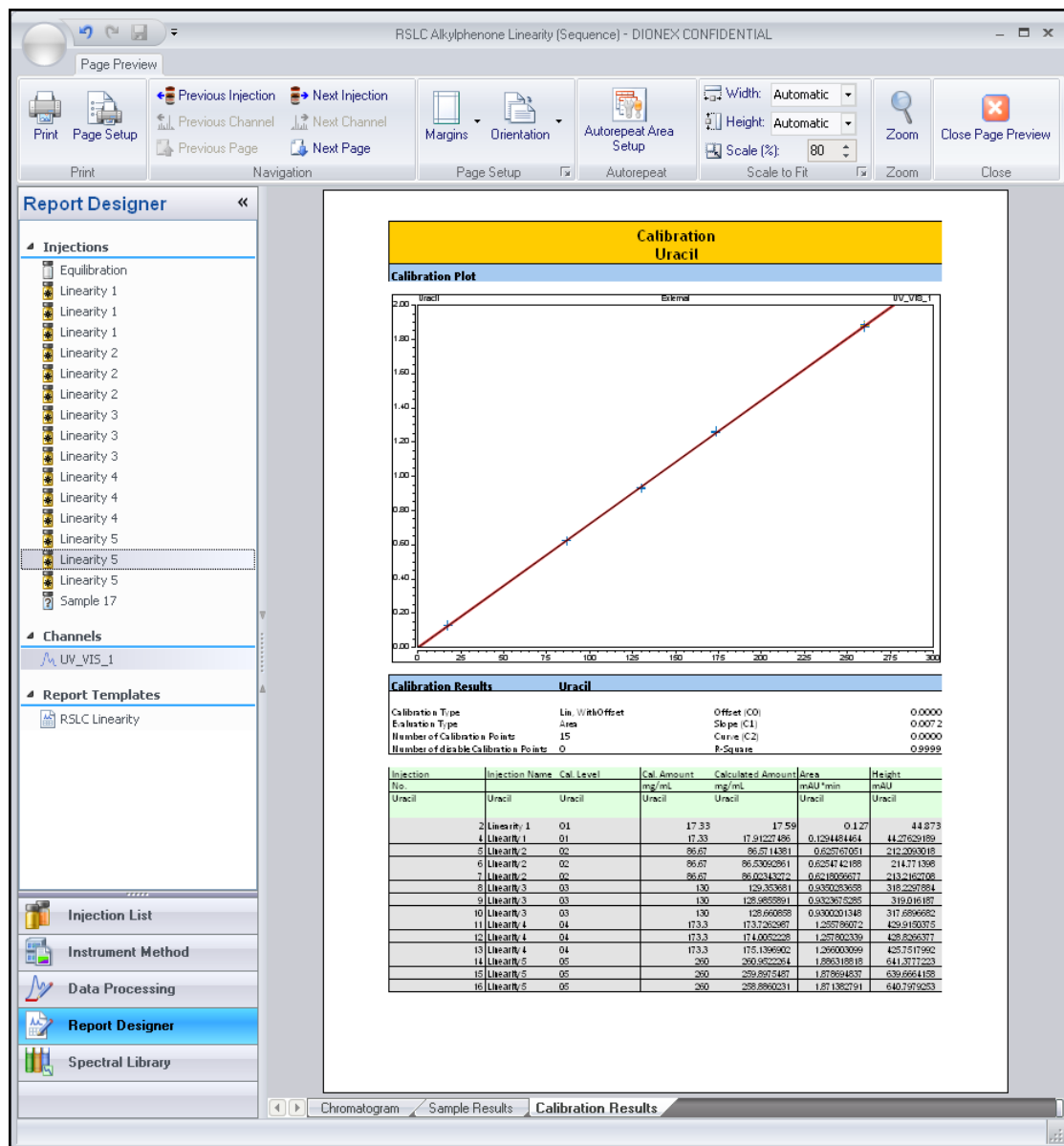


# New Ribbon Interface

- Provides contextual access to commands and options in the Studio
- Calibration Plot options via Contextual Ribbon:



# Chromatography Studio: Report Designer



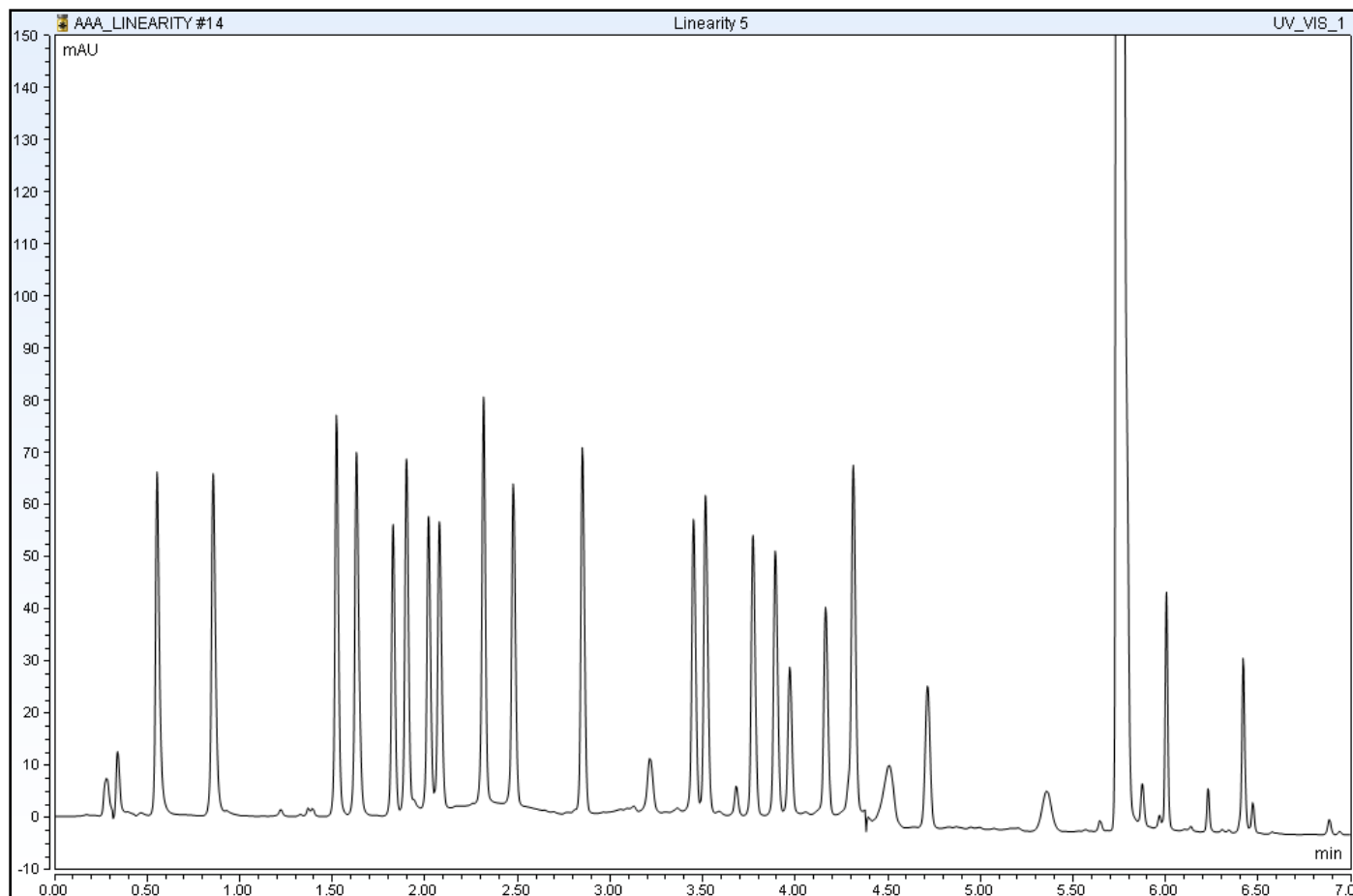
- Fully customizable report templates
- Built-in spreadsheet capabilities

---

# **Chromeleon 7: Peak Detection and Integration**

---

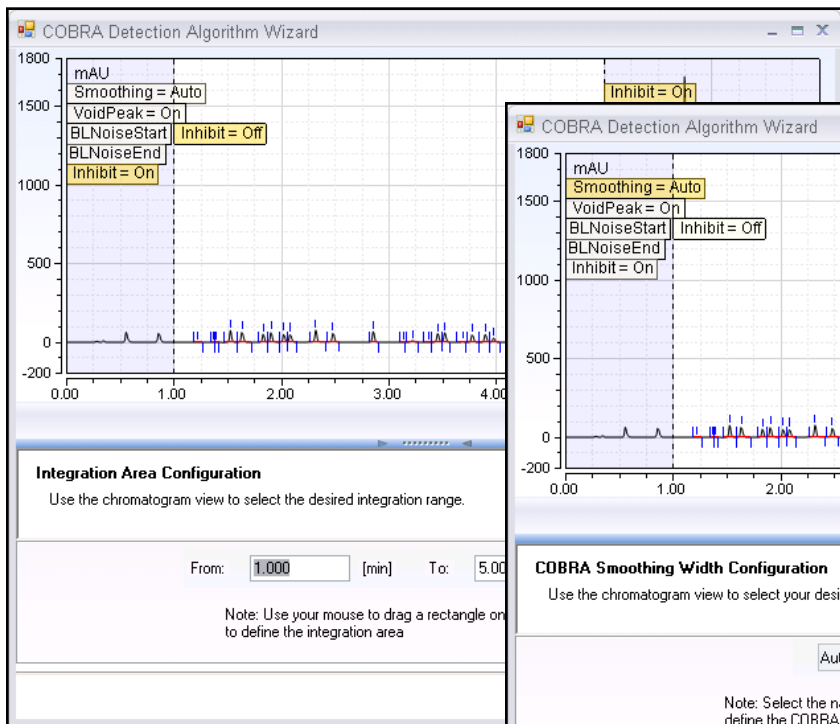
# Cobra™ Peak Detection Algorithm



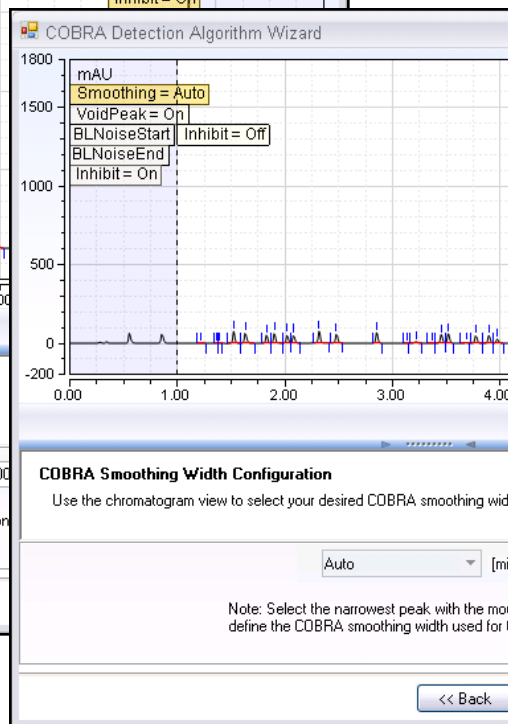
# Cobra™ Peak Detection Algorithm



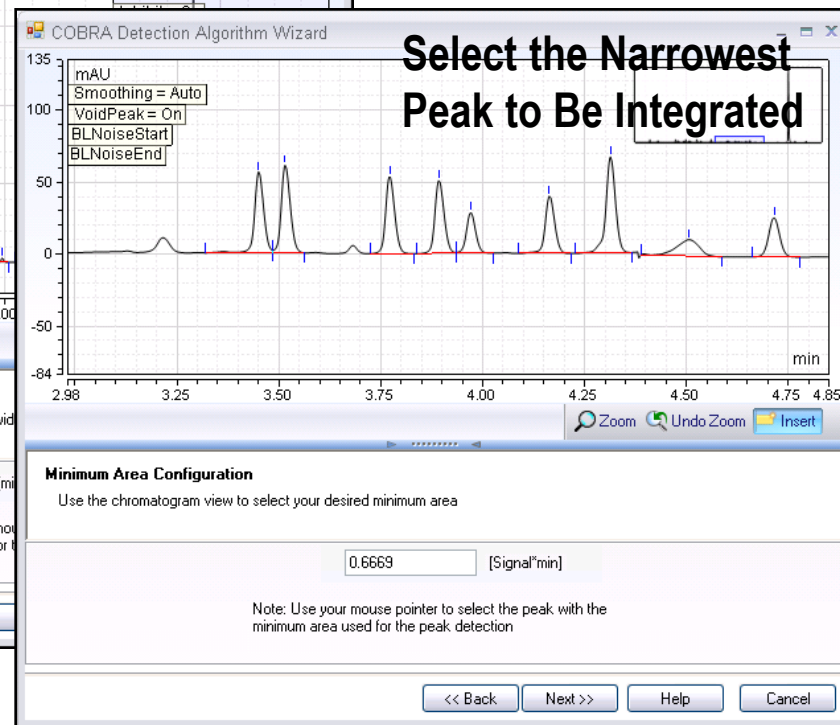
Start Cobra Wizard



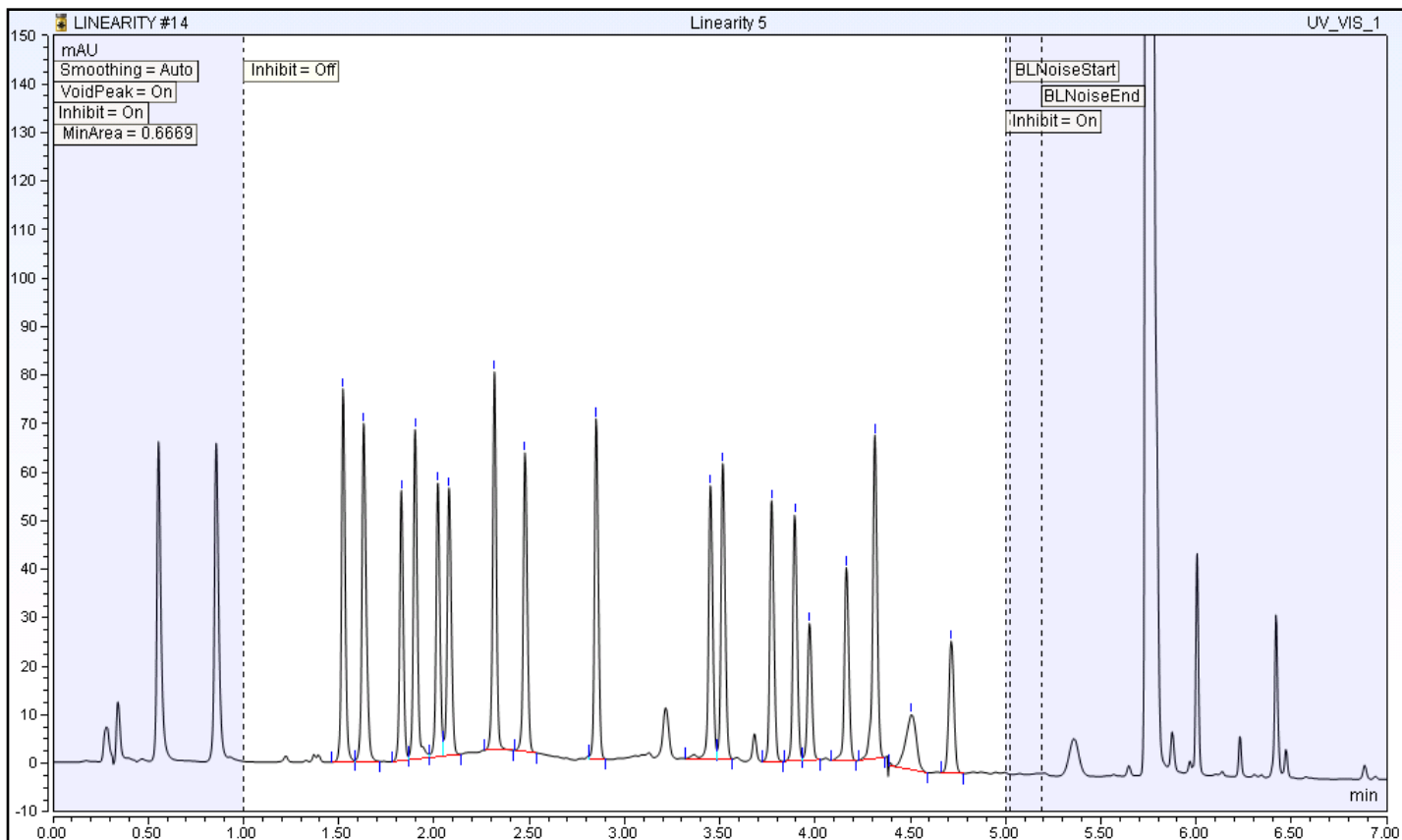
Define the Integration Range



Select the Smallest Peak to Be Integrated



# Cobra™ Peak Detection Algorithm

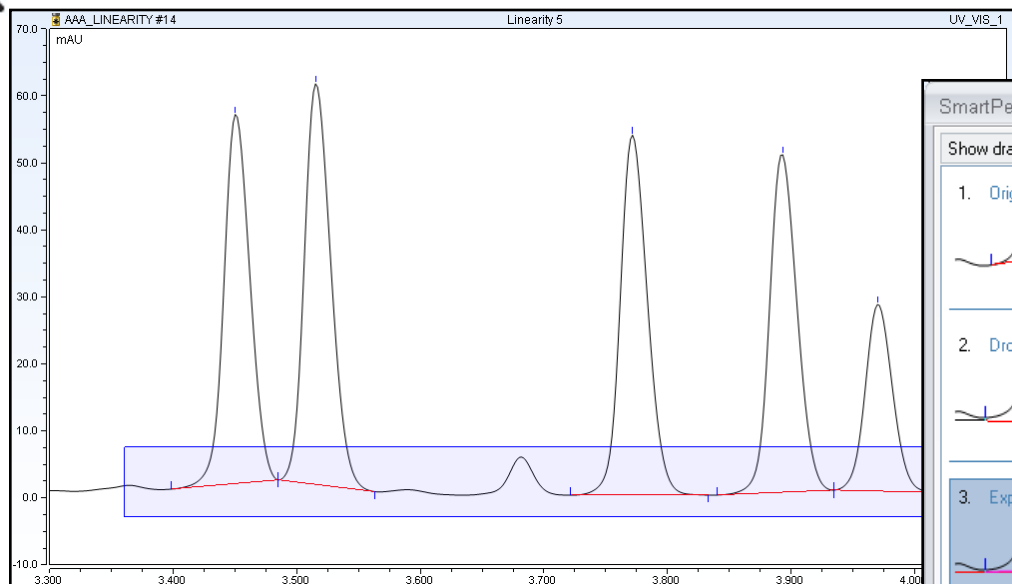


**And Your Integration Is Done!**

# SmartPeaks™ Integration Assistant

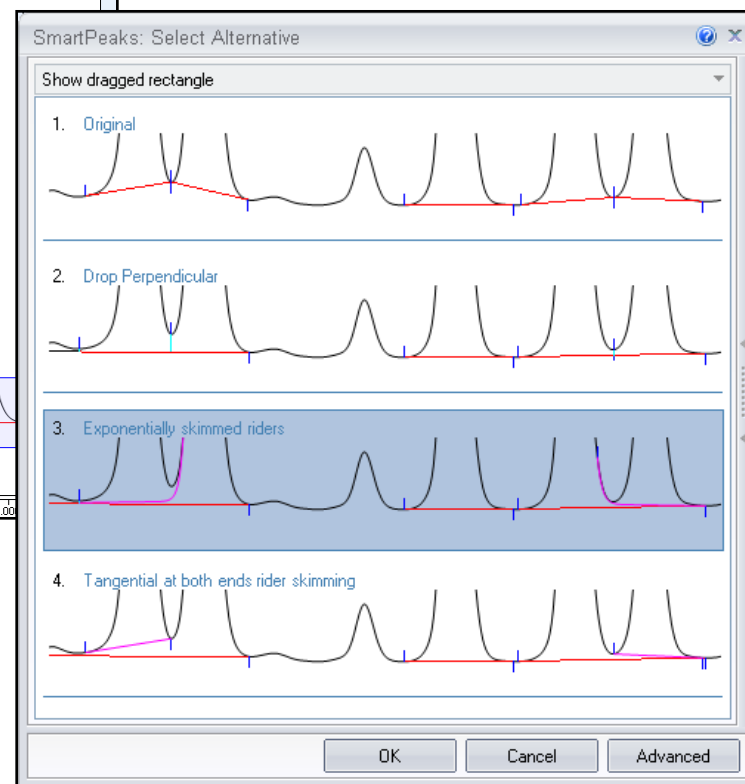


## Activate SmartPeaks Wizard

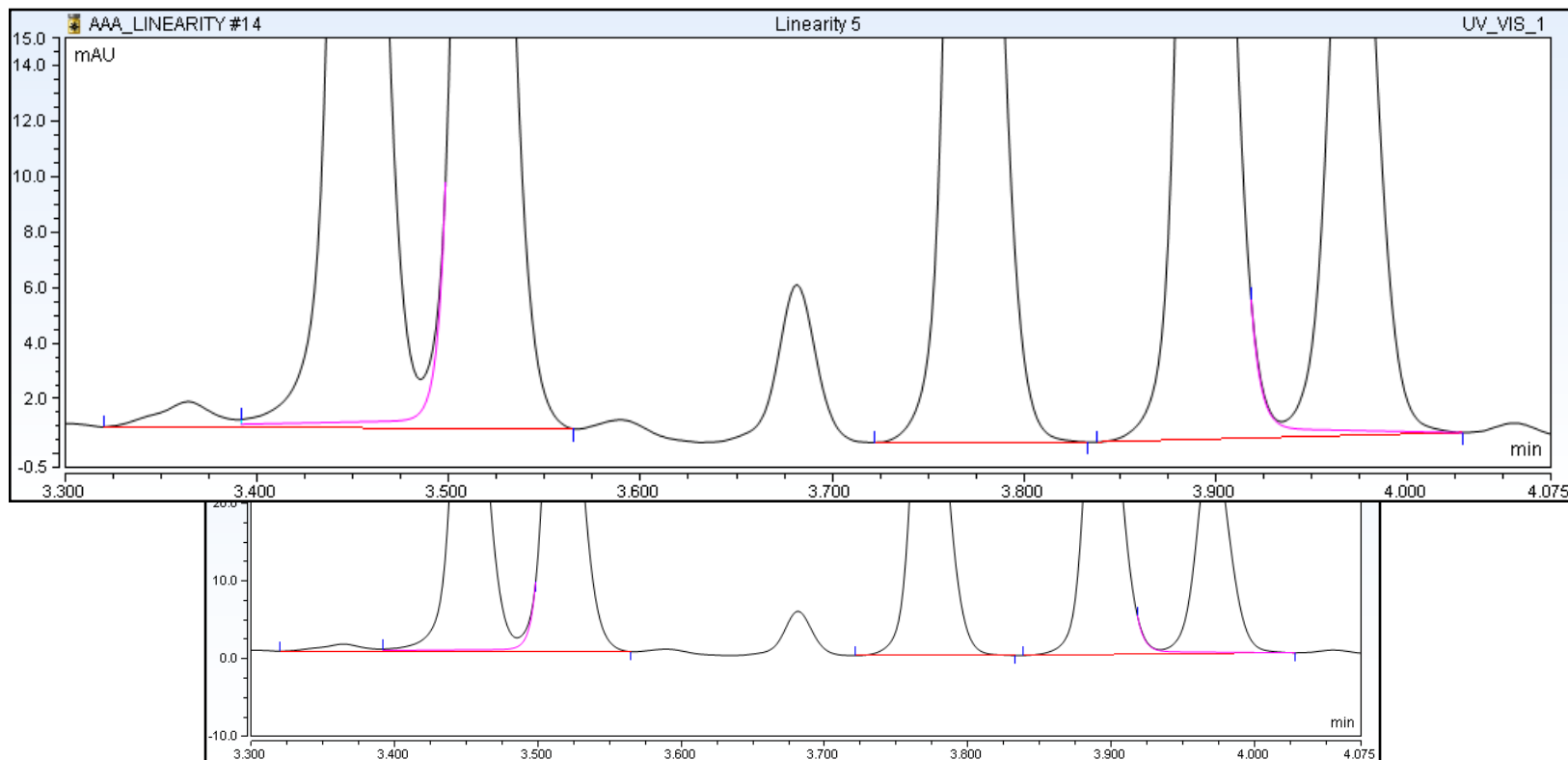


**Select Area of Interest**

**Select the Integration You Want**



# SmartPeaks™ Integration Assistant



**And Your Integration Is Done!**

---

# Chromeleon 7 eWorkflows

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# eWorkflows

---

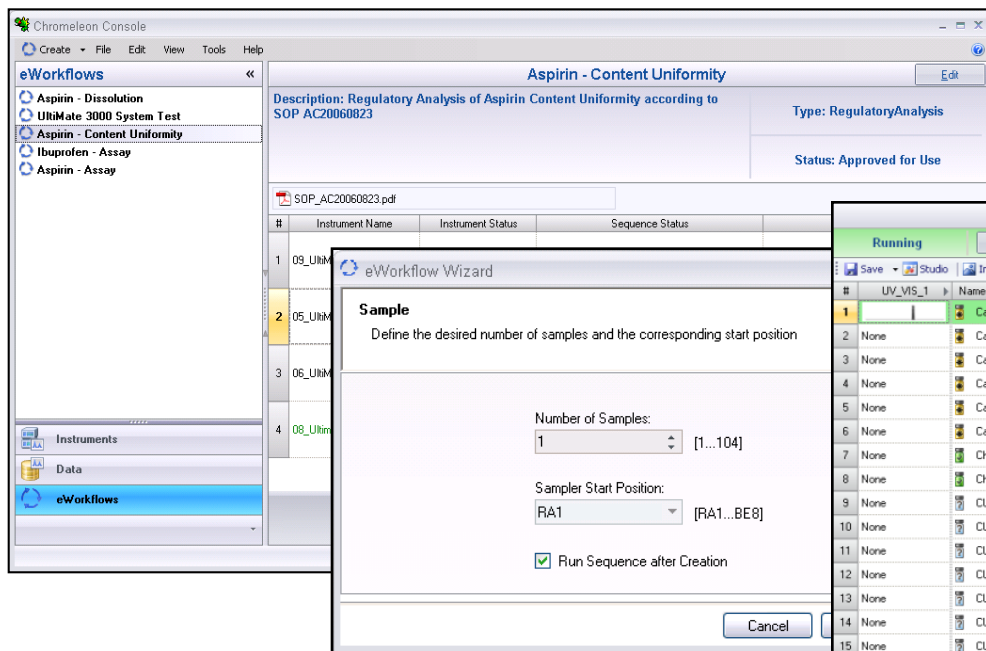
- High-level automation of all chromatography processes
- Useful for all laboratory applications, such as:
  - Quality Analysis / Quality Control
  - Method development
  - Research and development
  - Walk-up analysis
- Take you from samples to results in only a few steps
- Easily customized to suit diverse applications and user skill levels

# eWorkflows: All Aspects of a Chromatographic Analysis

---

- Instruments on which the analysis can be run
- All associated files:
  - Instrument methods
  - Processing methods
  - Reports
  - Spectral libraries
  - Documents with description of method
- Template for sequence name and storage location
- Custom variables
- Rules for sequence layout

# eWorkflow for a Regulated USP/EP Method



Sequence Is Created and  
Can Be Immediately Run

Running

Stop Now

CU\_Aspirin\_20090119

05\_Ultimate3000\_1 (Running)

| #  | UV_VIS_1 | Name                 | Type       | Level | Position | Volume [μl] | Pharmacopeia | Dosage Form        | Status  | Inje |
|----|----------|----------------------|------------|-------|----------|-------------|--------------|--------------------|---------|------|
| 1  |          | Calibration          | Standard   | 01    | RA1      | 10.000      | EP           | Common Dosage Form | Running | 19/  |
| 2  | None     | Calibration          | Standard   | 01    | RA1      | 10.000      | EP           | Common Dosage Form | Idle    |      |
| 3  | None     | Calibration          | Standard   | 02    | RA2      | 10.000      | EP           | Common Dosage Form | Idle    |      |
| 4  | None     | Calibration          | Standard   | 02    | RA2      | 10.000      | EP           | Common Dosage Form | Idle    |      |
| 5  | None     | Calibration          | Standard   | 03    | RA3      | 10.000      | EP           | Common Dosage Form | Idle    |      |
| 6  | None     | Calibration          | Standard   | 03    | RA3      | 10.000      | EP           | Common Dosage Form | Idle    |      |
| 7  | None     | Check Standard       | Validation | 04    | RA4      | 10.000      | EP           | Common Dosage Form | Idle    |      |
| 8  | None     | Check Standard       | Validation | 04    | RA4      | 10.000      | EP           | Common Dosage Form | Idle    |      |
| 9  | None     | CUT_Asp_86315 No. 1  | Unknown    |       | RA5      | 10.000      | EP           | Common Dosage Form | Idle    |      |
| 10 | None     | CUT_Asp_86315 No. 2  | Unknown    |       | RA6      | 10.000      | EP           | Common Dosage Form | Idle    |      |
| 11 | None     | CUT_Asp_86315 No. 3  | Unknown    |       | RA7      | 10.000      | EP           | Common Dosage Form | Idle    |      |
| 12 | None     | CUT_Asp_86315 No. 4  | Unknown    |       | RA8      | 10.000      | EP           | Common Dosage Form | Idle    |      |
| 13 | None     | CUT_Asp_86315 No. 5  | Unknown    |       | RB1      | 10.000      | EP           | Common Dosage Form | Idle    |      |
| 14 | None     | CUT_Asp_86315 No. 6  | Unknown    |       | RB2      | 10.000      | EP           | Common Dosage Form | Idle    |      |
| 15 | None     | CUT_Asp_86315 No. 7  | Unknown    |       | RB3      | 10.000      | EP           | Common Dosage Form | Idle    |      |
| 16 | None     | CUT_Asp_86315 No. 8  | Unknown    |       | RB4      | 10.000      | EP           | Common Dosage Form | Idle    |      |
| 17 | None     | CUT_Asp_86315 No. 9  | Unknown    |       | RB5      | 10.000      | EP           | Common Dosage Form | Idle    |      |
| 18 | None     | CUT_Asp_86315 No. 10 | Unknown    |       | RB6      | 10.000      | EP           | Common Dosage Form | Idle    |      |
| 19 | None     | Check Standard       | Validation | 04    | RA4      | 10.000      | EP           | Common Dosage Form | Idle    |      |
| 20 | None     | Check Standard       | Validation | 04    | RA4      | 10.000      | EP           | Common Dosage Form | Idle    |      |

Click here to add a new injection

| Name        | Type              | Date Modified       | Comment                   |
|-------------|-------------------|---------------------|---------------------------|
| Aspirin CUT | Processing Method | 19/01/2009 11:55 AM |                           |
| Aspirin CUT | Report Definition | 19/01/2009 11:55 AM |                           |
| Aspirin CUT | Instrument Method | 19/01/2009 11:55 AM | Aspirin CUT on Ultimate_1 |
| Aspirin CUT | View Settings     | 19/01/2009 11:55 AM |                           |

Associated Items Custom Variables

Choose eWorkflow,  
Select Instrument,  
and Click "Start"

Enter Number of  
Samples and  
Start Position

# eWorkflow for a Regulated USP/EP Method

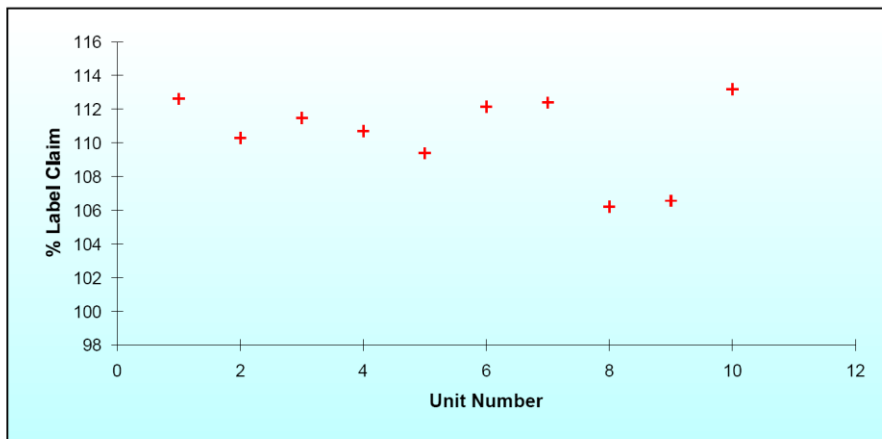
## Uniformity of Dosage Units Report

### General

|                      |                     |                                 |                     |
|----------------------|---------------------|---------------------------------|---------------------|
| Product Batch Number | 86315               | Target Content <i>T</i>         | 102.0               |
| Peak Name            | Aspirin             | Correction Factor               | 1.050               |
| CUT Number           | 186781              | Max. Acceptance Value <i>L1</i> | 15.0                |
| Channel              | UV_VIS_1            | Lower Amount Limit              | Not needed if n=10! |
| Dosage Form          | Common Dosage Forms | Upper Amount Limit              | Not needed if n=10! |
| Pharmacopeia         | EP                  |                                 |                     |

### Results

|                             |                        |
|-----------------------------|------------------------|
| Mean                        | <b>n = 10</b><br>110.5 |
| Standard Deviation <i>s</i> | 2.5                    |
| Reference Value <i>M</i>    | 102.0                  |
| Acceptance Value <i>AV</i>  | 14.4                   |
| Test Result                 | <b>Test passed</b>     |



## This eWorkflow Also:

- Processes all data
- Calculates all results

---

# Closing Remarks

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# Usability in Practice: Key Attributes of Chromeleon 7

- **Visual:** Taking advantage of the human brain's fast visual processing
- **Contextual:** Displaying items only when and where they are relevant
- **Predictable:** Appearing and behaving consistently, and as expected
- **Discoverable:** Inviting exploration without creating distraction
- **Helpful:** Allowing only valid choices, displaying useful tips, providing easy access to more information

ISO Slide Number

# Chromeleon 7—Simply Intelligent



- Provides the **intelligent functionality** needed to generate results
- Minimizes time and effort through **Operational Simplicity™**
  - New user interface with Console for navigation, Studio for analysis
  - Cobra™ peak detection algorithm and SmartPeaks™ integration assistant
  - eWorkflows—the framework for operational simplicity
- Establishes new benchmarks for usability and productivity

# Thanks for attending!

