QUANTO USER GUIDE · IFRA / SUPERCELL

Upgrade from SuperCell to Quanto

For IFRA allergen labs moving from MassHunter Quant + SuperCell to a single Quanto batch.

SuperCell solved a hard IFRA problem: four acquisition methods, four MassHunter Quant batches, and a decision tree across polarities, SIM sets, and dilutions. Quanto keeps that science — and removes the scaffolding.

SuperCell today

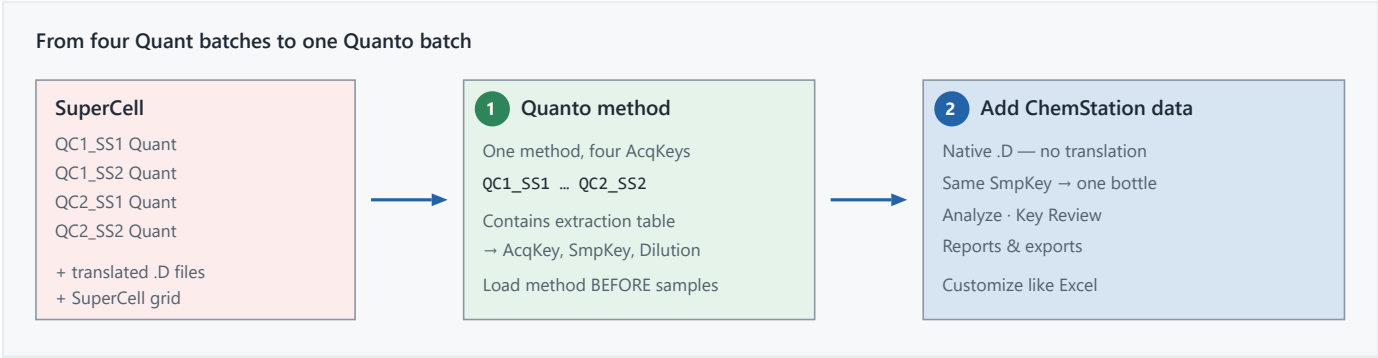
- **4 methods × 4 Agilent Quant instances**
- Data files must be **translated** for MassHunter
- Fixed multi-batch grid + decision tree
- External Quant always in the loop

Quanto instead

- **1 method, 1 batch**, no external Quant
- Loads **un-translated ChemStation** `.D` files
- AcqKey / SmpKey replace the four-batch layout
- Ease of use and speed are unmatched — highly customizable, fast reports and exports

Demo included. Quanto ships with an IFRA example batch, method, and sample-metadata extraction table. With a SuperCell-style naming scheme it should work more or less out of the box on your data.

1. Process overview

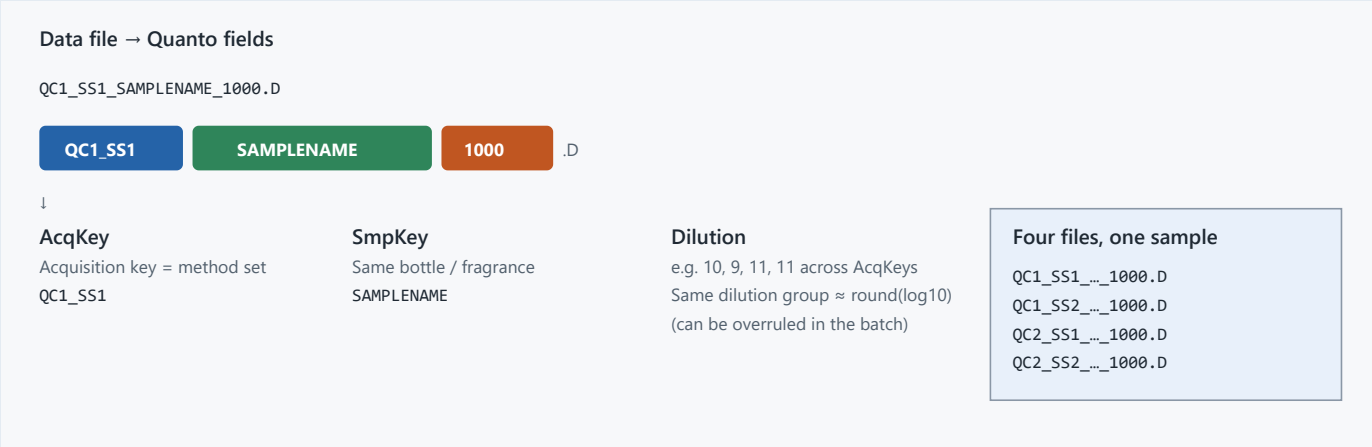


Keep your IFRA acquisition layout; drop the four Quant instances and the translation step.

2. SuperCell file naming (fixed scheme)

SuperCell expects a strict naming pattern so the four methods and dilutions line up.

Piece	Meaning
`QC1`	Instrument 1 — **apolar** column
`QC2`	Instrument 2 — **polar** column
`SS1` / `SS2`	SIM set 1 / SIM set 2
Methods	`QC1_SS1.M`, `QC1_SS2.M`, `QC2_SS1.M`, `QC2_SS2.M`
Data file	`QC1_SS1_SAMPLENAME_1000.D` (example dilution token `1000`)



Confirm a similar scheme in file names or sample names so extraction can fill AcqKey and SmpKey automatically.

3. How that maps in Quanto

Quanto field	Role for IFRA / SuperCell upgrades
AcqKey	What SuperCell treated as a separate Quant method/batch — e.g. `QC1_SS1`. Analyte names may repeat across AcqKeys; the pair (name + AcqKey) is unique.
SmpKey	Logical sample / bottle. Injections with the same SmpKey are combined for review (Key Review picks winners across AcqKeys).
Dilution	Per injection. Values such as 10, 9, 11, 11 on the four AcqKeys are recognized as the same dilution group (rounded power of 10) unless you override.
Extraction table	On the method. RegEx from file name / path → AcqKey, SmpKey, SampleType, Dose, Dilution when you Add samples.

Related guides: Method design, Sample metadata extraction, Key Review.

> **Order matters.** Create or load the Quanto *method first* (with extraction rules), then add data files. The method owns the extraction; the batch uses it when samples are added.

4. Analyte names and groups

In SuperCell, compounds with identical **Group Names** are summed for the IFRA total. Suffixes on names such as **Farnesol** and **Galaxolide** define which peaks belong together so that all bracket / isomer numbers are present without duplicating the group.

On the **apolar** column (`QC1`), **Farnesol (1)** and **Farnesol (2)**, and **Galaxolide (1)** and **Galaxolide (2)**, are treated as **co-eluting** peak pairs — the suffixes keep the required bracket numbers while the shared group name still sums correctly.

Suffixes → shared group (example pattern)

Peaks (distinct AcqKey / RT)

`Farnesol (1)`
`Farnesol (2)`
`Galaxolide (1)`
`Galaxolide (2)`

Co-eluting on apolar (QC1)
Farnesol (1,2) · Galaxolide (1,2)

→

Group name (summed)

Farnesol

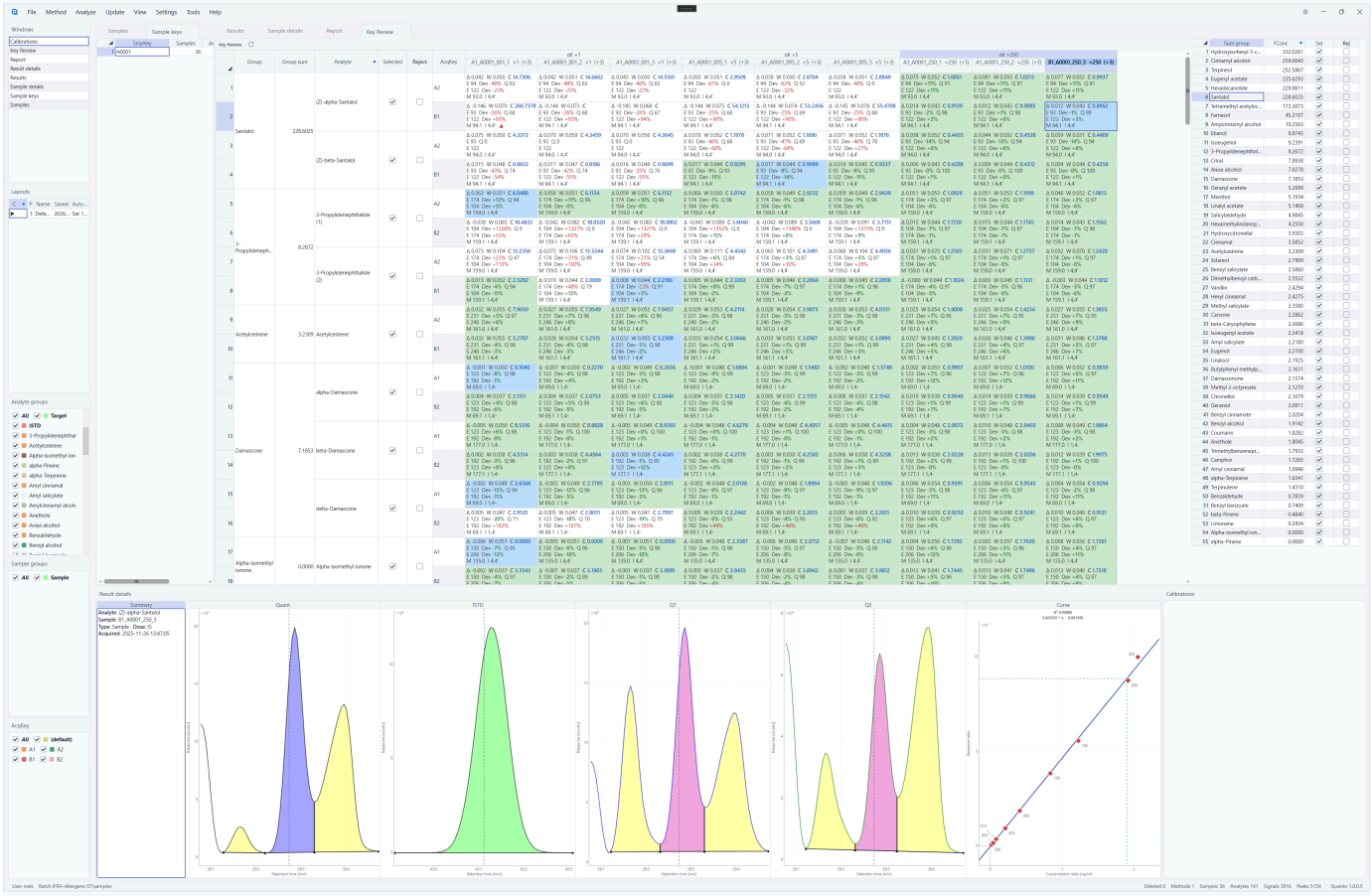
Galaxolide

All required bracket numbers present
No duplicate group entries

Farnesol (1, 2) and Galaxolide (1, 2) co-elute on apolar; suffixes + shared group names keep IFRA summing correct in Quanto.

5. Reviewing data

For reviewing data, use **Sample keys** and **Key Review** views.



IFRA Allergens example batch. Review results with Sample keys and Key Review.

6. Suggested upgrade checklist

1. Install Quanto and open the **IFRA example** batch / method (see Getting started).
2. Inspect the method's **extraction table** — confirm RegEx match your `QC*_SS*_…` names (or adapt them).
3. Confirm analyte names / groups (Farnesol, Galaxolide, …) match your SuperCell Compound Groups.
4. Add a small set of un-translated ChemStation `.D` files; verify AcqKey, SmpKey, and Dilution fill correctly.
5. Run Analyze, review with Key Review across AcqKeys, then try a report/export template.
6. Scale up: append remaining AcqKeys / historical methods as needed (Append import → new AcqKey).

7. Why labs switch

- **One tool** — no four Quant instances, no translation pipeline.
- **Native ChemStation** — load `.D` as acquired.
- **Speed** — interactive review; batch recalculation in well under a second on typical IFRA-sized methods.
- **Customization** — Excel-like reports and exports without fighting MassHunter report templates.

Questions or a guided migration on your data: niels@waleson.eu. Product pages: Quanto · SuperCell.