



Ion chromatography

Automatic calibration curve selection in ion chromatography with Chromeleon 7 CDS

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Keywords

Dynamic detector range, data export, Intelligent Run Control, IRC, processing method, Report Designer, System Suitability Test, SST

Goal

To provide instructions for an example on dividing a large concentration range calibration into three smaller segments, thereby complying with linearity requirements, and then automatically selecting the appropriate calibration segment for the amount calculation and reporting using the Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) software

Introduction

Modern analytical techniques need to be automated, flexible, robust, and adaptable to the challenges of real samples. Unlike working with synthetic standards, the analytical reality is best described as a mélange of different analytes, varying sample matrices, and often disparate concentration ratios. These already complex scenarios are further constrained by the analytical framework, such as the linear working range of the detection system or the specification of the calibration model to quantify unknown samples. Modern ion chromatography (IC) can address several of the experimental challenges, e.g., through the use of high capacity columns, modern 4- μm resins, electrolytic eluent generation, continuously regenerated membrane-based suppressors, and Thermo Scientific™ Dionex™ Reagent-Free™ Ion Chromatography (RFIC™) instrument setups, which continuously produce high purity eluents and regenerants through electrolytic reactions.¹

However, some national and international standards require linear calibration or limit the calibration range,^{2,3} though the dynamic detector range—not necessarily the linear dynamic range—allows the calibration and quantification over several orders of magnitude. Other standard procedures permit choosing the calibration model and do not restrict the concentration range.^{4,5} This is the analyst's dilemma: Complying with the rules while working efficiently and economically.

To illustrate the application of a novel Chromeleon software report and export option to overcome this hurdle, we used a common IC application with a carbonate-based eluent

with suppressed conductivity detection. In the suppressor, the dissolved salts are converted to "carbonic acid" from the eluent and the corresponding acids, which are usually more strongly dissociated, from the analytes. The simultaneous presence of a strongly dissociated acid and a weaker one often leads to second-order correlations of the analyte's peak area or height and the concentration.⁶

This work describes an automated approach to calibrate over a wider dynamic detector range, dividing this span into a set of linear calibrations, which are then automatically selected from, to quantify the unknown samples.

By using the integrated tools of the Chromeleon CDS, namely System Suitability Tests (SST), Intelligent Run Control (IRC), and formula functions, intelligent decisions are automatically made. The software selects the optimum linear calibration function based on the analyte's peak area and creates a report (Figure 1) ready to be exported in text format to Microsoft[™] Excel[™] or a format amenable to a laboratory information management system (LIMS). All steps are performed within a single processing method.

Process overview

In this work, we decided to divide the chosen dynamic range into three segments. The Chromeleon software uses a processing method to determine the concentration of the target compounds using three predefined calibration curves. These calibration curves are linked to detector channels created from the original data acquisition channel. The calibration is performed with external standard solutions, which are injected in the order of increasing concentration. After assigning the standard

chromatograms to the individual calibration and channel, three different calibration curves are available in one processing method. The selection of the best-suited calibration curve is based on the automatic comparison of the analyte's peak area with the peak areas of corresponding standards using formula functions in the report spreadsheets. Depending on the operator's selection, the final report can be printed or exported, e.g., to a LIMS.

Note: A European Windows[™] setting was used (decimal separator: comma, list separator: semicolon) to develop this Technical Note. If an *Invalid formula syntax* warning appears on your PC, check which character is set as the list separator in your regional settings on the Windows Control Panel. If a different character is defined as the list separator, use this character in the following examples in place of the semicolon.

Equipment

The approach can be used with any Thermo Scientific[™] Dionex[™] IC configuration including

- Thermo Scientific[™] Dionex[™] ICS-6000 HPIC[™] system
- Thermo Scientific[™] Dionex[™] Integrion[™] HPIC system
- Thermo Scientific[™] Dionex[™] Aquion[™] IC system
- Thermo Scientific[™] Dionex[™] Easion[™] IC system
- Thermo Scientific[™] Dionex[™] AS-AP autosampler
- Thermo Scientific[™] Dionex[™] AS-DV autosampler
- Chromeleon Chromatography Data System software version 7.2 or above

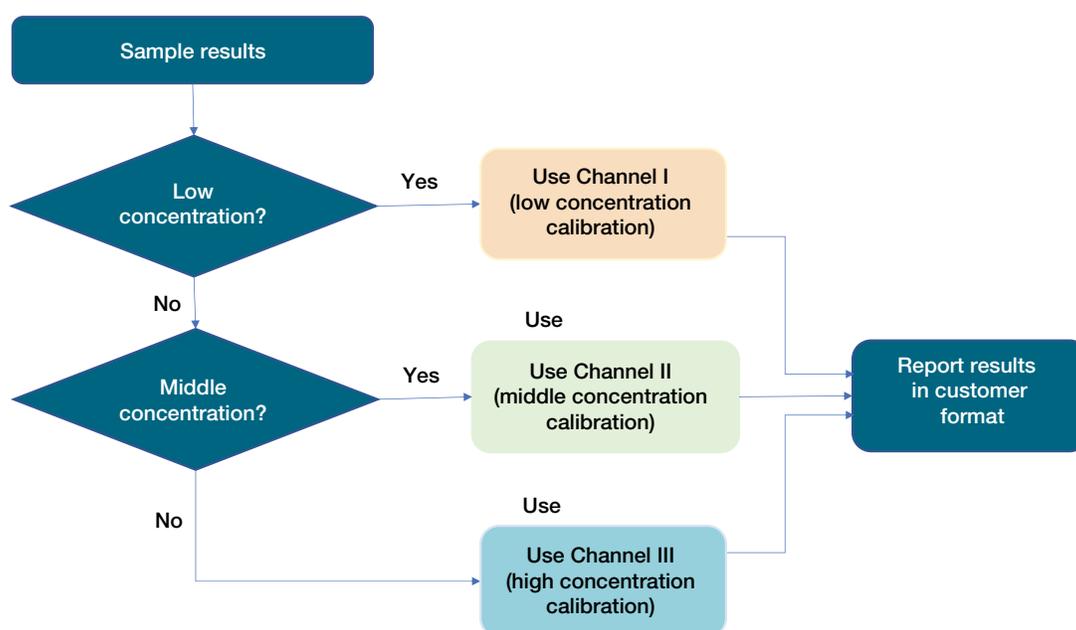


Figure 1. Flow chart of the Chromeleon 7 CDS automatic calibration selection process

Conditions

Parameter	Value
IC system	Dionex ICS-6000 with Dionex AS-AP autosampler*
Columns	Thermo Scientific™ Dionex™ IonPac™ AS22 (4 × 250 mm) with Thermo Scientific™ Dionex™ IonPac™ AG22 (4 × 50 mm)
Eluent	4.5 mM Na ₂ CO ₃ 1.4 mM NaHCO ₃
Flow rate	1.2 mL/min
Injection volume	25 µL
Temperature	30 °C (column compartment) 20 °C (detector compartment)
Backpressure	≈ 1,500 psi 100 psi = 0.6894 MPa)
Suppressed conductivity detection	Thermo Scientific™ Dionex™ Dynamically Regenerated Suppressor ADRS (4 mm), regeneration current = 31 mA, AutoSuppression™ recycle mode
Background conductance	< 21 µS/cm
Run time	< 15 min

*Any Thermo Scientific Dionex IC system configuration and analytical method can be used with the calibration and reporting option described in this note.

The approach

Calibration strategy

We decided to calibrate over several orders of magnitude of mass concentration for each analyte (Table 1, page 6). To comply with demands for a linear calibration and a limited concentration range (max. two orders), we covered the calibrated range for each anion with ten calibration levels. These ranges are divided into three segments with four levels each. Some of the calibration standards (see the marked standards in Figure 2) were injected twice so that the repetitive injections could be assigned to separate segments and channels (see below). This approach ensures that the entire calibrated range is covered.

Create additional data channels in Chromeleon CDS software

Additional data channels must be created to split the calibrated range and assign the respective calibration runs to the individual calibration segment.

There are two ways to generate additional data channels in Chromeleon CDS software:

- Use the Copy Channel function
- Use the SST/IRC option

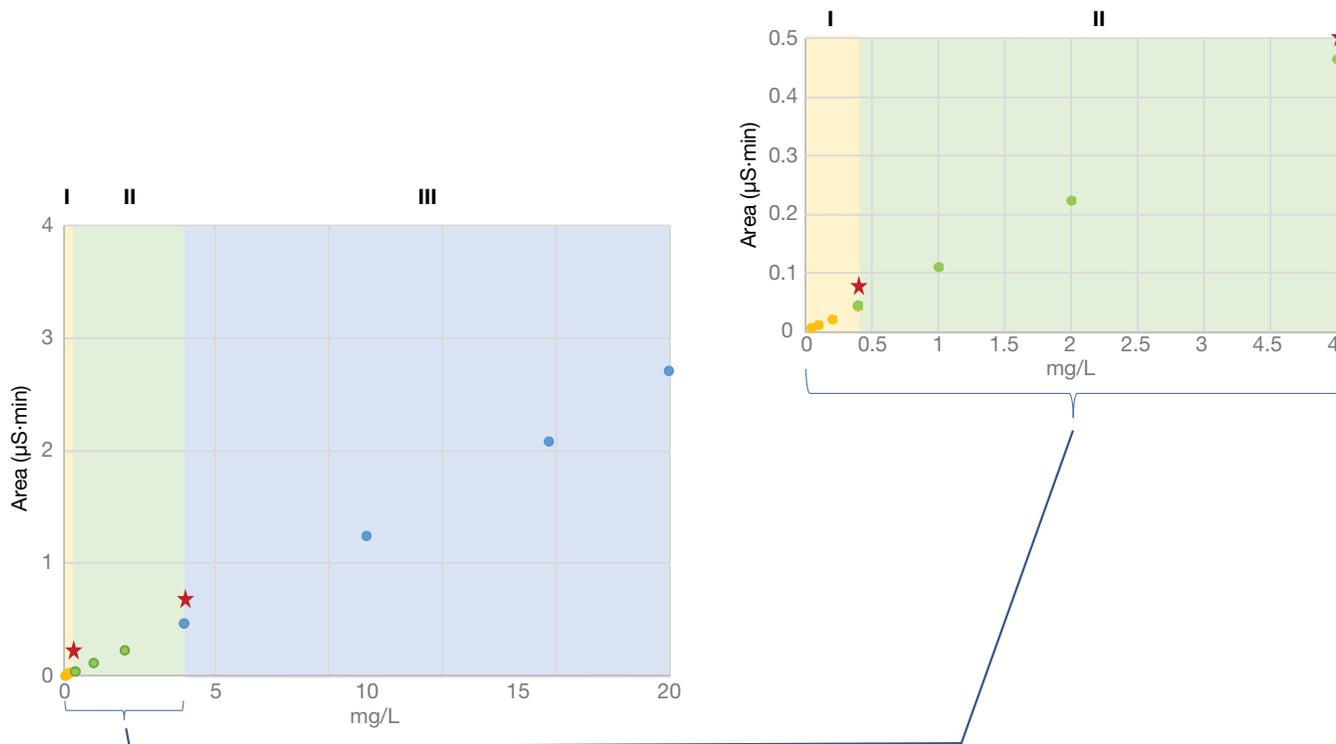


Figure 2. Calibrated range divided into three segments (example: chloride). I: low concentration range, II: middle concentration range, III: high concentration range. The standards marked with a star were measured twice to allow assignment to two separate segments.

To create a copy from the chromatogram's context menu

1. Open a chromatogram from the sequence.
2. Right mouse click on the chromatogram and select "Copy Channel" (Figure 3). Either accept the proposed name for the result channel or enter a new one.
3. Select "All" to apply the copy channel operation to all samples within the current sequence.

In this example, where three channels (calibration segments) are created, we would do this twice. Use this option for an already existing sequence.

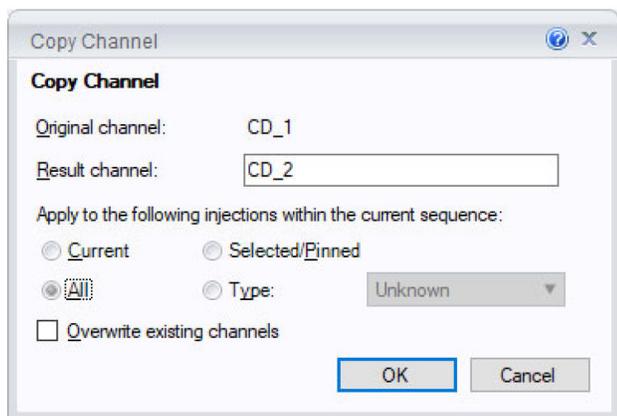


Figure 3. Copy channel from the context menu

Copy channels using the SST/IRC option

This approach makes the channels available automatically after a sample has been run. Open the processing method. Select the SST/IRC tab.

1. From the SST/IRC tab of the processing method, select "Click here to add a new test case" to start the wizard (Figure 4).
2. For automatic calibration, select "Create an unconditional test case" and click "Next".
3. Enter the "Test case name" and click "Next". On the next page, select "Apply to all injections".
4. Select "Copy Channel" from the list of available actions on the following page, pick the original channel (e.g., CD_1).
5. Click "Add" and name the result channel.



Figure 4. Selecting the SST/IRC option in the processing method

Repeat adding the "Copy Channel" action until the required channel number is obtained; for our exercise, we created two additional channels (CD_2 and CD_3, Figure 5). Use this option to copy channels automatically during a sequence for each new sample.

Split the original calibration

The next step is to split the original wide range calibration into three calibrations, each with a narrower concentration range. The processing method is set up once. It becomes available for use, and the configuration steps described below need not be repeated. For our experiment, we decided to split the original calibration into three smaller segments. The calibration was set to "Linear with offset" in the processing method to comply with linear regression requirements.^{2,3}

The "low concentration" standards (calibration levels "Low 1" to "Low 4", Figure 6A) are tagged to Channel 1 (CH_1) by *disabling* the standards reserved for the other channels.

1. Go to the "Calibration Tab" of the processing method and disable middle and high concentration standards for CH_1.
2. Double-click in the cell area around the checkbox to access the select options (Figure 6A). Select "All Components," then uncheck "All Channels". Mark the channels to be disabled. Click "OK" to accept. The highlighted and unchecked (!) red channel remains enabled, and the standard level is assigned to a specific channel and therefore to a specific calibration (Figure 6B).
3. Repeat the steps for the middle concentration levels and Channel 2 (calibration level "Mid 1" to "Mid 4"; CH_2) and the high concentration levels and Channel 3 (calibration levels "High 1" to "High 4"; CH_3).

Note: To facilitate the steps above, we renamed the calibration levels. To edit the level names, double-click the level field in the injection list, and enter the new name.

Note: The dialog box in Figure 6B is used to select the channels to be *disabled*. Hence, the checked (ticked) channels are disabled, while the unchecked (not ticked) channels remain active.

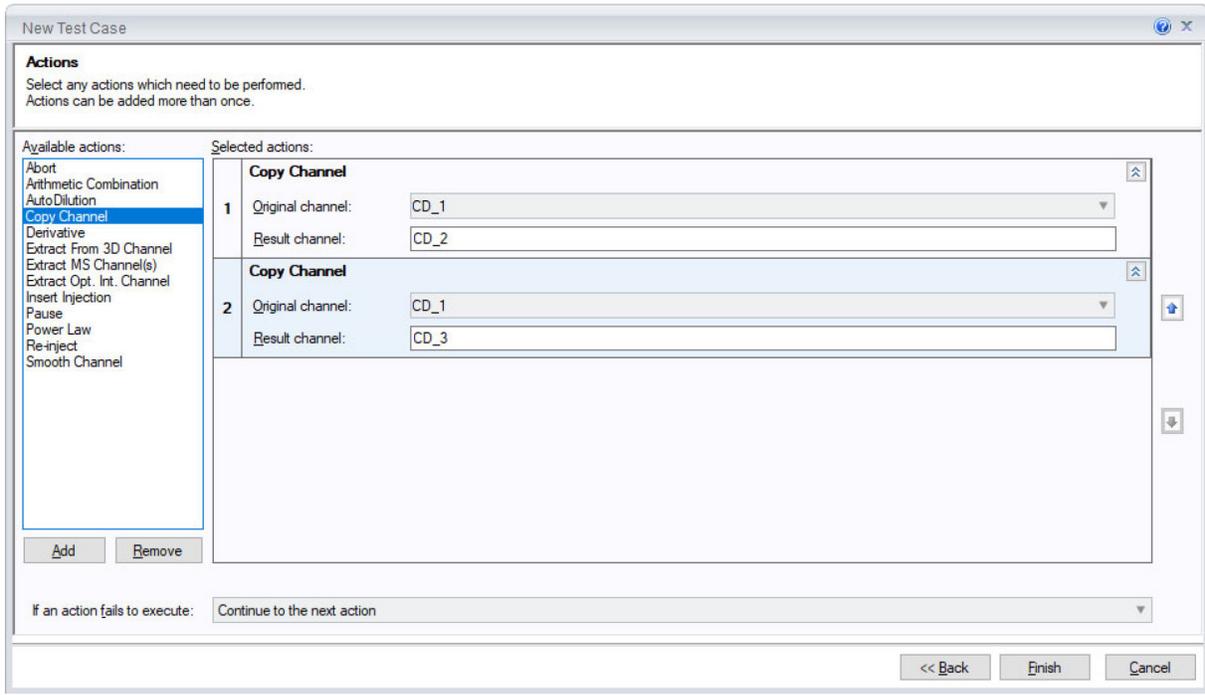


Figure 5. "Copy Channel" option in SST/IRC

(A)

#	Enabled	Name	Level	Position	Volume	Weight	IntStd	Dilution
1	<input checked="" type="checkbox"/>	STD (1)	Low 1	1	25.0 [µl]	1,0000	1,0000	1,0000
2	<input checked="" type="checkbox"/>				25.0 [µl]	1,0000	1,0000	1,0000
3	<input checked="" type="checkbox"/>				25.0 [µl]	1,0000	1,0000	1,0000
4	<input checked="" type="checkbox"/>	STD (4)	Low 4	4	25.0 [µl]	1,0000	1,0000	1,0000
5	<input checked="" type="checkbox"/>	STD (4)	Mid 1	4	25.0 [µl]	1,0000	1,0000	1,0000
6	<input checked="" type="checkbox"/>	STD (5)	Mid 2	5	25.0 [µl]	1,0000	1,0000	1,0000
7	<input checked="" type="checkbox"/>	STD (6)	Mid 3	6	25.0 [µl]	1,0000	1,0000	1,0000
8	<input checked="" type="checkbox"/>	STD (7)	Mid 4	7	25.0 [µl]	1,0000	1,0000	1,0000
9	<input checked="" type="checkbox"/>	STD (7)	High 1	7	25.0 [µl]	1,0000	1,0000	1,0000
10	<input checked="" type="checkbox"/>	STD (8)	High 2	8	25.0 [µl]	1,0000	1,0000	1,0000
11	<input checked="" type="checkbox"/>	STD (9)	High 3	9	25.0 [µl]	1,0000	1,0000	1,0000
12	<input checked="" type="checkbox"/>	STD (10)	High 4	10	25.0 [µl]	1,0000	1,0000	1,0000

(B)

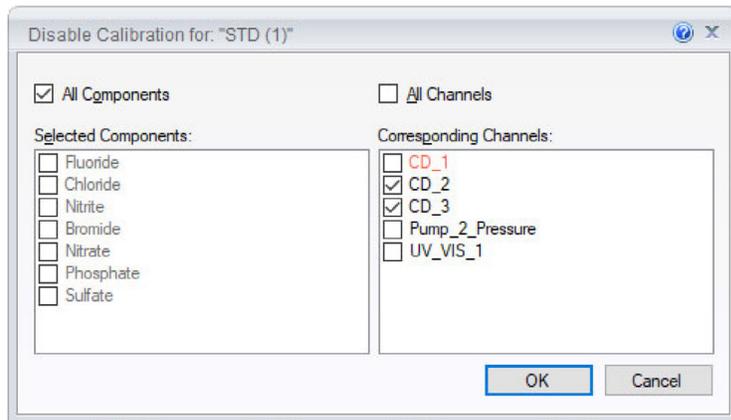


Figure 6. Assigning the selected calibration level (STD(1)) for ALL components to Channel 1

As a result, three calibration curves are established, one for each channel and component (Figure 7). The calibration performance for our example for each channel and analyte is demonstrated in Table 1. The squared correlation coefficients (r^2 , coefficient of determination) for all linear analyte calibrations are greater than

0.998, indicating a good approximation of the measured values to the chosen linear calibration model. Based on the laboratory's application need, the covered concentration range, split ranges, and the number of calibration levels can be adapted.

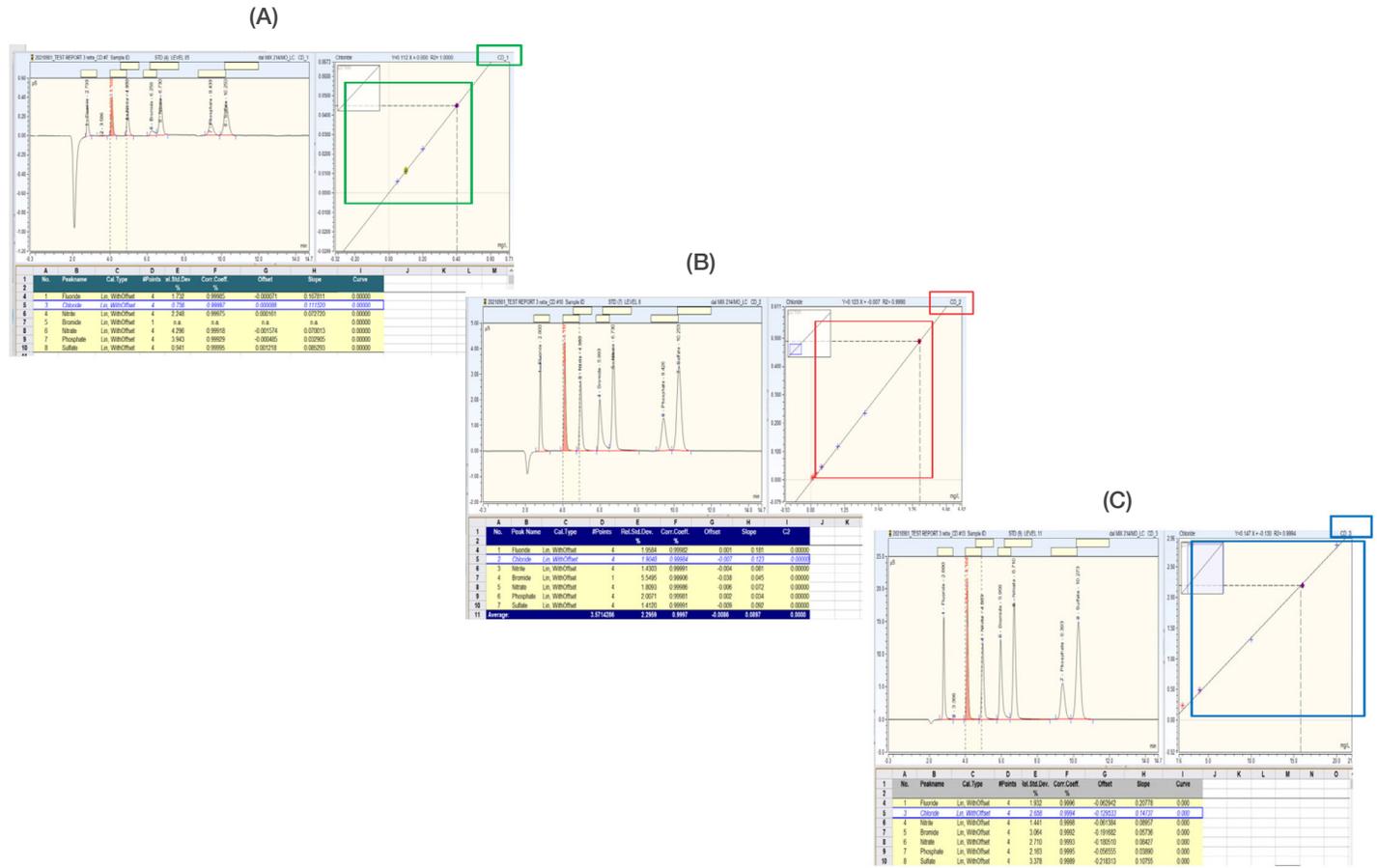


Figure 7. The original wide calibration range is divided into three smaller segments. (A) Channel 1: Low concentration calibration; (B) Channel 2: Middle concentration calibration; (C) Channel 3: High concentration calibration.

Table 1. Calibration data after the automatic splitting of the total calibrated range*

Peak name	Calibration type	Total calibrated range (mg/L)	Calibration range (mg/L)	Coefficient of determination (r^2)	Calibration range (mg/L)	Coefficient of determination (r^2)	Calibration range (mg/L)	Coefficient of determination (r^2)
			CD_1 (Low)		CD_2 (Middle)		CD_3 (High)	
Fluoride	Lin, With Offset	0.025–2	0.025–0.2	0.9996	0.2–1	0.9998	1–5	0.9997
Chloride	Lin, With Offset	0.05–10	0.05–0.4	0.9999	0.4–2	0.9998	2–10	0.9993
Nitrite	Lin, With Offset	0.0625–10	0.0625–0.5	0.9999	0.5–2.5	0.9999	2.5–12.5	0.9997
Nitrate	Lin, With Offset	0.125–10	0.125–1	0.9985	1–5	0.9996	5–25	0.9992
Phosphate	Lin, With Offset	0.125–20	0.125–1	0.9998	1–5	0.9998	5–25	0.9996
Sulfate	Lin, With Offset	0.125–10	0.125–1	0.9998	1–5	0.9999	5–25	0.999

*Based on the laboratory's application need, the concentration range, split ranges, and calibration levels can be adapted.

How to define the area range for quantification

Maximum peak areas

The optimum calibration curve based on the component's peak area has to be selected. The selection process uses the peak area maxima of the low and middle concentration calibration. If the analyte's peak area is below the maximum of the low concentration calibration, the analyte is quantified with this calibration segment. If the unknown's peak area is between the maxima of the low and the middle calibration, then the middle calibration function is used. All other peak areas are evaluated with the high concentration calibration function.

First, the maximum peak areas for the low and middle concentration calibration ranges are identified. In the "Report Designer", create a "Calibration" spreadsheet and modify the template to match the example given in Figure 8.

1. Open the Report Designer.
2. Select "Insert" from the Ribbon, then "Blank" to create a new, empty spreadsheet.
3. Select "Peak Summary" from the "Report Table" option.
4. Build the summary report using the insert or append option to create the interactive report columns (defined by the red triangles in the corners of the populated table, Figure 8).
5. Select "Calibration Standard" from the "Include Injection Type" option from the Ribbon and uncheck the sample types (Matrix, Blank, Spiked, Unspiked).
6. Rename the sheet to "Calibration". Figure 8 shows the table used for this example.

Once the report is set up, it becomes available for use, and the configuration steps described above are not repeated.

Chromeleon CDS supports user-defined spreadsheet formulas analogous to Microsoft Excel to perform calculations not included as standard Chromeleon CDS report variables.⁷ Formulas are equations that perform calculations on values in your worksheet. A formula always starts with an equal sign (=). Formula entry and syntax are the same as used in Microsoft Excel.

According to Figure 1, the selection process requires criteria to assign the optimum calibration curve. These selection criteria are defined by the maximum peak areas of the low concentration and middle concentration calibrations. These values can be automatically identified using the MAX()-formula in the spreadsheet.

In contrast to conventional spreadsheets with fixed contents, Chromeleon CDS report tables are interactive. Depending on the data generated—in our case, the number of calibration levels or repetitive injections of standards—the range of cells to be processed with the MAX()-formula may vary. We developed an automatic adjustment of the ranges based on formula functions that address individual cells in the spreadsheet (Table 2).

Define the number of standard injections used for the low and middle calibration

1. Place the cursor outside the interactive table range (marked by the red triangles in the corners of the respective table section), e.g., cell "C30" (Figure 9).
2. Type "=COUNTIF(C7:C18;"OK")"; this returns the number of assigned calibration injections for the "low calibration" of channel 1. The cell ranges may vary depending on the number of calibration levels and repetitive injections.
3. Place the cursor in cell "D30".
4. Type "=COUNTIF(D7:D18;"OK")"; this returns the number of assigned calibration injections for the "middle calibration" of channel 2.

	A	B	C	D	E	F	G	H	I
1									
2									
3	No.	Injection Name	Calibration Point Status	Calibration Point Status	Area	Area	Area	Area	Area
4			CD_1	CD_2	$\mu\text{S}^*\text{min}$	$\mu\text{S}^*\text{min}$	$\mu\text{S}^*\text{min}$	$\mu\text{S}^*\text{min}$	$\mu\text{S}^*\text{min}$
5			Fluoride	Fluoride	CD_1	CD_1	CD_1	CD_1	CD_1
6			Chloride	Nitrite	Chloride	Nitrate	Phosphate	Sulfate	
7	3	STD (1)	Ok	Disabled	0,006	0,005	0,008	0,004	0,011
8	4	STD (2)	Ok	Disabled	0,011	0,009	0,016	0,008	0,023
9	5	STD (3)	Ok	Disabled	0,022	0,018	0,031	0,015	0,042
10	6	STD (4)	Ok	Disabled	0,044	0,035	0,070	0,031	0,083
11	7	STD (4)	Disabled	Ok	0,044	0,035	0,071	0,033	0,084
12	8	STD (5)	Disabled	Ok	0,110	0,089	0,160	0,080	0,207
13	9	STD (6)	Disabled	Ok	0,224	0,181	0,310	0,159	0,420
14	10	STD (7)	Disabled	Ok	0,465	0,372	0,643	0,329	0,861
15	11	STD (7)	Disabled	Disabled	0,463	0,369	0,640	0,329	0,860
16	12	STD (8)	Disabled	Disabled	1,249	0,968	1,732	0,859	2,270
17	13	STD (9)	Disabled	Disabled	2,083	1,575	2,896	1,401	3,727
18	14	STD (10)	Disabled	Disabled	2,717	2,024	3,785	1,806	4,899
19									

Figure 8. Newly created summary table, named "Calibration"

Table 2. Formula functions used for automatic identification of the peak area maxima of the calibrations

Formula function	Description
= ADDRESS()	ADDRESS creates a cell address as text.
= COLUMN()	COLUMN returns the column number of the supplied reference.
= COUNTIF()	COUNTIF returns the number of cells within a range that meets the given criteria.
= INDIRECT()	INDIRECT returns the contents of the cell referenced by the specified cell.
= MAX()	MAX returns the largest value in the specified list of numbers.
= ROW()	ROW returns the row number of the supplied reference.

Note: See the Chromeleon Help for details on the syntax under "Formula Functions".

Define the line numbers for the middle and low calibration

The calibration solutions are injected in the order of increasing concentration. The "middle calibration" has to start immediately after the "low calibration" ends.

1. Place the cursor in a free cell outside the interactive range, e.g., "B32" (Figure 9).
2. Type "=ROW(A7)"; this returns the first line number after the table header and therefore is the beginning of the "low calibration".
3. Place the cursor in cell "B33".
4. Type "=B32-1+C30"; this returns the last line number of the "low calibration".
5. Place the cursor in cell "B34".
6. Type "=B33+1"; this returns the first line number of the "middle calibration".
7. Place the cursor in cell "B35".
8. Type "=B34-1+D30"; this returns the last line number of the "middle calibration".

Define the row numbers of the analyte peak areas

To locate the cells within the spreadsheet, we need to define the row numbers in which the peak areas of the individual analyte are displayed.

1. Place the cursor in a free cell outside the interactive range on top of the respective peak area column, e.g., "E2" (Figure 9).
2. Type "=COLUMN()"; this returns the column number (e.g., "5" for column "E").
3. Copy the formula for the remaining anions (see below).

Instead of repeating all the steps for the remaining anions, the formulas can be copied. To copy formulas, including the

formatting, into adjacent cells, use the "fill handle", the small black square in the lower-right corner of the selected cells. When pointing at it, the mouse cursor changes to a black cross. Drag the fill handle over the cell range to the right. The cell references are automatically adapted, and the respective column numbers are displayed.

Create the cell addresses

As we have specified the row and column numbers of the range delimiters for the "low calibration" and "middle calibration", we can use the ADDRESS function to obtain the address of the respective cells in the worksheet.

1. Place the cursor in a free cell outside the interactive range, e.g., "E38" (Figure 9).
2. Type "=ADDRESS(\$B\$32;E\$2)"; this returns a text "\$E\$7", which is the cell address of the first peak area of the low concentration calibration for fluoride in our case.
3. Place the cursor in cell "E39".
4. Type "=ADDRESS(\$B\$33;E\$2)"; this returns a text "\$E\$10", which is the cell address of the last peak area of the low concentration calibration for fluoride in our case.
5. Place the cursor in cell "E40".
6. Type "=ADDRESS(\$B\$34;E\$2)"; this returns a text "\$E\$11", which is the cell address of the first peak area of the middle concentration calibration for fluoride in our case.
7. Place the cursor in cell "E41".
8. Type "=ADDRESS(\$B\$35;E\$2)"; this returns a text "\$E\$14", which is the cell address of the last peak area of the middle concentration calibration for fluoride in our case.
9. Mark the cells "E38" to "E41" and copy the formulas to the right by dragging the fill handle. The cell references are automatically adapted, and the respective cell addresses are displayed.

Determine the maximum peak areas

Next, the MAX function automatically determines the maximum peak areas of the "low calibration" and the "middle calibration". The range delimiters for the MAX-evaluation are referenced using the INDIRECT function. INDIRECT returns the contents (e.g., "\$E\$7") and not the function referenced by the specified cell.

1. Place the cursor in a free cell outside the interactive range, e.g., "E24" (Figure 9).
2. Type " =MAX(INDIRECT(E\$38):INDIRECT(E\$39))"; this returns the maximum peak area value of the "low calibration" for fluoride in our test case.
3. Place the cursor in cell "E25".
4. Type " =MAX(INDIRECT(E\$40):INDIRECT(E\$41))"; this returns the maximum peak area value of the "middle calibration" for fluoride in our test case.
5. Mark the cells "E24" and "E25", and copy the formulas to the right by dragging the fill handle. The cell references are automatically adapted, and the respective peak area maxima are displayed.

Selection of the calibration function (channel)

1. Open a chromatogram from the sequence.
2. In the Chromeleon Studio, open the "Report Designer".
3. From the taskbar, select "Insert" then "Blank" from the Ribbon.
4. From the taskbar, select "Insert" then "Peak Summary" from the Ribbon.
5. Rename the new table to "Results".
6. Modify this table by adding the analytes' amount columns for each channel (Figure 10). Make sure that the order of the columns (Area(CD_1), Amount (CD_3), Amount (CD_2), Amount (CD_1)) is identical for each analyte.
7. Scroll to the right end of this table, and create a column for each analyte titled, e.g., "Amount Calc." (Figure 10B).

(A)

	A	B	C	D	E	F	G	H	I	J	K	L
1												
2												
3												
4												
5												
6												
7	3	STD (1)	Ok	Disabled	0.005	0.006	0.005	0.008	0.004	0.011		
8	4	STD (2)	Ok	Disabled	0.008	0.011	0.009	0.016	0.008	0.023		
9	5	STD (3)	Ok	Disabled	0.017	0.022	0.018	0.031	0.015	0.042		
10	6	STD (4)	Ok	Disabled	0.033	0.044	0.035	0.070	0.031	0.083		
11	7	STD (4)	Disabled	Ok	0.032	0.044	0.035	0.071	0.033	0.084		
12	8	STD (5)	Disabled	Ok	0.080	0.110	0.089	0.160	0.080	0.207		
13	9	STD (6)	Disabled	Ok	0.162	0.224	0.181	0.310	0.159	0.420		
14	10	STD (7)	Disabled	Ok	0.336	0.465	0.372	0.643	0.329	0.861		
15	11	STD (7)	Disabled	Ok	0.336	0.463	0.369	0.640	0.329	0.860		
16	12	STD (8)	Disabled	Ok	0.897	1.249	0.968	1.732	0.859	2.270		
17	13	STD (9)	Disabled	Ok	1.467	2.083	1.575	2.896	1.401	3.727		
18	14	STD (10)	Disabled	Ok	1.889	2.717	2.024	3.785	1.806	4.899		
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31												
32		First row										
33		End row calib low										
34		First row mid calib.										
35		End row middle calib.										
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(B)

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33		End row calib low										
34		First row mid calib.										
35		End row middle calib.										
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41												
42												

Figure 9. Example for a Calibration tab in the Report Designer using the automated peak area evaluation. (A) Final table, (B) Final table showing functions; only part of the table is displayed for space reasons.

As indicated above and shown in Figure 1, the optimum calibration function selection follows two logical tests. The tests can be described like this:

- If the analyte peak area is less than the low concentration peak area maximum, then use CH_1.
- Otherwise, if the analyte peak area is less than the middle concentration area, then use Amount of CH_2, otherwise use Amount of CH_3.

Such decisions can be arranged using the IF()-function in the spreadsheet. Its general syntax is “=IF(logical_test, [value_if_true], [value_if_false])”, and the two logical tests described above can be combined in one formula.

For the example given (Figure 10), enter for

- Amount Calc. (Fluoride), cell AA6:
“=IF(C6<Calibration!\$E\$24;F6;IF(C6<Calibration!\$E\$25;E6;D6))”
- Amount Calc. (Chloride), cell AB6:
“=IF(G6<Calibration!\$F\$24;J6;IF(G6<Calibration!\$F\$25;I6;H6))”
- Amount Calc. (Nitrite), cell AC6:
“=IF(K6<Calibration!\$G\$24;N6;IF(K6<Calibration!\$G\$25;M6;L6))”

- Amount Calc. (Nitrate), cell AD6:
“=IF(O6<Calibration!\$H\$24;R6;IF(O6<Calibration!\$H\$25;Q6;P6))”
- Amount Calc. (Phosphate), cell AE6:
“=IF(S6<Calibration!\$I\$24;V6;IF(S6<Calibration!\$I\$25;U6;T6))”
- Amount Calc. (Sulfate), cell AF6:
“=IF(W6<Calibration!\$J\$24;Z6;IF(W6<Calibration!\$J\$25;Y6;X6))”

Please note that the syntax is analogous to Microsoft Excel. The use of two "\$"-signs, one before and one after the cell letter (e.g., “\$E\$”), locks the reference to the cell. In our case, this fixes the reference to the corresponding calibration peak area maximum. After verifying that the cell references in the previously entered formula produce the expected result, select the formula cells and drag the fill handle down over the cell range to be populated. The cell references are automatically adapted, and the selected sample results are displayed (Figure 11).

The table design can be optimized by the “Hide columns” and cell formatting options in the Report Designer (Figure 12).

The “Results” table can be used to print the sample results.

(A)

A1													
	A	B	C	D	E	F	G	H	I	J	K	L	M
1													
2	No.	Injection Na	Area	Amount	Amount	Amount	Area	Amount	Amount	Amount	Area	Amount	Amount
3			$\mu\text{S}^*\text{min}$	mg/L	mg/L	mg/L	$\mu\text{S}^*\text{min}$	mg/L	mg/L	mg/L	$\mu\text{S}^*\text{min}$	mg/L	mg/L
4			CD_1	CD_3	CD_2	CD_1	CD_1	CD_3	CD_2	CD_1	CD_1	CD_3	CD_2
5			Fluoride	Fluoride	Fluoride	Fluoride	Chloride	Chloride	Chloride	Chloride	Nitrite	Nitrite	Nitrite
6	3,000	STD (1)	0,005	0,339	0,055	0,027	0,006	0,927	0,101	0,052	0,005	0,699	0,117
7	4,000	STD (2)	0,008	0,355	0,073	0,047	0,011	0,963	0,144	0,099	0,009	0,747	0,170
8	5,000	STD (3)	0,017	0,400	0,124	0,100	0,022	1,041	0,237	0,199	0,018	0,862	0,296
9	6,000	STD (4)	0,033	0,483	0,218	0,200	0,044	1,198	0,425	0,401	0,035	1,071	0,526
10	7,000	STD (4)	0,032	0,481	0,215	0,197	0,044	1,199	0,426	0,402	0,035	1,070	0,524
11	8,000	STD (5)	0,080	0,726	0,495	0,492	0,110	1,673	0,992	1,011	0,089	1,721	1,240
12	9,000	STD (6)	0,162	1,151	0,980	1,003	0,224	2,485	1,964	2,056	0,181	2,842	2,472
13	10,000	STD (7)	0,336	2,054	2,010	2,090	0,465	4,202	4,017	4,264	0,372	5,155	5,014
14	11,000	STD (7)	0,336	2,052	2,007	2,086	0,463	4,191	4,003	4,249	0,369	5,124	4,981
15	12,000	STD (8)	0,897	4,956	5,318	5,578	1,249	9,797	10,708	11,460	0,968	12,396	12,973
16	13,000	STD (9)	1,467	7,903	8,678	9,122	2,083	15,745	17,821	19,109	1,575	19,762	21,069
17	14,000	STD (10)	1,889	10,090	11,171	11,751	2,717	20,267	23,229	24,926	2,024	25,218	27,065
18	16,000	3268 MO/13	0,035	0,493	0,229	0,212	0,118	1,728	1,058	1,082	0,077	1,577	1,081
19	17,000	3268 MO/14	0,359	2,170	2,142	2,229	1,304	10,187	11,174	11,961	0,809	10,466	10,852

(B)

AA6												
	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF
1												
2	Amount	Amount	Area	Amount	Amount	Amount	Amount Calc.					
3	mg/L	mg/L	$\mu\text{S}^*\text{min}$	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
4	CD_2	CD_1	CD_1	CD_3	CD_2	CD_1	Fluoride	Chloride	Nitrite	Nitrate	Phosphate	Sulfate
5	Phosphat	Phosphat	Sulfate	Sulfate	Sulfate	Sulfate						
6	0,205	0,127	0,011	2,019	0,215	0,118						
7	0,338	0,255	0,023	2,122	0,334	0,261						
8	0,544	0,489	0,042	2,322	0,565	0,494						
9	1,025	1,004	0,083	2,730	1,037	1,001						
10	1,066	1,048	0,084	2,741	1,051	1,016						
11	2,484	2,563	0,207	3,976	2,479	2,548						

Figure 10. Newly created "Results" report. (A) Calculated amounts for the individual channels. The screenshot shows the columns for fluoride and chloride. The remaining columns follow to the right. (B) Appended amount columns ("Amount Calc.") used for automatic result selection.

AA6 =IF(C6<Calibration!\$E\$24;F6;IF(C6<Calibration!\$E\$25;E6;D6))												
	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF
1												
2	Amount	Amount	Area	Amount	Amount	Amount	Amount Calc.					
3	mg/L	mg/L	µS*min	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
4	CD_2	CD_1	CD_1	CD_3	CD_2	CD_1	Fluoride	Chloride	Nitrite	Nitrate	Phosphate	Sulfate
5	Phosphate	Phosphate	Sulfate	Sulfate	Sulfate	Sulfate						
6	0,205	0,127	0,011	2,019	0,215	0,118	0,03	0,05	0,06	0,14	0,13	0,12
7	0,338	0,255	0,023	2,122	0,334	0,261	0,05	0,10	0,12	0,25	0,25	0,26
8	0,544	0,489	0,042	2,322	0,565	0,494	0,10	0,20	0,25	0,47	0,49	0,49
9	1,025	1,004	0,083	2,730	1,037	1,001	0,22	0,43	0,53	1,08	1,03	1,04
10	1,066	1,048	0,084	2,741	1,051	1,016	0,20	0,43	0,50	1,09	1,07	1,05
11	2,484	2,563	0,207	3,976	2,479	2,548	0,50	0,99	1,24	2,49	2,48	2,48
12	4,904	5,149	0,420	6,101	4,940	5,188	0,98	1,96	2,47	4,85	4,90	4,94
13	10,045	10,642	0,861	10,500	10,030	10,649	2,05	4,20	5,15	10,55	10,32	10,50
14	10,027	10,623	0,860	10,489	10,017	10,635	2,01	4,00	4,98	10,02	10,03	10,02
15	26,085	27,782	2,270	24,570	26,314	28,119	4,96	9,80	12,40	24,46	24,73	24,57
16	42,491	45,314	3,727	39,120	43,154	46,186	7,90	15,75	19,76	39,33	39,47	39,12
17	54,766	58,431	4,899	50,821	56,696	60,715	10,09	20,27	25,22	50,70	50,50	50,82
18	2,148	2,204	0,088	2,783	1,099	1,068	0,23	1,06	1,08	1,18	2,15	1,10
19	21,796	23,199	0,899	10,878	10,468	11,118	2,17	10,19	10,47	10,96	20,88	10,88

Figure 11. "Results" spreadsheet with logical IF()-formula for automatic result selection

AA6 =IF(C6<Calibration!\$E\$24;F6;IF(C6<Calibration!\$E\$25;E6;D6))								
	A	B	AA	AB	AC	AD	AE	AF
1								
2	No.	Injection Name	Amount Calc.					
3			mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
4			Fluoride	Chloride	Nitrite	Nitrate	Phosphate	Sulfate
5								
6	3,000	STD (1)	0,03	0,05	0,06	0,14	0,13	0,12
7	4,000	STD (2)	0,05	0,10	0,12	0,25	0,25	0,26
8	5,000	STD (3)	0,10	0,20	0,25	0,47	0,49	0,49
9	6,000	STD (4)	0,22	0,43	0,53	1,08	1,03	1,04
10	7,000	STD (4)	0,20	0,43	0,50	1,09	1,07	1,05
11	8,000	STD (5)	0,50	0,99	1,24	2,49	2,48	2,48
12	9,000	STD (6)	0,98	1,96	2,47	4,85	4,90	4,94
13	10,000	STD (7)	2,05	4,20	5,15	10,55	10,32	10,50
14	11,000	STD (7)	2,01	4,00	4,98	10,02	10,03	10,02
15	12,000	STD (8)	4,96	9,80	12,40	24,46	24,73	24,57
16	13,000	STD (9)	7,90	15,75	19,76	39,33	39,47	39,12
17	14,000	STD (10)	10,09	20,27	25,22	50,70	50,50	50,82
18	16,000	3268 MO/13 LOW LEVEL	0,23	1,06	1,08	1,18	2,15	1,10
19	17,000	3268 MO/14 HIGH LEVEL	2,17	10,19	10,47	10,96	20,88	10,88

Figure 12. Simplified and adjusted layout of the "Results" table.

Summary

The flexible reporting options of Chromeleon 7 CDS software allow easy adaptation to specific calibration and laboratory routines. The calibrated dynamic detector range can be segmented, and the peak results automatically attributed. After the laboratory defined process is arranged, only minimal user interaction is needed. Productivity increases, and transcription errors are avoided, resulting in significant time savings while

securing data reliability. In addition, the high adaptability of Chromeleon CDS software simplifies data export, e.g., to a LIMS, contributing to the integration process of workflows and results in modern laboratories. Before using the process described here to generate analytical data in a laboratory, the form sheets and included formulas must be validated according to the laboratory standards.

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