QUANTO USER GUIDE

Compatibility

Single/triple quad, SIM/MRM/SCAN, MassHunter / ChemStation / SCIEX data and methods.

What Quanto can read today: instruments, acquisition modes, raw data, and vendor methods. Formats land through **add-ins** under `AddIns\` (see Installation and folders and Creating add-ins).

Platform

Item	Requirement
OS	Windows 10 or 11, **64-bit only**
Runtime	.NET 10 Desktop Runtime (x64), unless your installer bundles it
Host	WPF desktop (`Quanto.WPF.exe`); not a service, not Linux

Sizing and Analyze performance: Hardware and performance.

Instruments and acquisition modes

Quanto is built for **GC/LC–MS quantitative** work on **single quadrupole** and **triple quadrupole (QQQ)** data.

Mode	Meaning in Quanto	Typical instrument
SCAN	Full-scan MS1 extracted-ion chromatogram (EIC)	Single quad GC-MS / MS1 scan
SIM	Selected-ion monitoring	Single quad
MRM / MS-MS	Multiple-reaction monitoring (precursor → product)	Triple quad (QQQ)
Combinations	Mixed modes in one sample (e.g. SCAN+SIM)	Supported where the vendor file exposes them

Internally, chromatogram extraction uses `ChromatogramAcquisitionMode` : `Auto` , `Scan` , `Sim` , `MsMs` . **Auto** detects from the file and tries alternates if a channel comes back empty. TIC for a mode is that mode's primary TIC — not a sum of mixed modes.

MassHunter `.D` : detector classifies SingleQuadrupole vs QQQ / MRM / SIM / SCAN from the embedded acquisition method and scan types.

ChemStation `.D` : modes are SCAN, SIM, or **ScanAndSim** (`data.ms` / `dataSim.ms`). SIM windows can come from classic `acqmeth.txt` .

SCIEX WIFF: MRM transitions from the WIFF (Clearcore2 / SCIEX APIs).

Raw data (data providers)

Vendor	Add-in (class)	What you point at	Notes
Agilent MassHunter	`AgilentMassHunterDataProvider`	`.D` sample folders	Reads MassHunter data; may use Agilent **TDA indexed-data** conversion (`TDAConverterConsole.exe`) when indexed data is required for chromatogram access
Agilent ChemStation / MSD	`AgilentChemStationDataProvider`	`.D` sample folders	**Reads ChemStation data natively** via Agilent MSDChem (`MSDChemDataFile`) — **no TDA / format conversion step**
SCIEX	`SciexWiff`	`.wiff` files	Reads SCIEX WIFF through Clearcore2 / SCIEX vendor DLLs

All three also implement sample discovery (`FindSamples`) and fill common bottle metadata when present (name, acquired time, instrument, position, dilution, dose/level hints).

Vendor native DLLs ship under:

- `AddIns\VendorSupportFiles\Agilent\`
- `AddIns\VendorSupportFiles\Sciex\`

Method import (method importers)

Source	Add-in (class)	What you point at	What comes in
MassHunter quant method	`AgilentMhMethod`	`.m` method folder (`…\DaMethod\Quant\quantitative.xml`) or `.quantmethod.xml`	Compounds, ISTD flags, transitions, expected RT, curve hints
MassHunter method **from data**	`AgilentMassHunterDataMethod`	`.D` data folder	Method inferred from acquisition / MRM content in the data file
ChemStation quant method	`AgilentCsMethod`	`.M` method folder containing `qdb.mth`	Compounds from ChemStation QDB
SCIEX method **from data**	`SciexWiffMethod`	`.wiff` file	MRM compounds / transitions built from the WIFF (standalone `.msm` is **not** supported with the current minimal SCIEX DLL set)
Quanto package	(built-in host path)	`.qtm`	Full Quanto method (analytes, quants, doses, ISTD links, types, optional stored calibration and reports)

Import UX: **Method** → **Load / Import** — **Replace** or **Append** (Append uses a new **AcqKey** for multi-instrument / Key Review). Details: Reports, import, and export.

Vendor methods do **not** set Quanto's Calibration mode; new work defaults to Initial calibration unless you change it.

Peak integration (integrators)

Integrator	Role
Quanto	Shipped high-performance peak detector (default on channels)
Slice	Placeholder / alternate integrator slot (extensibility sample)

Per-channel integrator name and settings live on the method; custom integrators are add-ins (see Creating add-ins).

Capability checklist

Capability	Status
Single Quad data (SCAN / SIM)	Supported (MassHunter + ChemStation)
Triple Quad / QQQ data (MRM)	Supported (MassHunter + SCIEX; ChemStation as exposed by MSDChem)
SCAN + SIM combinations	Supported where the file layout exposes both (e.g. ChemStation ScanAndSim)
Import MassHunter method	Yes (`.m` / `.quantmethod.xml`)
Import MassHunter method from data file	Yes (from `.D`)
Import ChemStation method	Yes (`.M` + `qdb.mth`)
Import SCIEX method from data file	Yes (from `.wiff`)
Read MassHunter data	Yes
Read ChemStation data without conversion	Yes (native MSDChem)
Read SCIEX data	Yes (`.wiff`)

Related

- Analyst import/export workflow: Reports, import, and export
- Install layout and permissions: Installation and folders
- Extending formats: Creating add-ins