

OpenLab CDS

Introducing the Custom Calculator

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Agilent OpenLab



Agilent CrossLab

OpenLab CDS

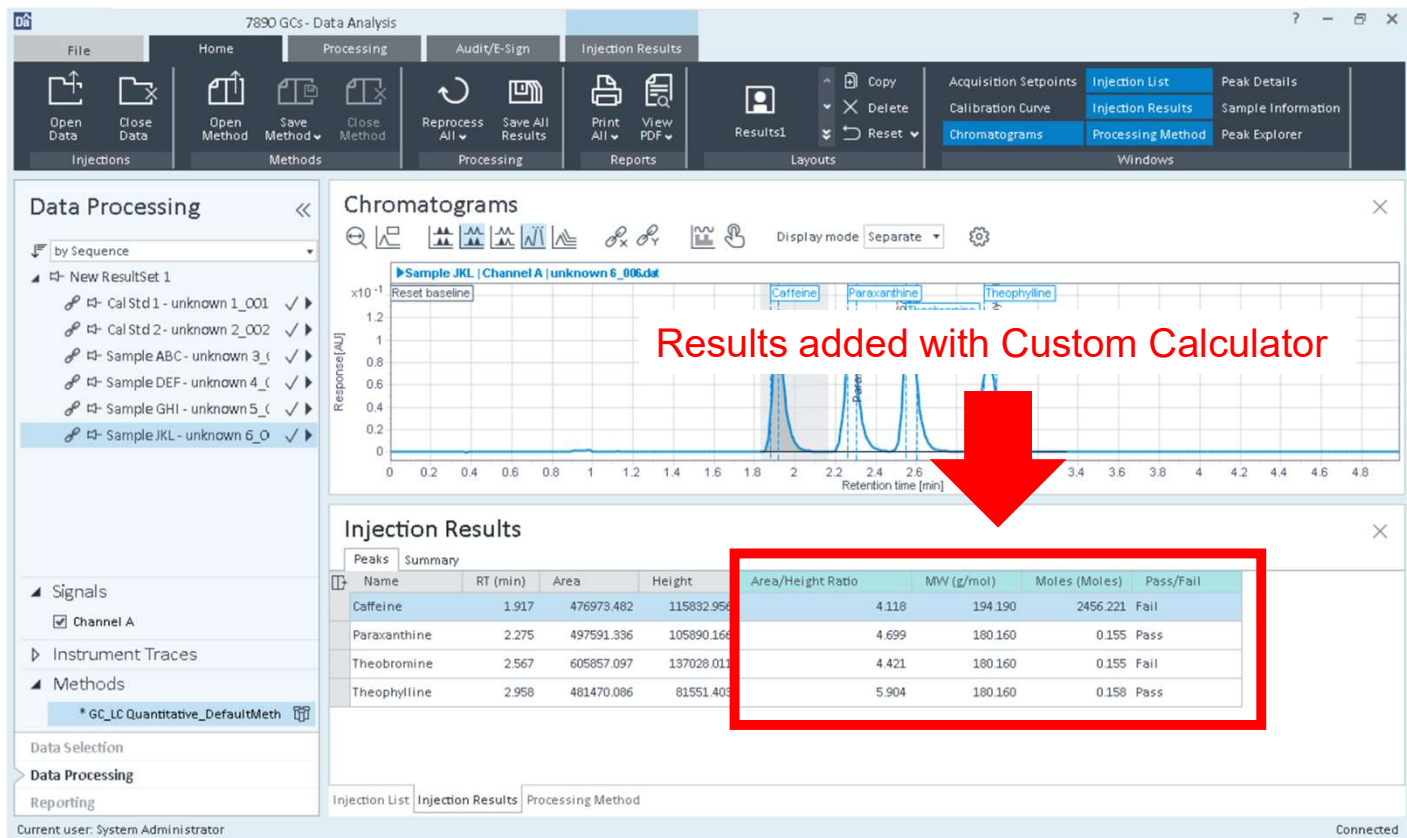
Introducing the Custom Calculator

What is the Custom Calculator?

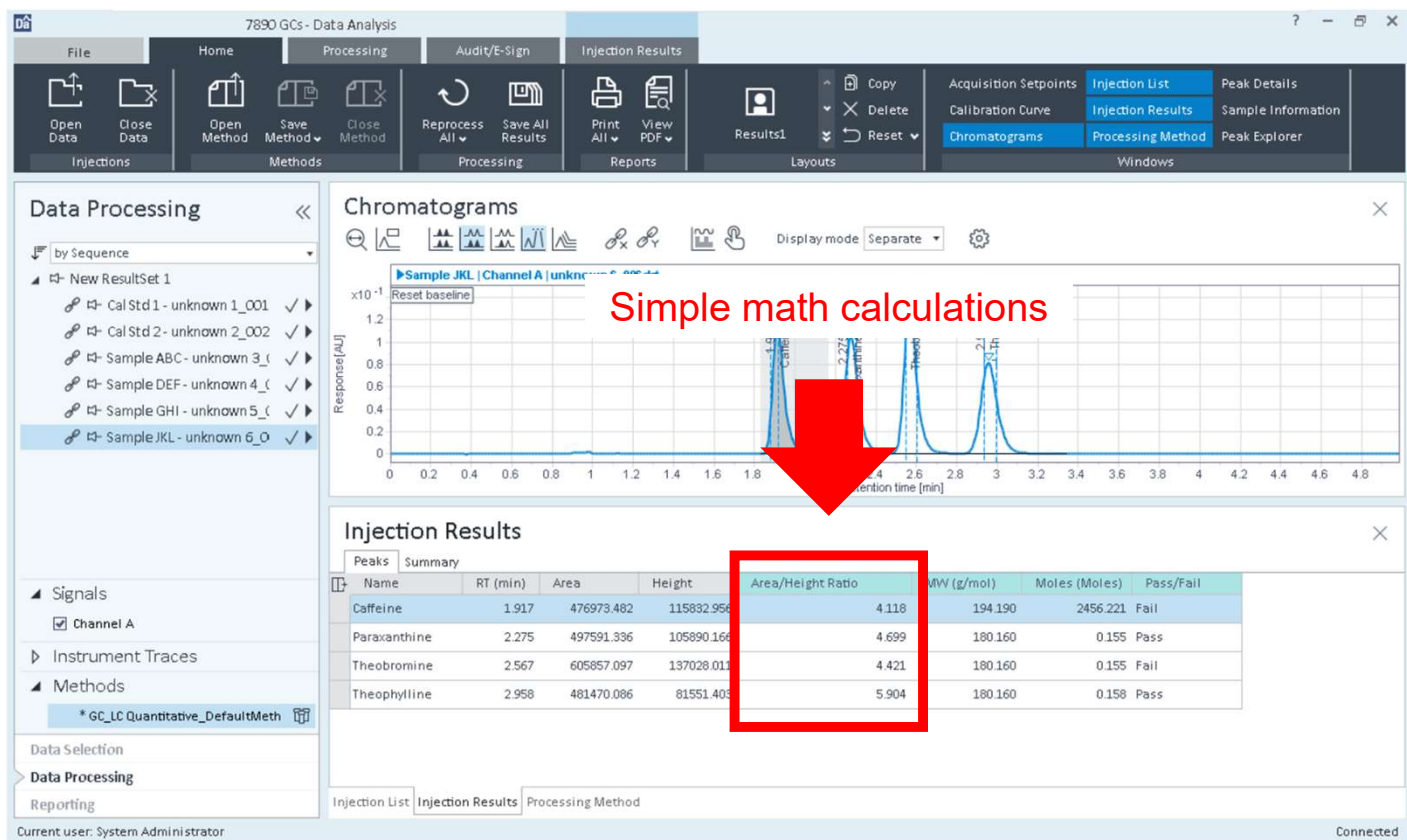
New to OpenLab CDS

- Allows users to extend the data system calculations
 - Simple math – apply a conversion factor
 - Add constants – physical constants per peak; MW, boiling point, density...
 - Logic expressions – check pass/fail criteria
 - Complex multistep calculations – RGA, fatty acids
- These calculated results appear in the data system results view.
- Enables data review inside OpenLab CDS without report generation
- Custom Calculations can be included in reports and exports
- Compliance
 - Each Custom Calculation file has its own audit trail
 - Restricted access to build / edit calculations

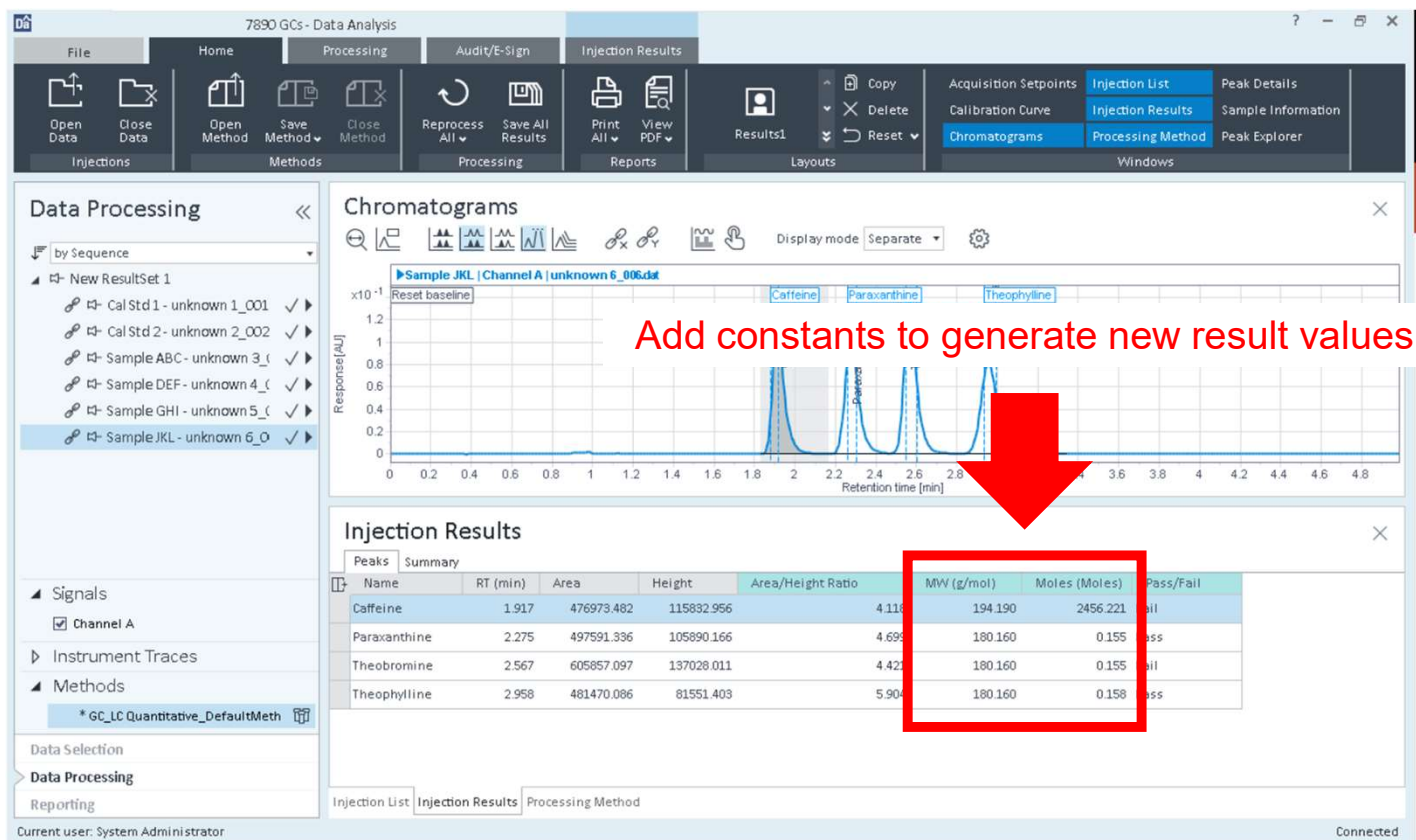
Results added with Custom Calculator



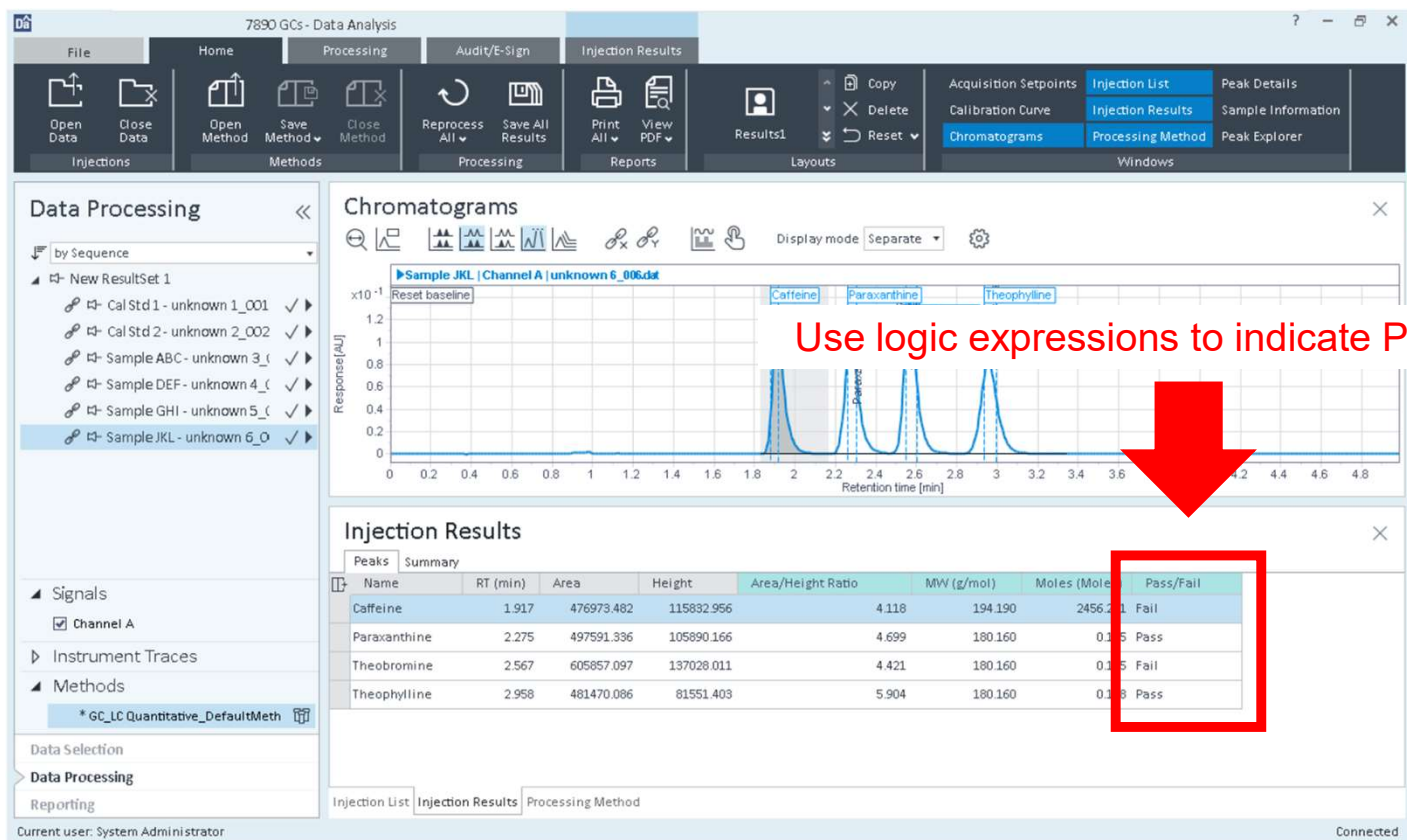
Results added with Custom Calculator



Results added with Custom Calculator



Results added with Custom Calculator



In this Webinar...

- **Launching the Custom Calculator Editor**
- **Add a basic math expression**
- **Add a constant file**
- **Use a constant to generate a new result**
- **Add a simple logic expression**
- **Use OpenLab CDS's Intelligent Reporter to create a report with Custom Calculation values**

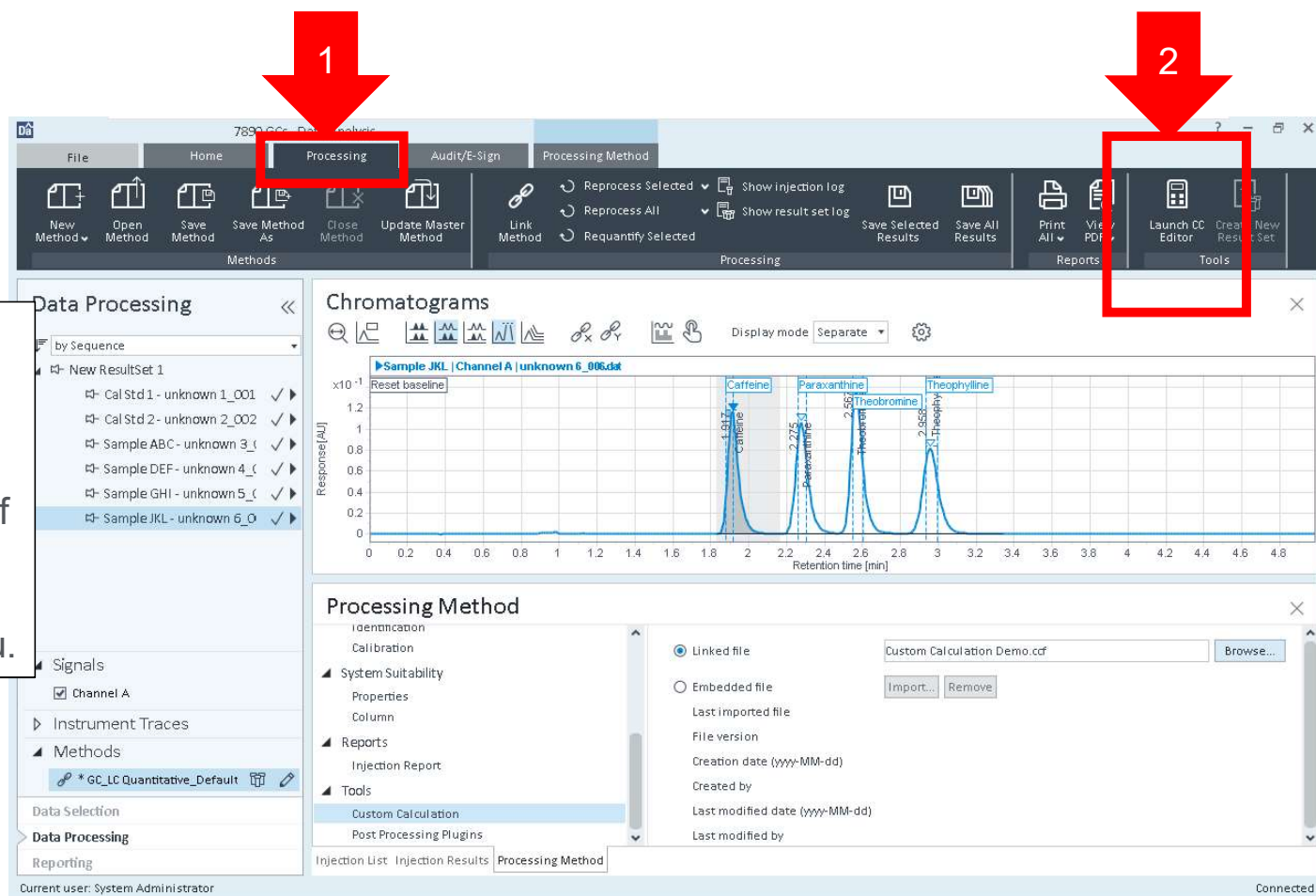
Custom Calculator

Launching the Custom Calculator Editor

Launching the Custom Calculator

The Custom Calculator is part of OpenLAB CDS's Data Analysis

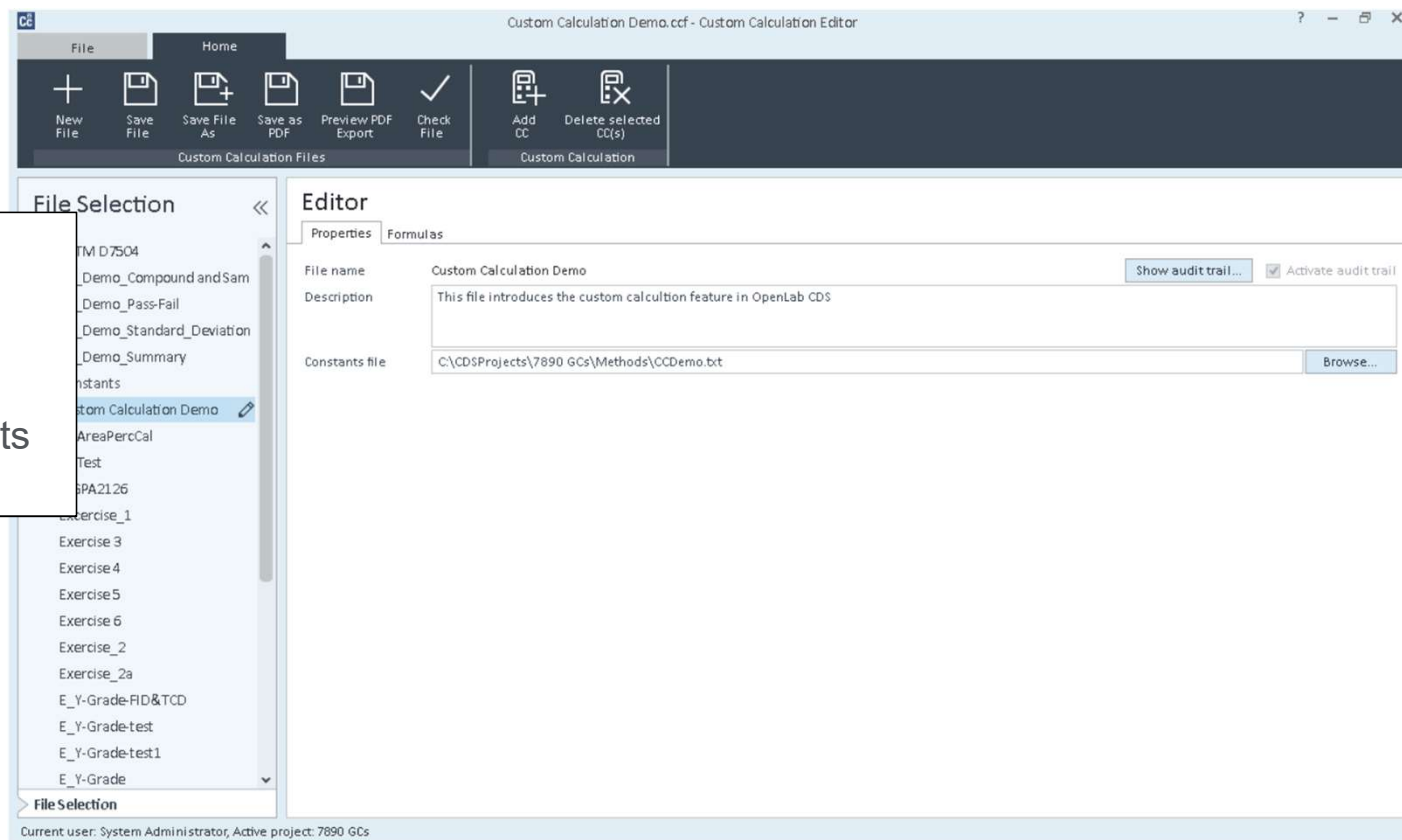
- 1.) In Data Analysis, switch to the Processing tab at the top of the window
- 2.) Then select the Launch CC Editor button in the Tools menu.



Custom Calculation Editor

The Editor's Properties Tab

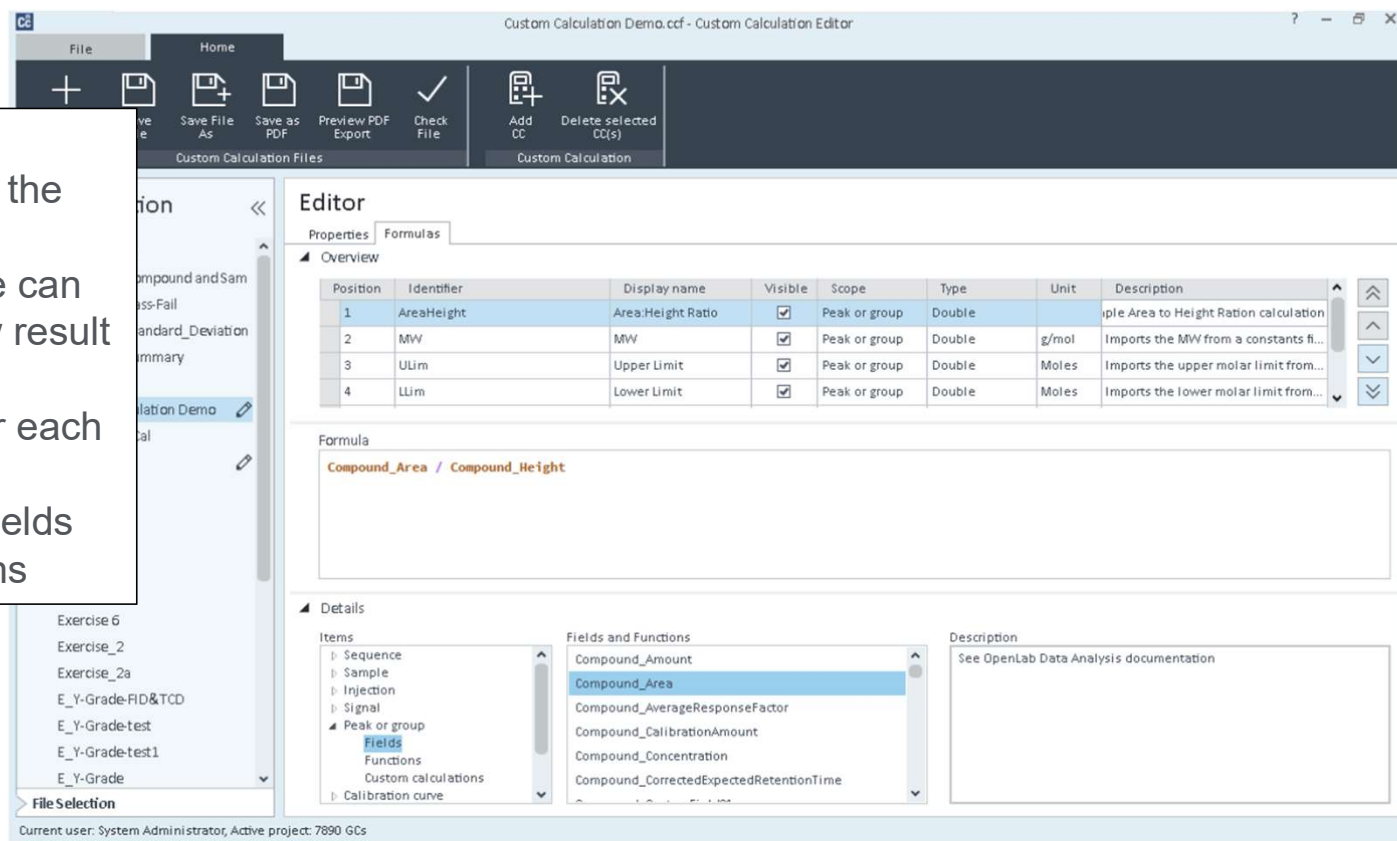
- The Custom Calculation File name
- Audit trail options
- A place to specify a Constants File



Custom Calculation Editor

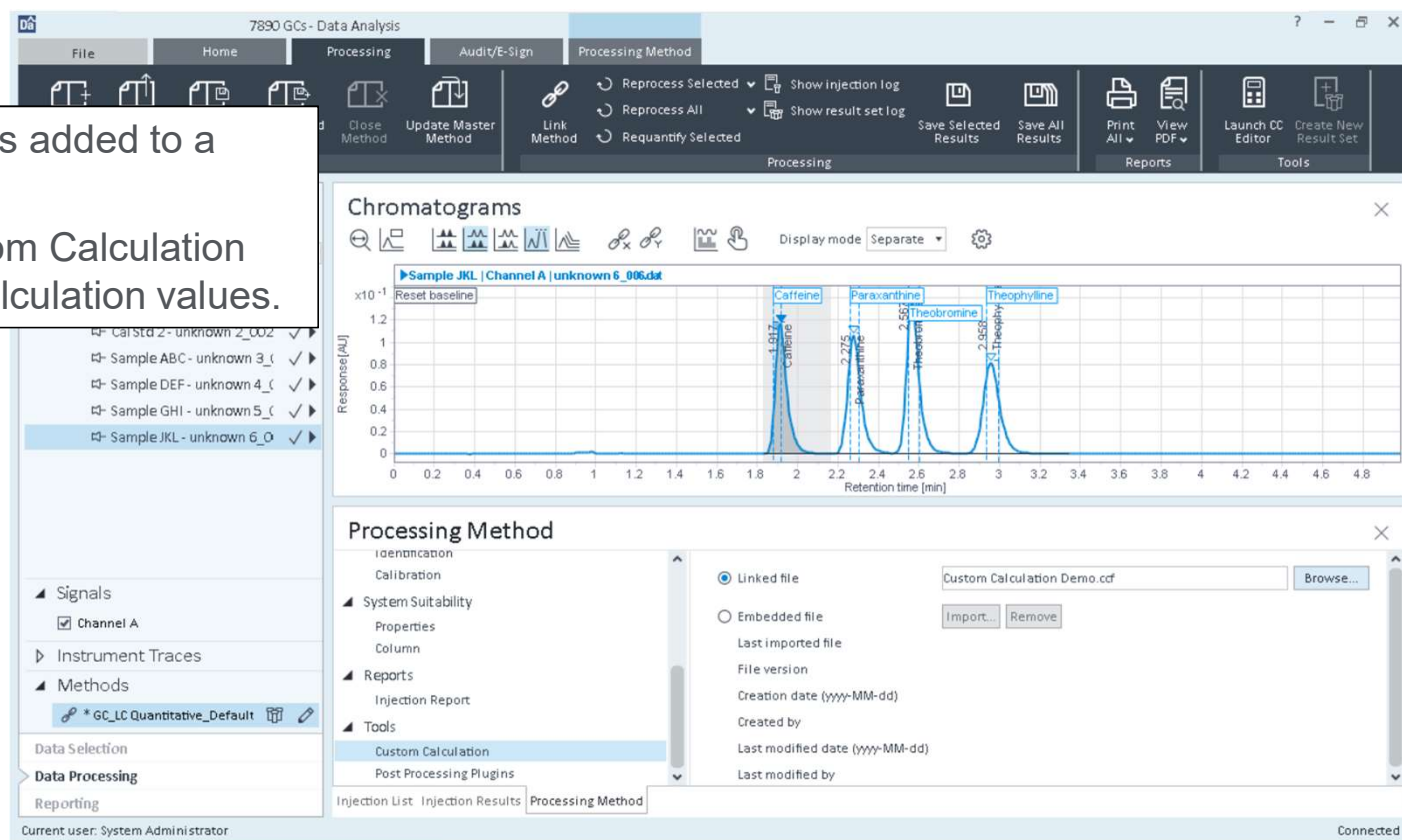
The Editor's Formula's tab:

- Overview: a list of all CCs in the file
One Custom Calculator file can generate one of many new result values.
- Formula: the expressions for each CC
- Details: The available data fields and commonly used functions



Adding Custom Calculation to a Processing Method

The Custom Calculation file is added to a Processing Method.
Data Processed with a Custom Calculation file, contains the specified calculation values.



Custom Calculator

Building expressions

Defining a Simple Math Expression

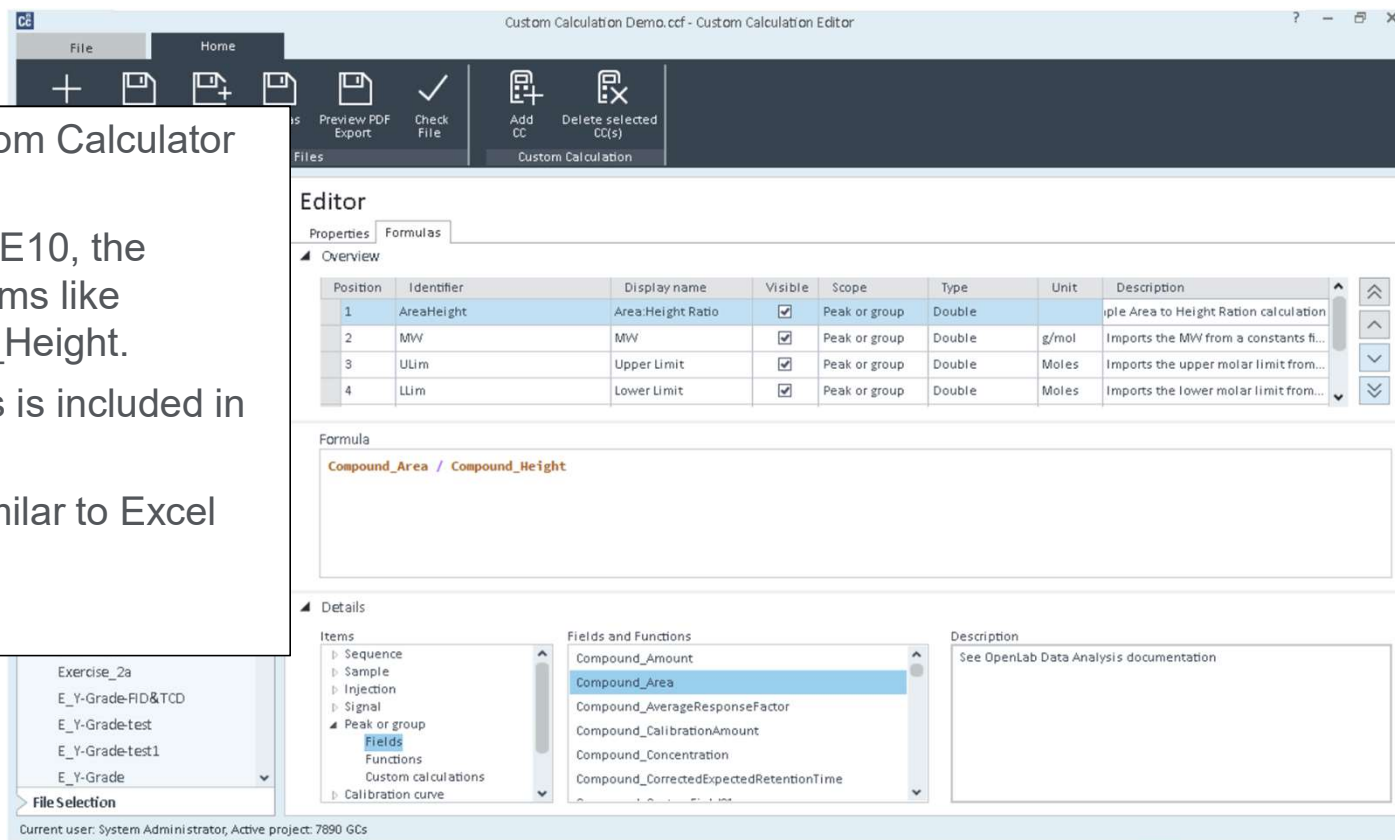
Basic Calculations in the Custom Calculator follow a MS Excel like syntax.

Rather than cell numbers: A1, E10, the expressions reference data items like Compound_Area, Compound_Height.

A list of all available data items is included in the Details area.

Use mathematical symbols similar to Excel for simple expressions:

$+$, $-$, $*$, and $/$

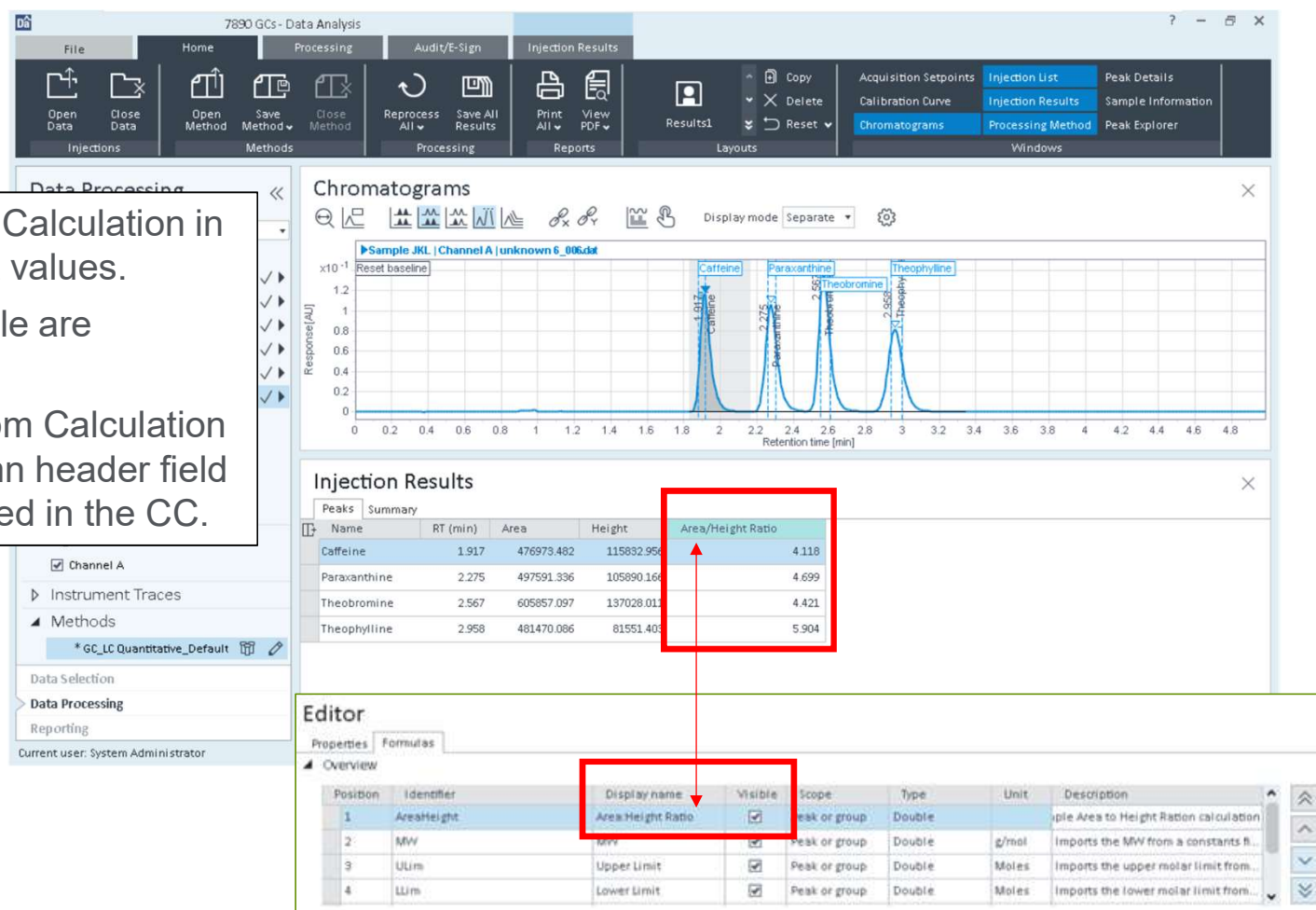


Results of a Simple Math Expression Inside OpenLab CDS

Data processed with a Custom Calculation in the method contains new result values.

Individual CCs marked as Visible are available in the results display.

Results generated with a Custom Calculation are displayed with a blue column header field using the Display Name specified in the CC.



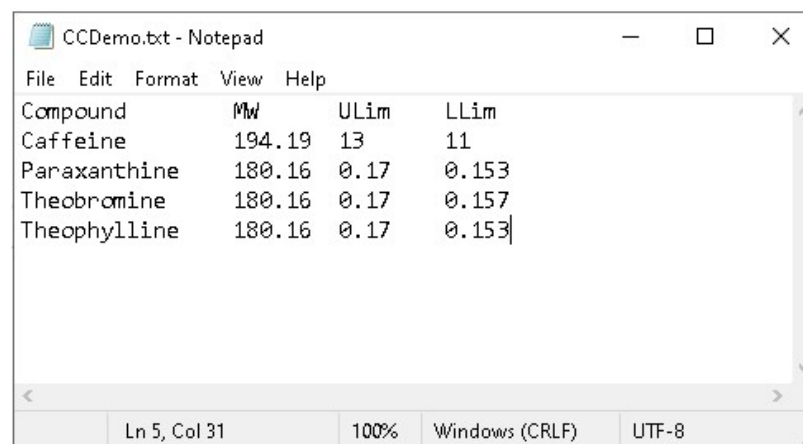
Adding Constants – Tab Delimited Text File

Compound Constants can be added to a Custom Calculation file via a tab delimited text file.

The first column of this file must contain the compound names – and these names must match – exactly – the peak names specified in the method Peak Table

One Constants file can be shared by many CC files.

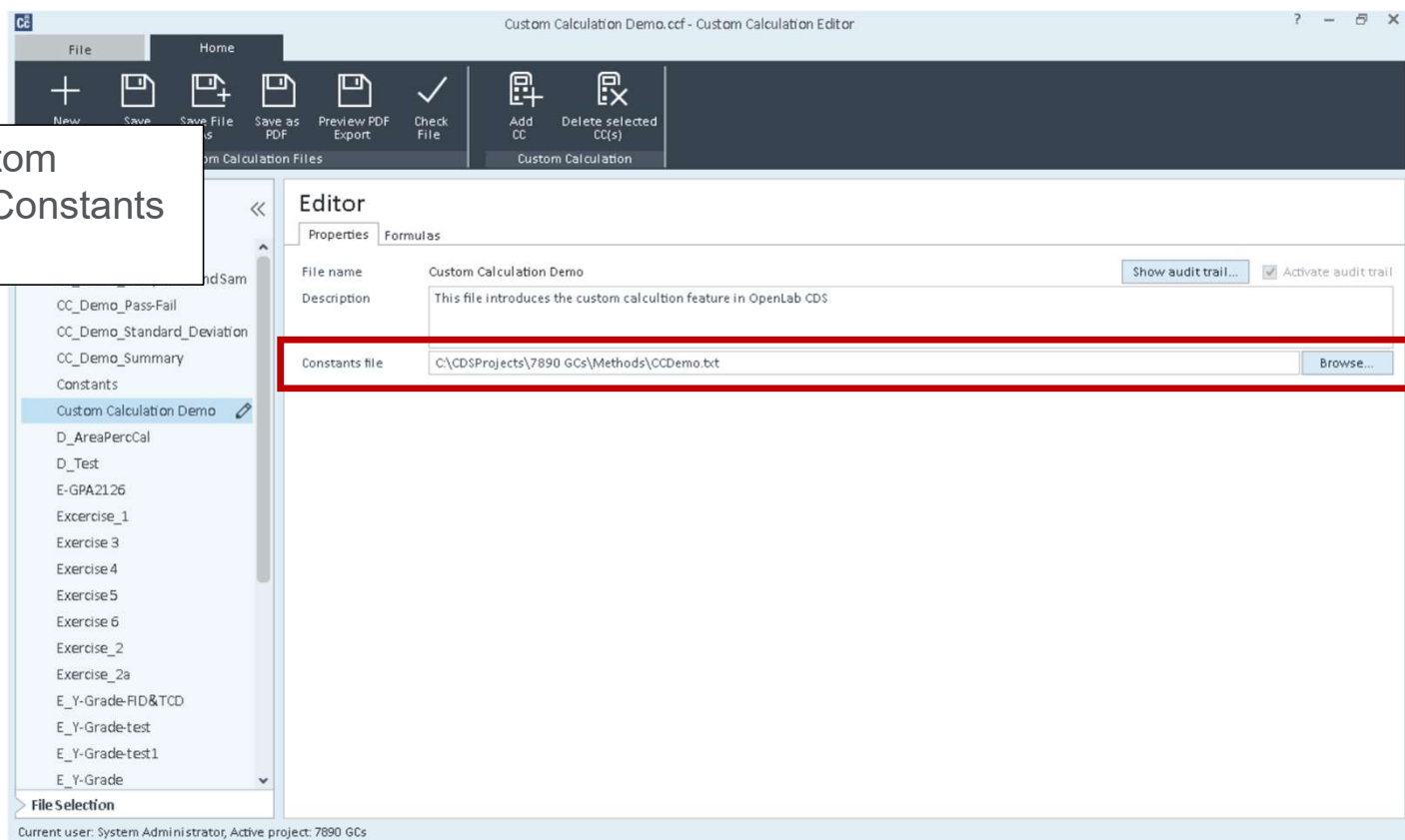
A CC file can use all, or just a portion of the information in the Constants file.



Compound	MW	ULim	LLim
Caffeine	194.19	13	11
Paraxanthine	180.16	0.17	0.153
Theobromine	180.16	0.17	0.157
Theophylline	180.16	0.17	0.153

Adding a Constants File to a Custom Calculation

On the Properties tab in the Custom Calculator Editor, browse to the Constants File.



Adding Constants to a Custom Calculation

The Function:

GetConstant("MW")

Is used to bring values from the Constant File into the Custom Calculation file.

The text **"MW"** should be the same text used in the header row of the Constant File.

CCDemo.txt - Notepad

Compound	MW	ULim	LLim
Caffeine	194.19	13	11
Paraxanthine	180.16	0.17	0.153
Theobromine	180.16	0.17	0.157
Theophylline	180.16	0.17	0.153

Ln 5, Col 31 100% Windows (CRLF) UTF-8

Custom Calculation Demo.ccf - Custom Calculation Editor

Save as PDF Preview PDF Export Check File Add CC Delete selected CC(s)

Editor

Properties Formulas

Overview

Position	Identifier	Display name	Visible	Scope	Type	Unit	Description
1	MW	MW	☒	Peak or group	Double	g/mol	Imports the MW from a constants file...
2	ULim	Upper Limit	☒	Peak or group	Double	Moles	Imports the upper molar limit from...
3	LLim	Lower Limit	☒	Peak or group	Double	Moles	Imports the lower molar limit from...
4	Moles	Moles	☒	Peak or group	Double	Moles	Calculates the moles of each peak

Formula

GetConstant("MW")

Details

Items

- Sequence
- Sample
- Injection
- Signal
- Peak or group
 - Fields
 - Functions
- Custom calculations
- Calibration curve

Fields and Functions

- AllMatchingPeaksAndGroups
- CalibrationCurve
- ExpectedSignalName
- GetBoolCC
- GetConstant
- GetCustomField

Description

Returns the value defined in the constant file for the specified constant for the current compound.

This implies that a constant file is defined in the CC file.

Syntax:

GetConstant(constant as a string) as a double

Example:

GetConstant("MW") returns the value of MW for the current

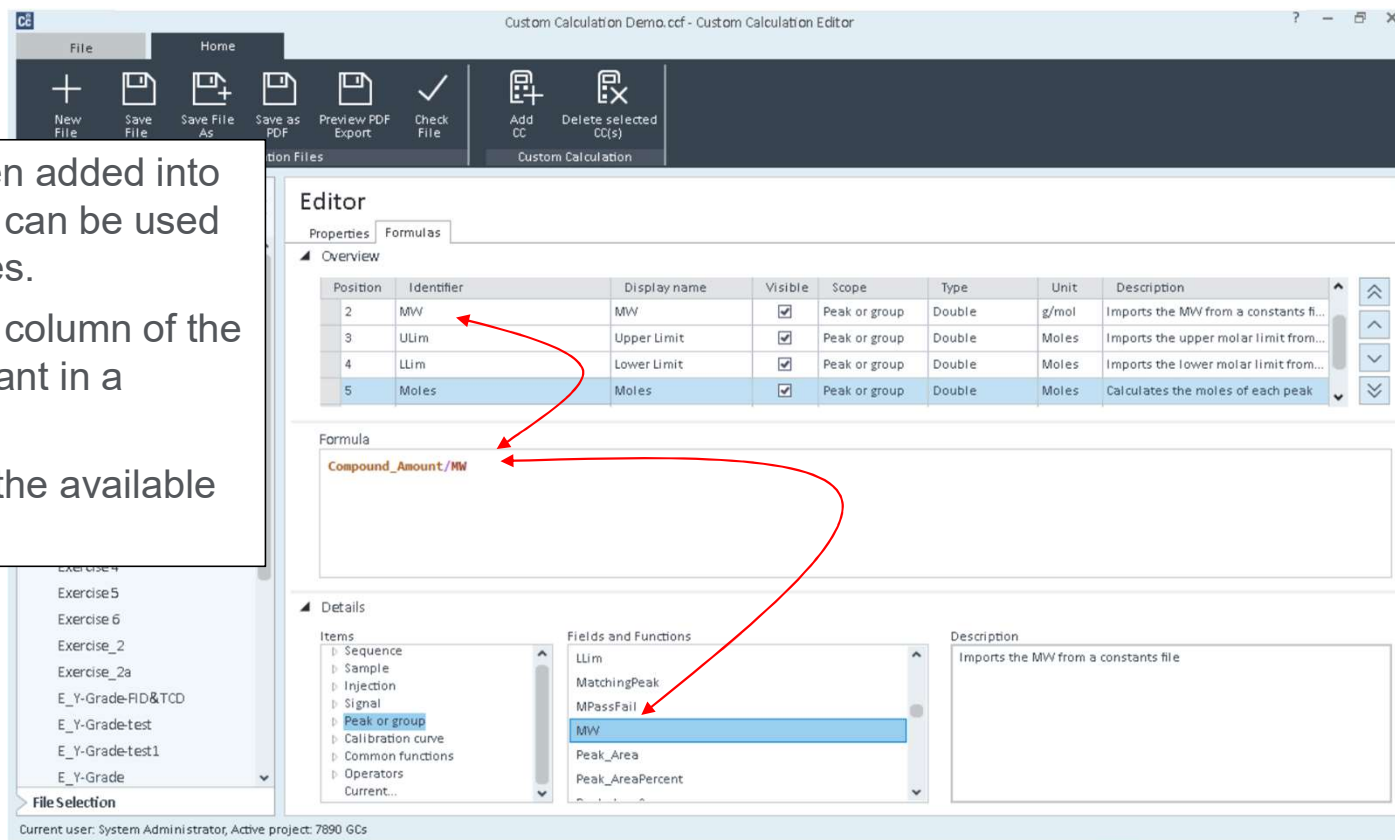
Active project: 7890 GCs

Using Constants in a Custom Calculation

Once the constants have been added into the Custom Calculation, they can be used to calculate new results values.

Use the entry in the Identifier column of the overview to specify the constant in a calculation.

Constants are also added to the available data items in the Details lists.

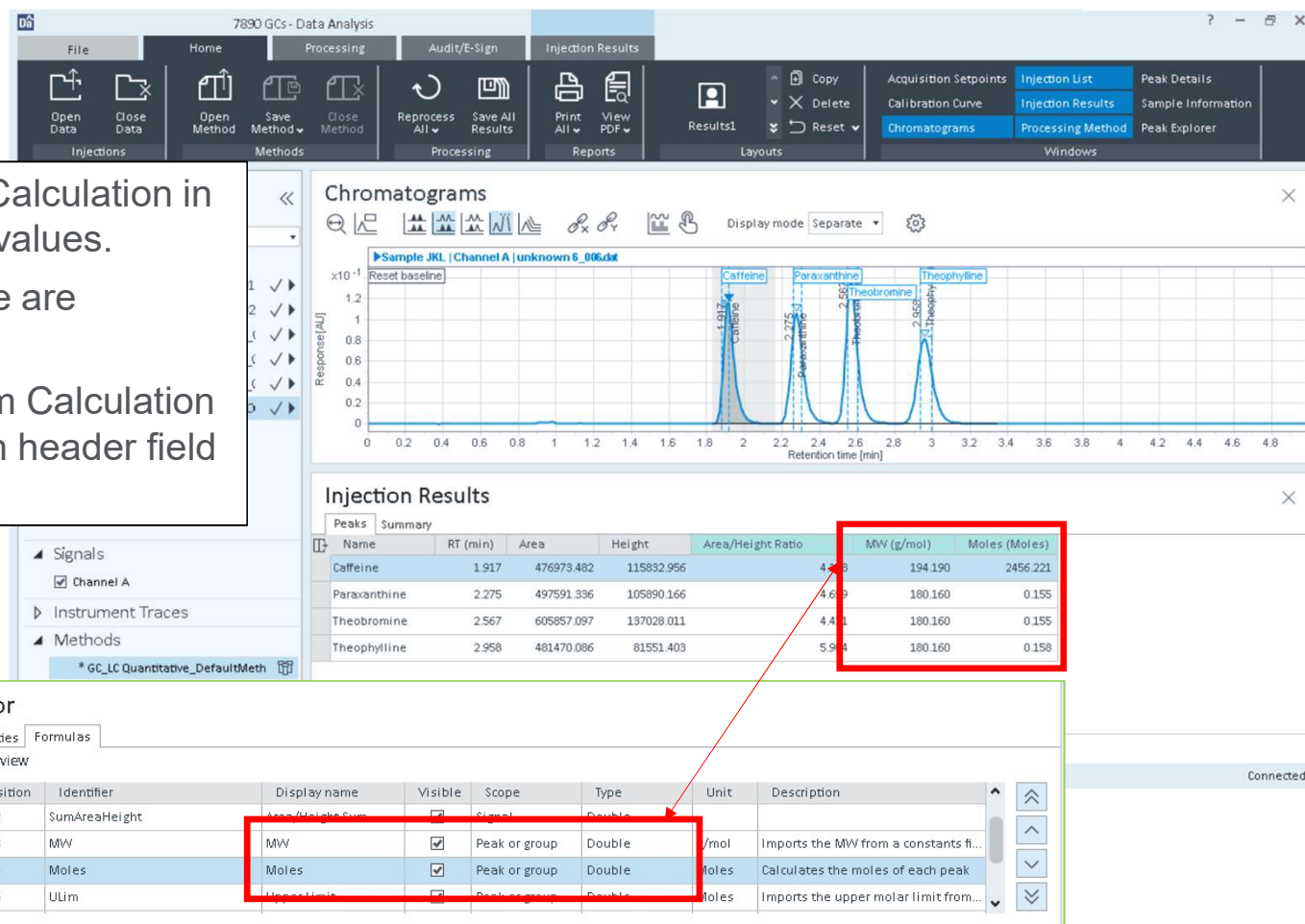


Constant Values and New Results Inside OpenLab CDS

Data processed with a Custom Calculation in the method contains new result values.

Individual CCs marked as Visible are available in the results display.

Results generated with a Custom Calculation are displayed with a blue column header field using the Display Name



Logic Statements in a Custom Calculation

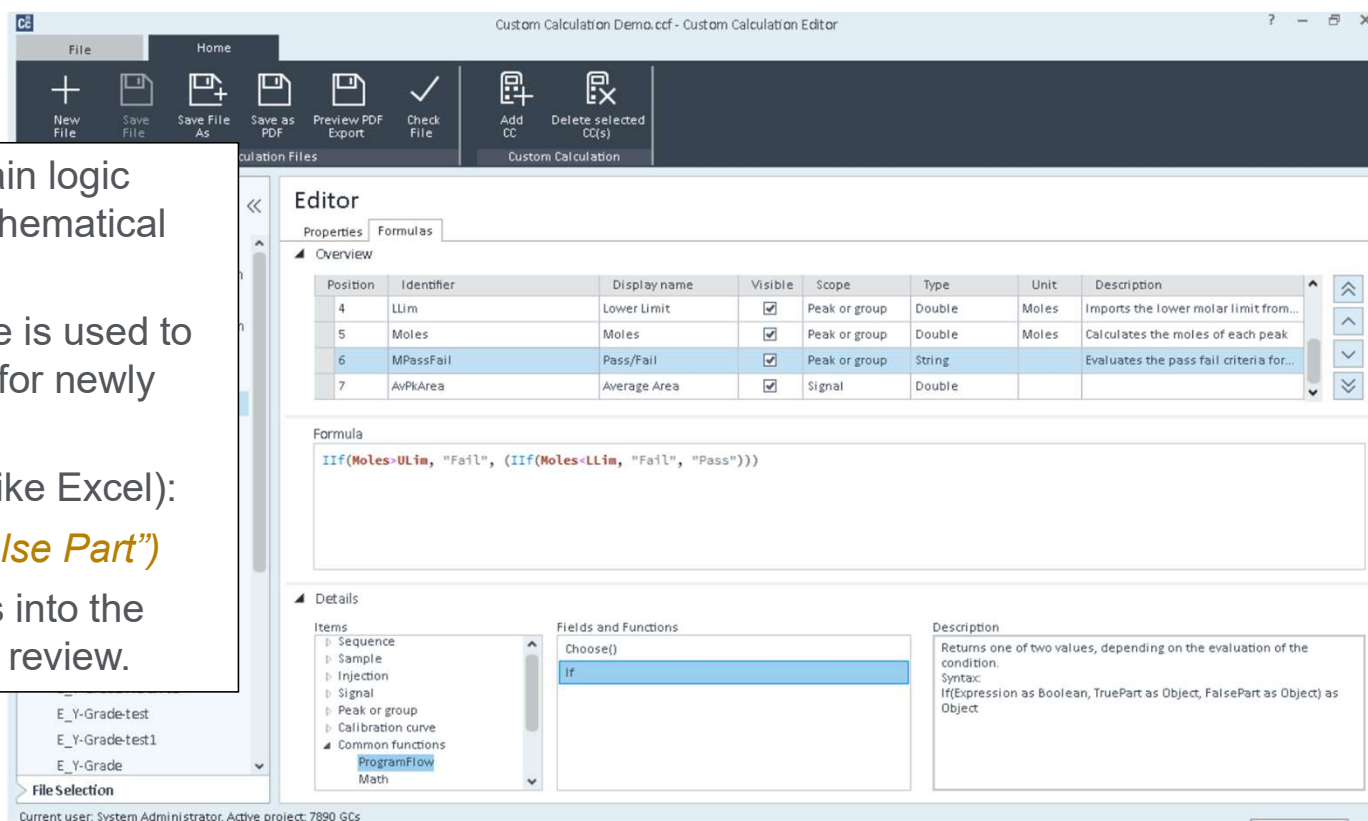
Custom Calculations can contain logic statements in addition to mathematical calculations.

In this example, a constants file is used to bring in upper and lower limits for newly calculated Moles result.

Using a logic expression (just like Excel):

IIF(Condition, "True Part", "False Part")

Can add Pass / Fail indications into the data system – simplifying Data review.

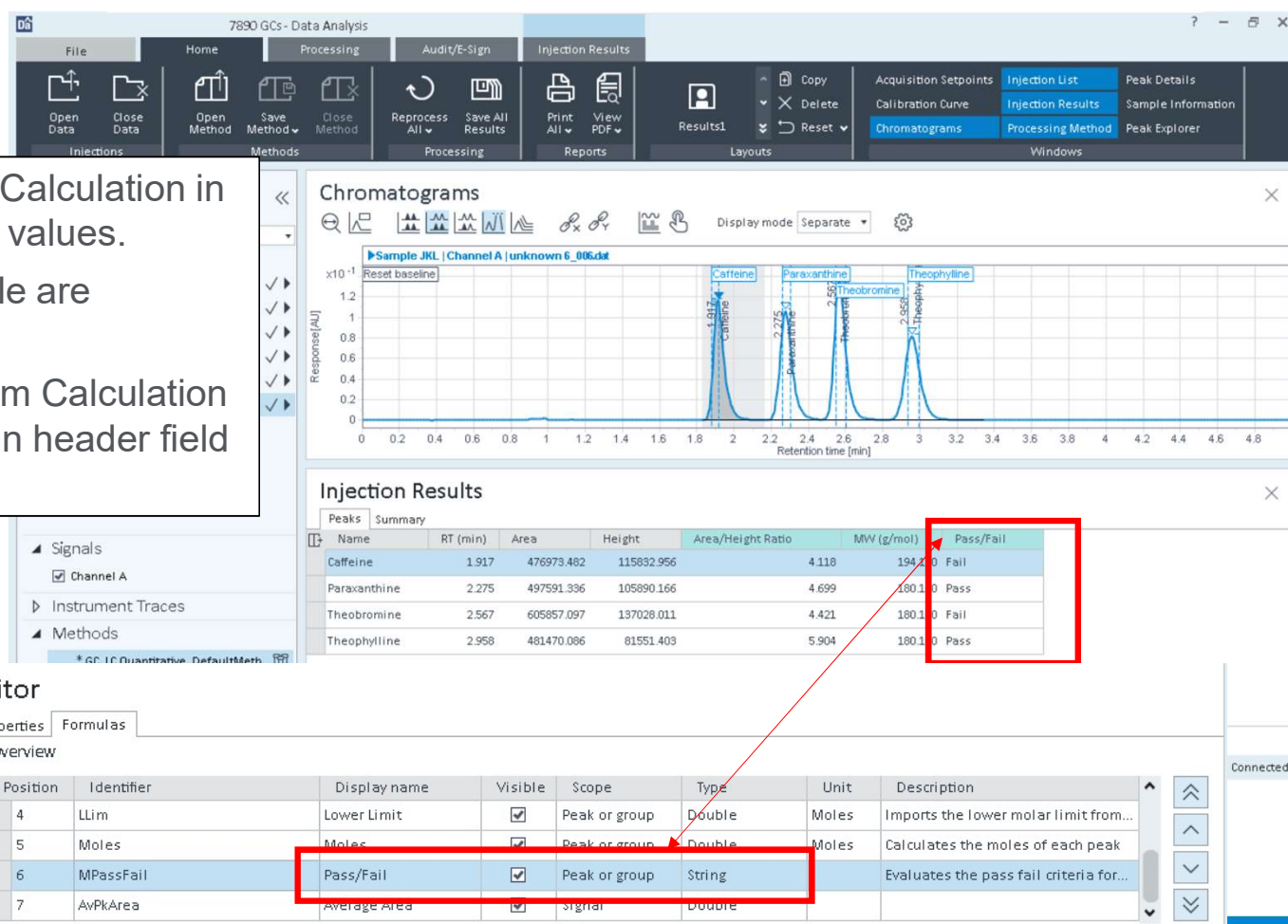


Logic Statements Inside CDS

Data processed with a Custom Calculation in the method contains new result values.

Individual CCs marked as Visible are available in the results display.

Results generated with a Custom Calculation are displayed with a blue column header field using the Display Name

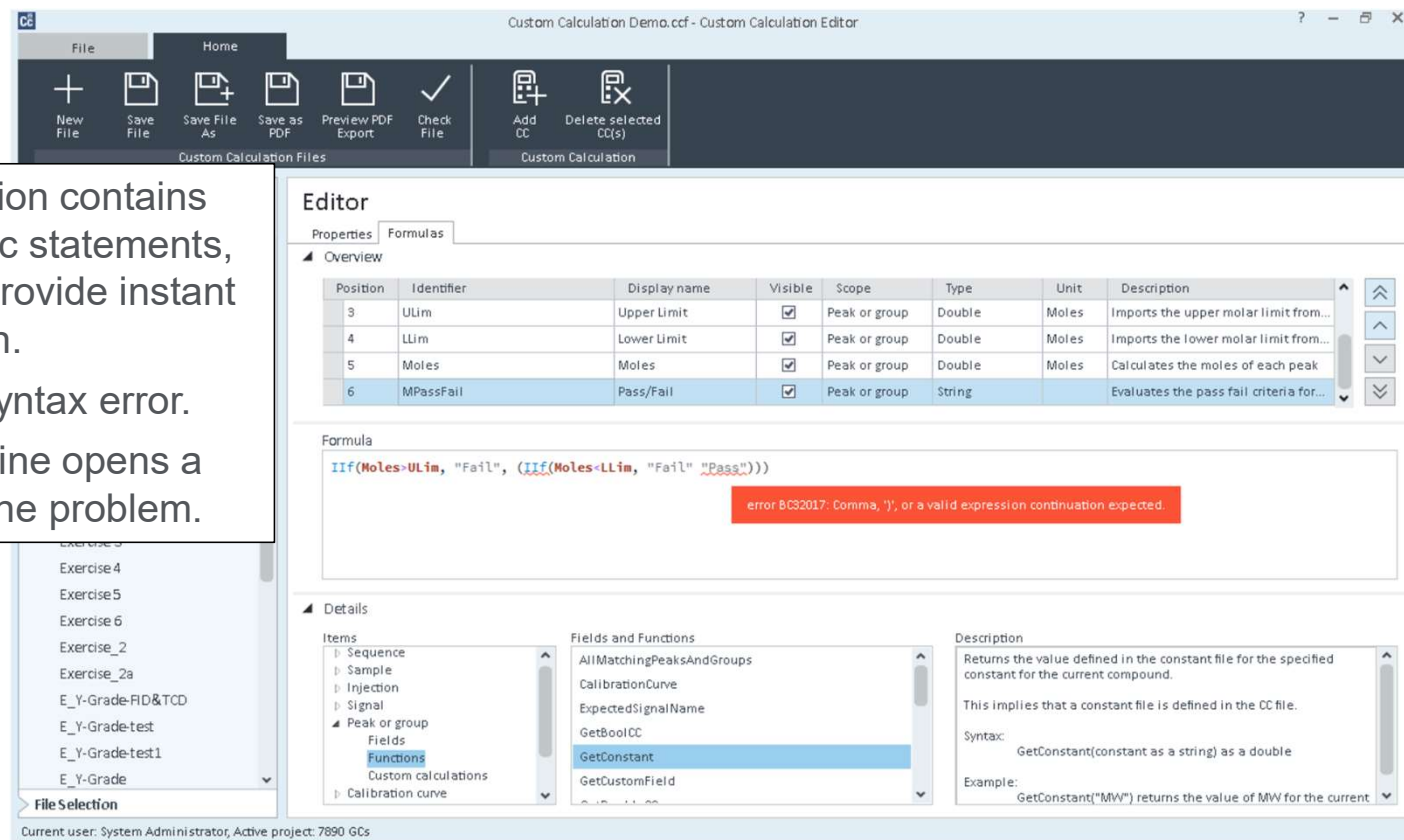


Error Checking in Custom Calculations

Whether the custom calculation contains simple math, or complex logic statements, the error checking features provide instant feedback on each expression.

A red underline indicates a syntax error.

Hovering over the red underline opens a tool tip with an indication of the problem.



Defining Summary Calculations

Custom Calculations also summarize results for a signal, Injection, or sequence.

In this summary calculation, the area for all peaks per signal are averaged.

Note – the Scope changes for this type calculation from Peak or Group (used when the calculation generates 1 value per peak or groups) to Signal (used when the calculation generates one value per signal).

The screenshot displays the 'Custom Calculation Editor' window. The 'Overview' tab is active, showing a table of calculation properties. A red arrow points from the 'Average Area' row in the table to the formula field.

Position	Identifier	Display name	Visible	Scope	Type	Unit	Description
4	LLim	Lower Limit	☒	Peak or group	Double	Moles	Imports the lower molar limit from...
5	Moles	Moles	☒	Peak or group	Double	Moles	Calculates the moles of each peak
6	MPassFail	Pass/Fail	☒	Peak or group	String		Evaluates the pass fail criteria for...
7	AvPkArea	Average Area	☒	Signal	Double		

Formula:

```
Average("Peak_Area", CurrentSignal.AllIdentifiedPeaks)
```

Details:

- Items: Calibration curve, Common functions, ProgramFlow, Math, Conversion, Text, Aggregate
- Fields and Functions: Average, Count, CountDistinct, First(), Last(), Max, ...
- Description: Returns the average value of a specified field or CC computed on a specified data source.
Syntax: `Average("field or CC", Datasource as a list) as a double`
Example: `Average("Peak_Area", CurrentSignal.AllPeaks)` returns the average of Peak_Area of all peaks within the current signal.

Current user: System Administrator, Active project: 7890 GCs

Summary Calculations Inside CDS

Editor

Properties Formulas

Overview

Position	Identifier	Display name	Visible	Scope	Type	Unit	Description
4	LLim	Lower Limit	☒	Peak or group	Double	Moles	Imports the lower molar limit from...
5	Moles	Moles	☒	Peak or group	Double	Moles	Calculates the moles of each peak
6	MPassFail	Pass/Fail	☒	Peak or group	String		Evaluates the pass fail criteria for...
7	AvPkArea	Average Area	☒	Signal	Double		

Custom Calculations for Summary results are viewed in the Summary tab of the Injection Results window.

Summary results are displayed in the Sequence, Injection, or Signal section based on the Scope of the calculation

Injection Results

Peaks Summary

Sequence

Injection

Signals

Name	Channel A
Average Area	515473

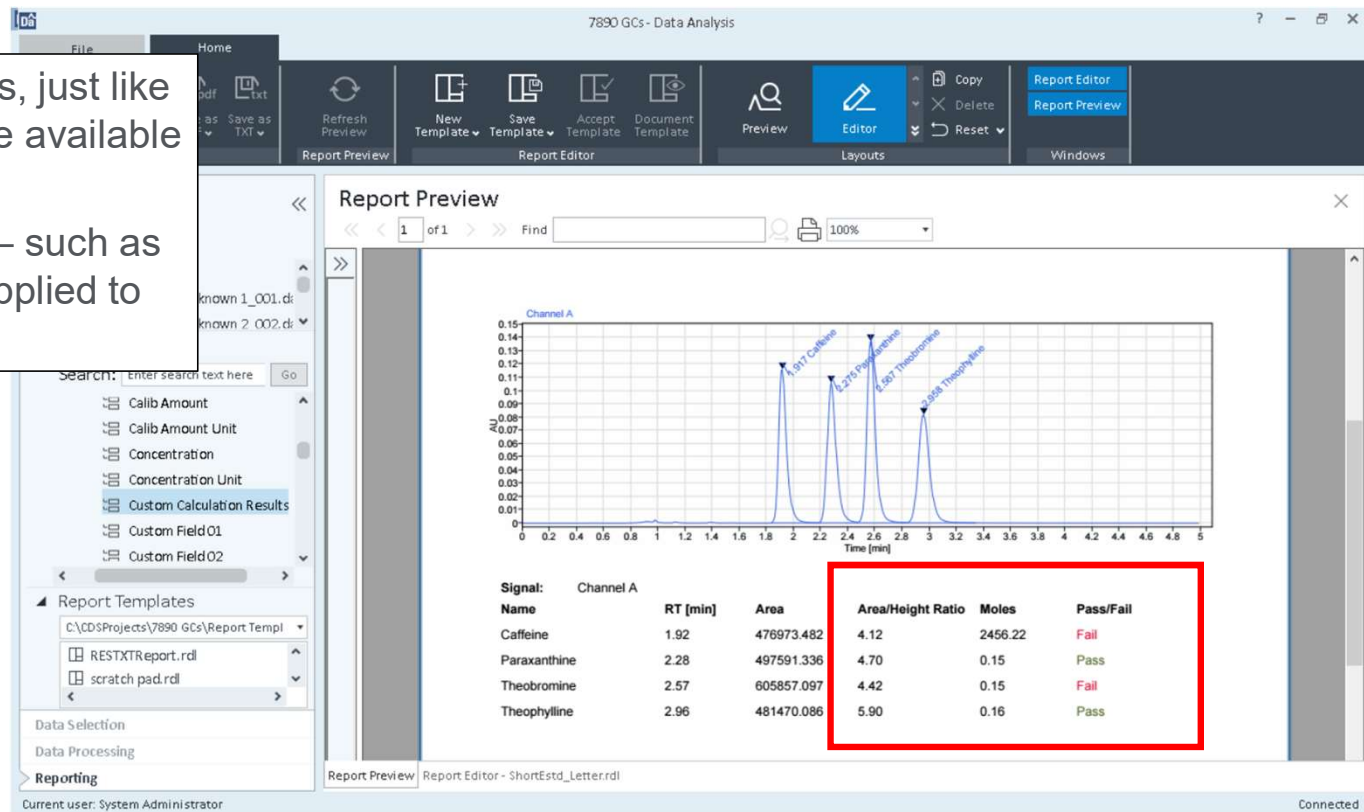
Custom Calculator

Adding Custom Calculation Values to a Report / Export

Reporting / Exporting Custom Calculations

Results from Custom Calculations, just like standards data system results are available for reporting and exporting.

All Intelligent Reporting features – such as conditional formatting – can be applied to custom results too!

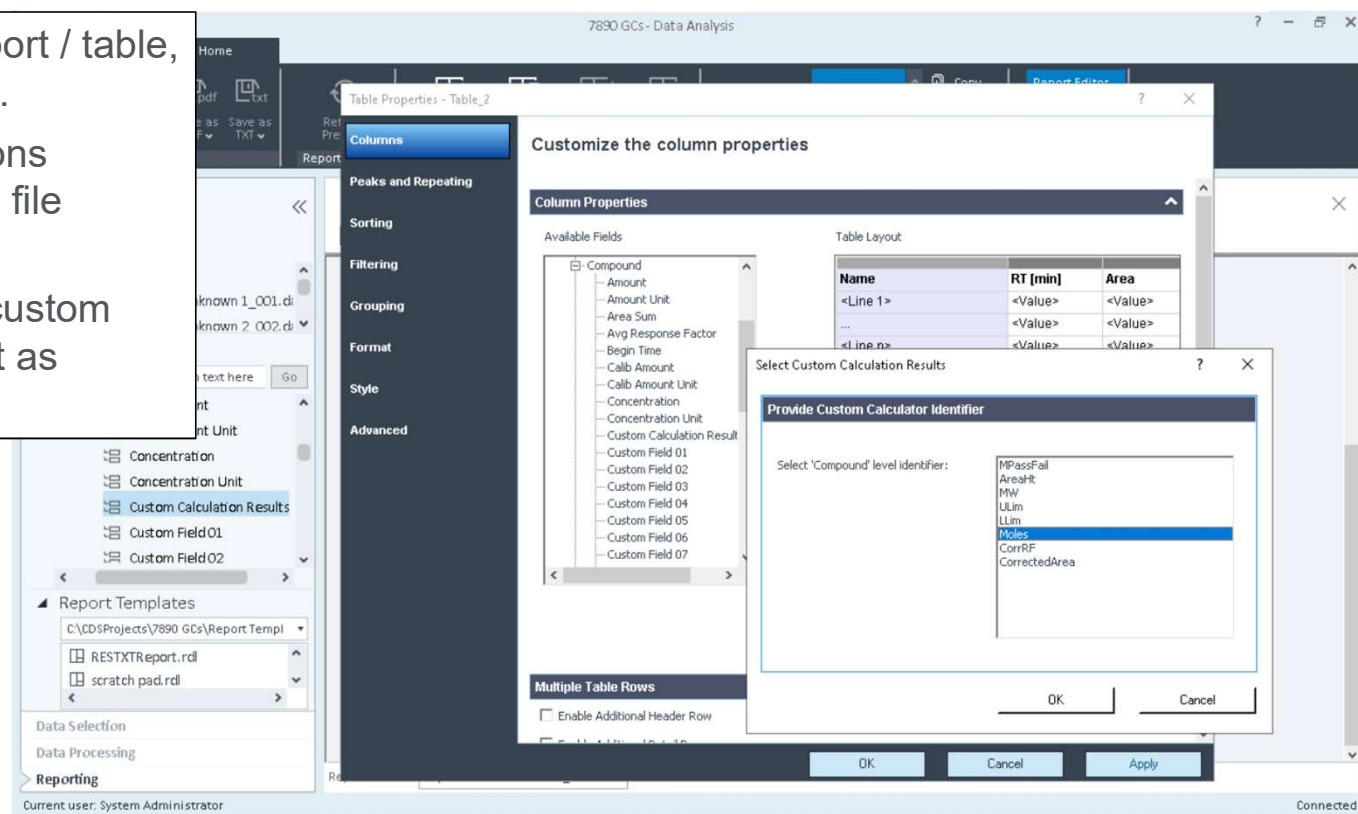


Reporting / Exporting Custom Calculations

When adding a data item to a report / table, select Custom Calculation Result.

A dialog with all custom calculations associated with the selected data file appears.

When specified as an export, the custom calculations included in the report are exported.



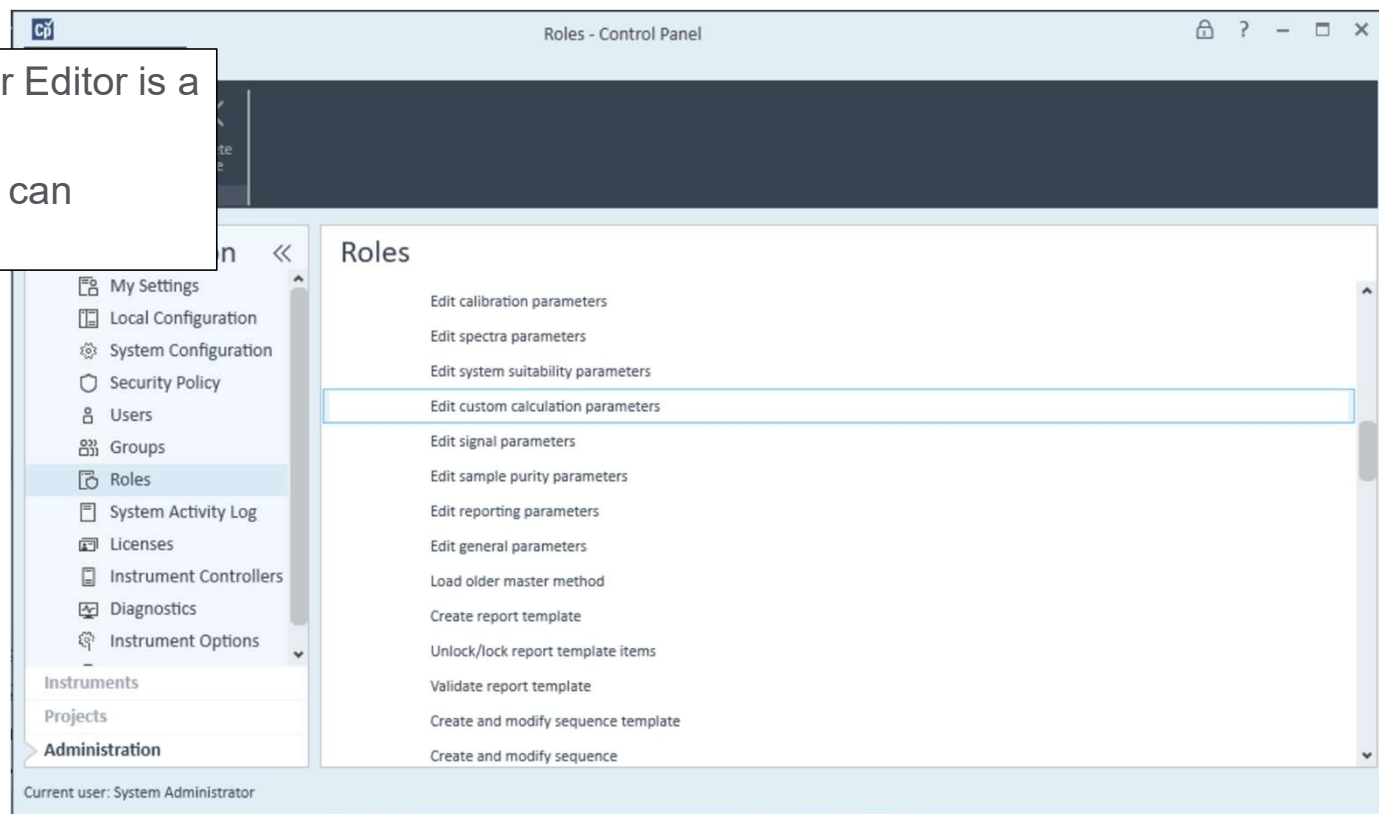
Custom Calculator

Extending Compliance Features to Custom Calculations

Compliance: Role Based Access to Custom Calculations

Access to the Custom Calculator Editor is a permissioned activity.

Users who have this permission can generate and edit CC files.

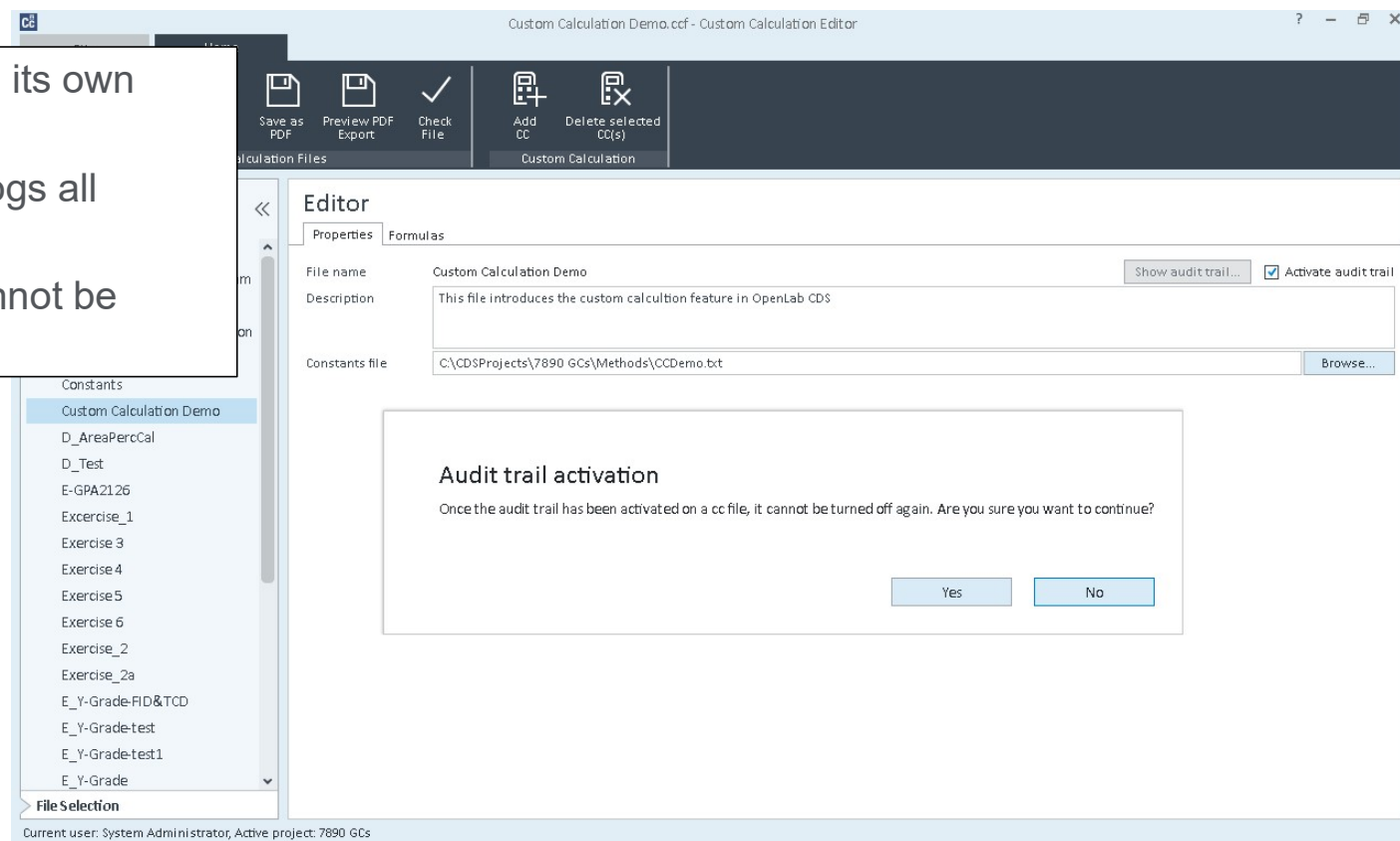


Compliance: Audit Trail for Custom Calculations

Each Custom Calculator file has its own Audit Trail.

When enabled, the audit trail logs all changes to the CC file.

Once enabled, the audit trail cannot be disabled.



Compliance: Audit Trail for Custom Calculations

The Custom Calculator file's Audit Trail enjoys the same features as the general method / data audit trails within OpenLab CDS.

- Who, what, when, and why
- Searchable entries
- Printing / exporting entries
- Audit Trail review

Audit Trail CC_Demo_Summary.ccf, Version 2015-30-06 14:48:41.028 (Number of entries: 371)

Find From 6/22/2015 To 6/30/2015 Filter Manual entry

(yyy-MM-dd)	Description	Host name	Reviewed	Reason	Category	Version
2015-06-30 07:43:33-07:00	Changed 'formula' from '"Min Peak Area: "&Cstr(FormatNumber(Min("Peak_Area", CurrentSignal.AllPeaks),5)) &" Max Peak Area: "&Cstr(FormatNumber(Max("Peak_Area", CurrentSignal.AllPeaks),5)) &" Sum: "&Cstr(FormatNumber(Sum("Peak_Area", CurrentSignal.AllPeaks),5))' to '"Min Peak Area: "&Cstr(FormatNumber(Min("Peak_Area", CurrentSignal.AllPeaks),5)) &" Max Peak Area: "&Cstr(FormatNumber(Max("Peak_Area", CurrentSignal.AllPeaks),5)) &" Sum: "&Cstr(FormatNumber(Sum("Peak_Area", CurrentSignal.AllPeaks),5))' for CC 'Peak_Areas_Current_Injection'.	FB15PC			Custom calculation	2015-30-06 14:43:33.809
2015-06-30 07:43:33-07:00	Saved file	FB15PC			CC File	2015-30-06 14:43:33.809
2015-06-30 07:39:06-07:00	Changed 'display name' from 'Used Calibration Peak(s) (Current Injection)' to 'Calibration Peak(s) (Current Injection)' for CC 'Name_of_Calib_Peaks_Injection'.	FB15PC			Custom calculation	2015-30-06 14:39:06.795
2015-06-30 07:39:06-07:00	Changed 'display name' from 'Used Calibration Peak Name(s) (All Available Signals)' to 'Calibration Peak Name(s) (All Available Signals)' for CC 'Name_of_Calib_Peaks_Signal'.	FB15PC			Custom calculation	2015-30-06 14:39:06.795

Version 2015-30-06 14:39:06.795 CC File (1 entries)
Version 2015-30-06 14:38:06.784 CC File (1 entries)

Review PDF Export... Print Close

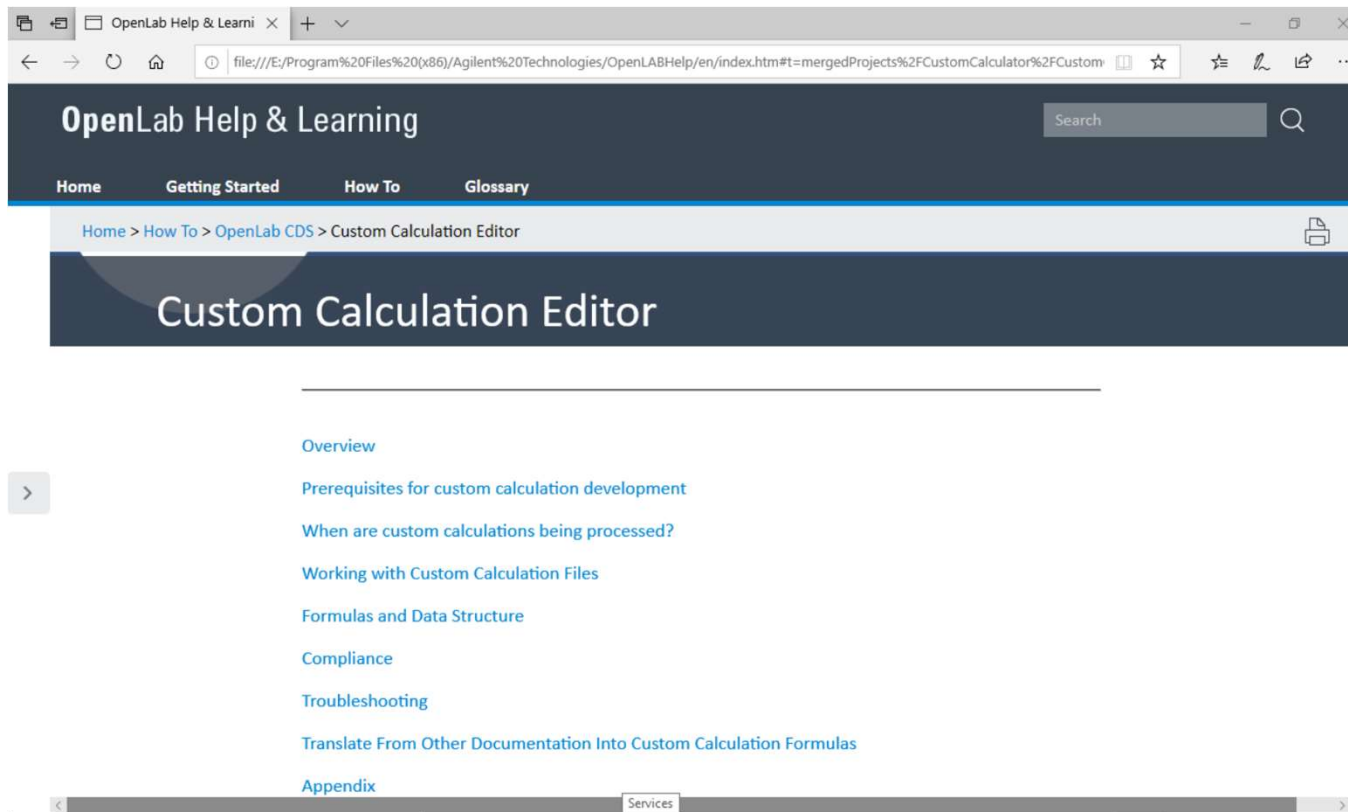
Custom Calculator

Additional Information

How Does Custom Calculator Work?

- Simple expressions are very similar to Excel in syntax
 - Custom Calculation formulas use VB.NET
 - More complex expressions can use Language Integrated Query (LINQ)
 - Any VB.NET expression can be used.
- Frequently used expressions are available in the Custom Calculations editor with typeahead search and syntax provided.
- Functions are error checked
- One Custom Calculation file can perform many calculations
 - An expression can consider Peak results, Signal, Injection, Sample, and Sequence information

For More Information - OpenLab CDS Help Learning



For More Information – Agilent University

The screenshot shows a web browser window displaying the Agilent University website. The URL in the address bar is https://inter.viewcentral.com/events/cust/catalog_detail.aspx?cid=agilent&pid=1&lid=1&tstamp=1585323482245&event_id=892&schedule_id=0&postingFor. The browser tabs include "Direct Download - Feature upd...", "Space: Agilent IT: Information...", and "Agilent Technologies". The website header features the "Agilent University" logo and navigation links: "Checkout", "Check Credit Key", "Buy Training Credits", "My Training & Account", "Login/Logout", "Welcome Video", and "Help". Below the header is a blue navigation bar with "All Courses", "Classroom", and "Online" options. The main content area is titled "COURSE INFORMATION" and includes a "Back" link. A thumbnail image shows a classroom setting with students and an instructor. The course title is "SW-OLII-3170c - OpenLAB 2 CDS Custom Reporting and Custom Calculations - 2 Day", followed by "Instructor-led/Conference" and "SW-OLII-3170c". The description states: "Are you tired of transferring your analysis data to other programs such as Excel for calculations and formatting. Do the standard reporting layouts lack information you need for your laboratory? Cut your data analysis workload by designing and creating custom reports that will execute automatically and save you time. Perform complex calculations and flag outliers without moving your data from OpenLAB CDS software." The course features include: "Display chromatograms, calibrations curves, and spectra exactly as needed for your application review.", "Construct custom tables with your required columns and formatting.", "Build custom control charts to assess analytical performance.", "Incorporate instrument specifics such as module information and Early Maintenance Feedback Counters into your report.", and "Create custom calculations and flag data that is out of specified ranges." The software used is "OpenLAB CDS Version 2.1 (Note: Sessions delivered in Waldbronn/Germany use most recent software versions)". The delivery is "Classroom with Laptops" and the duration is "2.00 day(s)".

Thank You

