QUANTO USER GUIDE

CalGroup & standard addition

Group bottles that share a curve; Calibration vs StdAdd mode; vs Initial/Bracket.

Use **CalGroup** when one batch needs more than one calibration story — for example two matrices, two instruments already merged under AcqKeys, or a **standard-addition** set beside a normal curve.

What CalGroup is

CalGroup is a label on bottles. Bottles with the same label share:

- One curve (or one standard-addition line)
- Blank-offset / blank-concentration picking when you use **Average (CalGroup)** or sequence modes that stay inside the group

Bottles with an empty CalGroup share the **default** group.

CalGroup is **not** a sample type. Sample types stay **Blank / Calibration / QC / Sample / Solvent**. Fortified amount still lives on **Dose**.

Mode: Calibration vs StdAdd

CalGroup Mode	What Quanto builds
Calibration	A normal ESTD or ISTD curve from the Calibration bottles in that group
StdAdd	A standard-addition line from the spiked Calibration bottles in that group; the shared native (unspiked) amount is taken from the addition line

For **StdAdd**:

1. Put the addition set in its own CalGroup and set Mode **StdAdd**.
2. Mark spiked bottles **Calibration** with the **spike increment** as Dose (not the total amount in the bottle).
3. Keep the unspiked native in that story as the native the line reports — see also Blank concentration if you also subtract a method blank toward NativeConc.

Recovery % for additions still uses the **spike increment** on Dose (`RecPct`).

CalGroup vs Initial / Bracket

Setting	Job
CalGroup	Which bottles share one curve / blank pool
Calibration mode = Initial	One curve in time for that group's cal set
Calibration mode = Bracket	Cut cal sets by acquisition time; each sample block uses surrounding cal sets **within the same CalGroup story**

You can bracket inside a group. You can also run two CalGroups side by side with Initial mode. Do not confuse CalGroup with AcqKey (instrument / imported method set) — AcqKey is for Key Review; CalGroup is for calibration grouping.

Blank offset and blank concentration

Blank-use modes that say **CalGroup** only average (or walk) blanks inside that group. **Average (overall)** ignores CalGroup and uses every eligible blank in the batch. Guides: Blank offset, Blank concentration.

Setup checklist

1. On Samples, fill **CalGroup** for bottles that belong together.
2. Set the group **Mode** to **Calibration** or **StdAdd**.
3. Confirm Calibration / QC doses (spike increment for StdAdd).
4. Choose Initial vs Bracket on the method.
5. Set Origin / Blank corr / Blank use if needed.
6. **Analyze**, then check the curve per group and Method Validation.

Related

- Set up an analysis
- Method design
- Bracket calibration
- Result limits & flags