

Key Review

Multi-instrument AcqKeys, QntKeys, SmpKey pick.

AcqKey is an acquisition set (an imported method, or an instrument). **QntKey** is one quantitation ion or transition. **SmpKey** is the reporting key that groups injections of the same physical sample.

Key Review is the matrix where those three meet: you see every AcqKey × QntKey × dilution for one SmpKey, then pick the result that reports.

Key Review □ one SmpKey, several instruments and ions

SmpKey SAMPLE-14 was injected on LC-QQQ and GC-MS, neat and 10x. Columns are QntKeys under dilution bands.

SmpKey SAMPLE-14						Dilution band 1x		Dilution band 10x
Group	Sum	Analyte	AcqKey	Sel	Rej	Q1	Q2	Q1 (10x)
Stimulants	12.4	Caffeine	LC-QQQ	☒		12.4 Q 195->138	11.9 Q 195->110	☐
		Caffeine	GC-MS			13.1 above curve	☐	1.28 diluted
Xanthines	3.1	Theobromine	LC-QQQ	☒		3.10 Q 181->138	fail ion ratio	☐

- ☒ Chosen result for this analyte on the SmpKey (reports use this)
- ☐ Failed qualifier / flag ☐ still visible, not auto-picked
- ☐ AcqKey = acquisition set (instrument or imported method). Q1 / Q2 = QntKey.
- Tick Reject to drop a row from Group sum. Auto-pick prefers a passing neat result over a diluted or above-curve one.
- The side Amount grid lists one concentration per SumGroup for the selected sample key.

Key Review matrix for SAMPLE-14 across LC-QQQ and GC-MS

Acquisition sets

AcqKey and QntKey □ how many methods fit in one batch

An AcqKey is an imported acquisition set. A QntKey is one quantitation ion / transition on that analyte.

AcqKey LC-QQQ
Imported MassHunter method

Caffeine
Q1 195 -> 138
Q2 195 -> 110

Theobromine
Q1 181 -> 138
ISTD caffeine-d9

AcqKey GC-MS
Appended second method

Caffeine
Q1 m/z 194
own curve and ISTD

Sample file
AcqKey = GC-MS
matches this slice

Same analyte name on two AcqKeys is allowed. Key Review stacks those rows. Navigator AcqKey checkboxes hide a whole instrument.

ISTD links stay inside an AcqKey unless you point a Quant at another Analyte|Quant explicitly.

Two AcqKeys, each with its own analytes, QntKeys, and ISTD

Key	Meaning
AcqKey	Slice of the method. Append a second vendor method to create one. Samples carry AcqKey so they match the right slice.
QntKey	One Quant on that analyte (Q1, Q2, ...). Each has its own curve and optional ISTD.
SmpKey	Manual override, or the auto key from the method extraction table. All files that share it compete for one reported result per analyte name.
Dilution band	$\log_{10}$ of Dilution (1→0, 10→1, 100→2). Columns group by band.

Navigator **AcqKey** checkboxes hide a whole instrument from every grid, including Key Review.

Open Key Review

View → **Key Review** (or the ribbon). It follows the current SmpKey.

Rows: **SumGroup** → **analyte name** → **AcqKey**.

Fixed columns: Group, Group sum, Analyte, Selected, Reject, AcqKey.

Then one super-cell per **QntKey** under each dilution band.

The side **Amount** grid lists one concentration per SumGroup (the group sum of accepted analytes).

How a cell is chosen

Auto-pick, per analyte name inside the SmpKey:

1. Skip rejected samples and results rejected for the key.
2. Prefer a result that is **not above the curve**.
3. Prefer the **lower dilution band** (neat over 10×).
4. You can override with **Selected**, or drop a row with **Reject**.

The green outline is the winner. Reports that call `Q.KeyCompound` read that winner.

Failed qualifier / ion-ratio cells stay visible so you can see why they lost.

Typical setups

Two instruments, same samples. Append the GC method as AcqKey `GC-MS`. Give both data files the same **SmpKey**. Key Review stacks LC and GC rows; pick one (or keep both in Group sum if they are different SumGroups).

Several ions, one instrument. One AcqKey, Q1 / Q2 / Q3 columns. Qualifier percent lives on the Quant; Key Review shows pass/fail in the super-cell.

Dilution series. Same SmpKey, Dilution 1 and 10. Auto-pick keeps the neat result when it is on-scale, and falls back to 10× when the neat point is above the curve.

Group sum

SumGroup on the AnalyteNames master (isomer family, residue group). Group sum adds accepted members. Bracketed isomer names can cover across SumGroups. Reject a row to keep it out of the sum without deleting the result.