

What your CDS calibration settings actually compute: Empower, Chromeleon and OpenLab.

Fit type, weighting and origin are three dropdowns in your processing method. Each one changes the equation behind every reported result, and the same name does not always mean the same math.

SUMMARY

Chromatography data systems give analysts flexible calibration settings: fit type, weighting, origin handling. This paper sets out, from vendor documentation, what Empower, Chromeleon and OpenLab CDS offer and report, shows that identical names can describe different equations, and works one data set through the choices to show how far a reported result can move. It closes with a checklist for documenting calibration settings.

THE SHORT VERSION

- 01 Fit type, weighting and origin handling each change the equation behind every reported result.
- 02 The same name can mean different math: Chromeleon's LIN is forced through the origin, while Empower's and OpenLab's Linear are not.
- 03 Record all three settings for every analyte, and judge the curve on back-calculated percent error, not the default statistics.

Three dropdowns, one equation.

A method is transferred from one site to another. The new lab rebuilds the processing method, picks "linear" from the fit type list, leaves weighting at its default, and runs the standards. The curve passes. The low-level results come out different from the sending lab's, and nobody can see why.

Every chromatography data system asks three questions when you build a calibration: which model, which weighting, and what to do with the origin. Waters Empower, Thermo Scientific Chromeleon and Agilent OpenLab CDS all answer them with dropdowns in the processing method. These systems are built for acquisition, control and secure records, and their calibration settings are flexible by design. That flexibility is exactly why the settings need to be understood and written down.

This article sets out what each system offers and reports, using only the vendors' own documentation [1] [5] [7].

Same name, different calibration curve.

The fit type names look interchangeable. They are not.

WHAT YOU WANT	WATERS EMPOWER 3	THERMO CHROMELEON 7	AGILENT OPENLAB CDS
Straight line with an intercept	Linear	Linear WithOffset (LOFF)	Linear, origin set to Ignore
Straight line through the origin	Linear through Zero	LIN	Linear, origin set to Force

WHAT YOU WANT	WATERS EMPOWER 3	THERMO CHROMELEON 7	AGILENT OPENLAB CDS
Quadratic with an intercept	Quadratic	Quadratic WithOffset (QUOFF); QUAD is the through-origin form	Quadratic, origin set to Ignore
Average response factor	Response factor	Average calibration factors (ACF)	Average RF
1/x² weighting	Not stated in public documentation	1/Amount ²	1/Amount ²

In Chromeleon, LIN is the straight line forced through the origin. The line with an intercept is Linear WithOffset ^[5]. In Empower, Linear has an intercept, and the forced versions sit in a separate group of "through zero" fits ^[2]. In OpenLab, Linear is a curve model, and the origin is a separate setting: Ignore, Include, Force or Connect ^[7].

So "use a linear fit" is not a complete instruction. A method that says only "linear" can produce two different equations depending on the system it is rebuilt in.

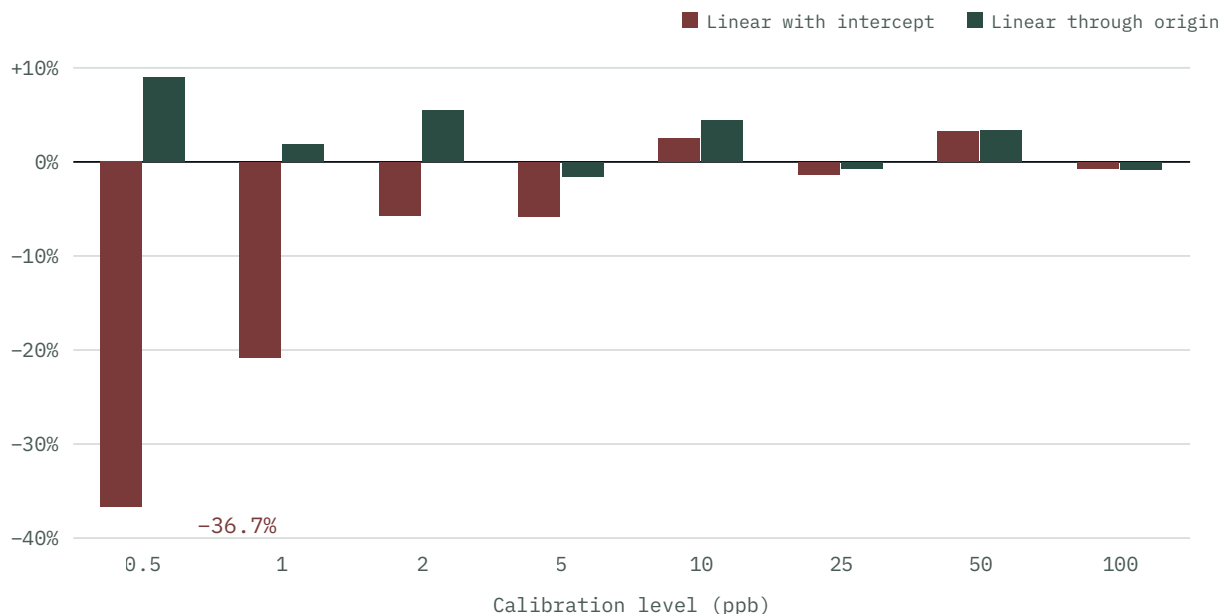
The same fit type name can describe two different equations.

One data set, three CDS settings.

Here is the eight-level calibration from [Insights 01](#), 0.5 to 100 ppb, run through three settings an analyst could reasonably pick. Each standard is back-calculated against its own curve.

LEVEL (PPB)	LINEAR WITH INTERCEPT (EMPOWER LINEAR, OPENLAB LINEAR + IGNORE)	LINEAR THROUGH ORIGIN (CHROMELEON LIN)	AVERAGE RESPONSE FACTOR
0.5	-36.7%	+9.0%	+6.2%
1	-20.8%	+1.9%	-0.7%
2	-5.7%	+5.4%	+2.7%
5	-5.8%	-1.5%	-4.0%
10	+2.5%	+4.4%	+1.8%
25	-1.3%	-0.7%	-3.3%
50	+3.2%	+3.3%	+0.7%
100	-0.7%	-0.8%	-3.4%

Illustrative data set from Insights 01, unweighted fits. Column labels give the setting names that produce each equation, per vendor documentation. Every value is computed from the responses in Insights 01.

-36.7%ERROR AT 0.5 PPB, LINEAR WITH
INTERCEPT**+9.0%**ERROR AT 0.5 PPB, LINEAR
THROUGH ORIGIN**46 points**SWING AT THE LOW STANDARD FROM
ONE SETTING**FIGURE 1 Percent error by level: intercept vs. through the origin**

Same data, same instrument, same word "linear". At the lowest standard, the line with an intercept reports -36.7%. The line through the origin reports +9.0%. That is a 46-point swing at the reporting limit, caused by one dropdown. Above 10 ppb the two settings agree within a few percent, which is why the difference is easy to miss.

Neither setting is wrong in itself. Whether the origin should be forced is a question for the data, covered in [Insights 08](#). What matters here is that the choice is made deliberately and recorded, because it decides the low-level results.

Weighting: the default is none.

All three systems offer weighting. In Empower it is set in the Weighting column of the processing method's Components tab, and the default is None ^[3]. OpenLab lists None, 1/Amount, 1/Amount², 1/Response and 1/Response², and normalizes amount weights to the smallest amount ^[7]. Thermo's technical note on Chromeleon uses 1/Amount² ^[5].

The default matters. An unweighted fit favors the top of the range, so a method built without a deliberate weighting choice is usually least accurate where accuracy matters most. [Insights 07](#) shows how to pick the weight from your own data.

One more detail: OpenLab offers weighting by amount or by response. They are not the same weight. If your SOP says $1/x$, confirm which axis x is in your system.

Origin: four options, one of them adds a point.

OpenLab makes the origin its own setting with four options. Ignore fits the standards only. Force passes the curve through zero. Connect draws a line to the origin without using it in the calculation. Include adds a point at zero amount and zero response to the calibration levels ^[7].

That last option deserves care in regulated work. EPA Method 8000D states that an X value of zero should not be included as a calibration point, whatever the model ^[9]. If a method transferred into OpenLab uses Include, the curve contains a standard that was never run.

In Empower and Chromeleon the origin is part of the fit type name rather than a separate field, which is one more reason the names in the table above need reading closely ^{[2][5]}.

What the CDS reports, and what it does not.

SYSTEM	FIT STATISTICS NAMED IN VENDOR DOCUMENTATION	BUILT-IN CURVE CHECK DESCRIBED
Empower 3	R , R^2 , standard error of calibration, RSD, RSD(E), RSS, and % Deviation for each calibration point	None found in public documentation
Chromeleon 7	r^2 , RSE (computed on amounts, including weights), RSD for average calibration factor curves, and relative amount deviation	None found in public documentation
OpenLab CDS	r , R^2 , residual standard deviation, standard deviation, RSD, and residual and relative residual per level	Warnings for too few points, a zero, negative or infinite slope, or a curve that cannot be calculated

Three things stand out.

First, r and R^2 are everywhere, and RSE is not. Chromeleon reports RSE ^[5]. The Empower and OpenLab documentation we reviewed describes RSD and residual statistics, but no statistic named RSE ^{[2][8]}.

Second, per-point error is computed differently. Empower's % Deviation formula depends on a System Policy. With the policy off, the default, it is the calculated value minus the standard's value, divided by the standard's value. With it on, the subtraction and the denominator change ^[4]. OpenLab defines its residuals on the fitted variable, which is normally the response ^[8]. For the line with an intercept in the example above, the lowest standard misses its response by -25.1% but its amount by -36.7%. Method 8000D's 30% limit applies to the amount ^[9].

Third, the built-in checks are structural, not statistical. OpenLab's "verification of the calibration curve" warns when there are too few points, when the slope is zero, negative or infinite, or when the curve cannot be calculated ^[6]. Those are useful guards. They do not test whether the curve is accurate at the reporting limit. We found no automatic acceptance check described in the public Empower or Chromeleon documentation.

A statistic can also look perfect by construction. Empower notes that a point-to-point fit always reports a correlation coefficient of 1 and a standard error of 0 ^[2].

A checklist for documenting CDS calibration settings.

01 **Name the equation, not just the fit type.**

Write "linear with intercept" or "linear through the origin" in the method, not "linear".

02 **Record the weighting and its axis.**

1/x² by amount is not 1/y² by response.

03 **Record the origin setting.**

And confirm no zero point is being added to the calibration.

04 **Re-check on transfer.**

When a method moves between systems, rebuild the settings from the written equation, then compare low-level results.

05 **Know which per-point error your CDS reports.**

Response residual or amount error, and which sign convention.

06 **Judge the curve on amount error and RSE.**

Calculate them if your system does not report them, and keep the calculation with the record.

Where WLTR fits.

Most labs accept the statistics their CDS reports by default and rarely compare one setting against another. Few can show, for a given analyte, what the result would have been under the alternatives.

WLTR is calibration data integrity infrastructure for regulated analytical laboratories. For each analyte, it derives nine calibration regression models: average response factor, plus linear and quadratic fits across four weightings each. It scores every model against fifteen ICAL parameters, including RSE. All of it is computed orthogonally to the CDS, under U.S. Patent 12,038,448 B2 ^[P].

CALIBRATION VERIFICATION

See every fit type, weighting and origin option computed side by side for your own ICAL data, orthogonally to your CDS.

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