NEXCHROM ANALYTICAL CHROMATOGRAPHY SOFTWARE

Take Control of Your Gas Chromatography Data

One application. Every step. From raw instrument data to certified results.

››› Built for accuracy ››› Built for simplicity ››› Built for you

No Cloud Required
Runs 100% locally. Your data never leaves your machine.

Fast & Lightweight
Browser-based UI. No heavy installs. Runs on any PC.

AI Assistant Planned Add-in
Questions about your own data and instrument documentation, answered by a local model.

Secure & Stand-Alone
No network needed. Full data integrity by design.

Complete Analytical Workflow

NexChrom guides you through every step — intuitively, accurately, and traceably.

1 Instrument & Sample Setup
Register GC instruments, locations, and samples. Import CDS data natively from Agilent and Scion / Bruker, or via CSV, Excel or text export from Thermo Fisher, InterScience, Shimadzu and others.

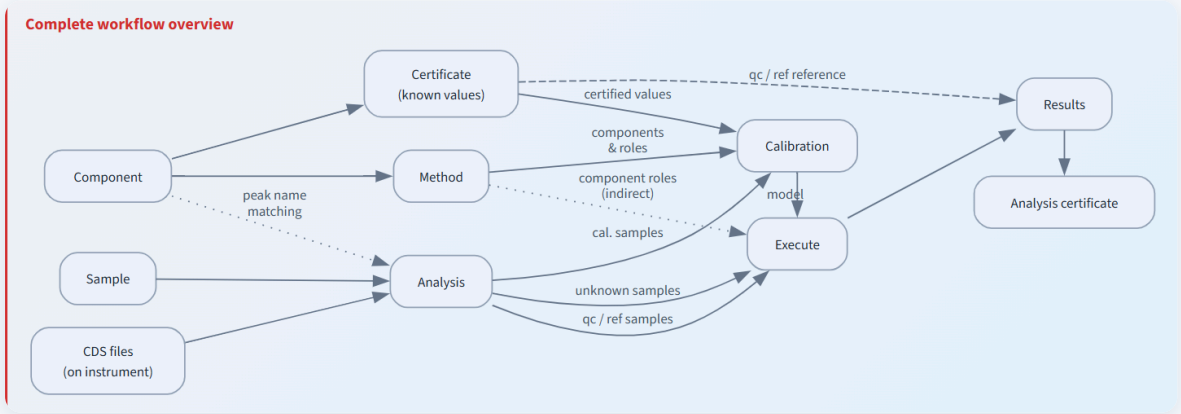
2 Method Configuration
Define analytical methods with component roles: direct (calibrated), indirect (via RRF), or fixed (certified value).

3 Calibration
Build polynomial calibration models per instrument with full regression statistics, covariance, and goodness-of-fit.

4 Execute & Calculate
Run calculations combining sample data, calibration model, and method. Results stored with full traceability.

5 Review & Approve
Inspect calculation results, approve or reject runs; the analysis certificate is issued with the approval.

6 Certificates
Generate analysis certificates. Import external reference certificates from PDF with OCR support.



Everything above lives inside a single application. The sample is registered once, CDS files stream in from the instrument, components and methods are re-used across runs, and the calibration model that produced each certificate is kept for later inspection. No exports to spreadsheets, no second tool for calibration, no separate certificate generator — data stays in one place and every result can be traced and re-inspected on demand.

INSTRUMENT & CDS COMPATIBILITY

Native: Agilent ChemStation (.D) • Scion / Bruker CompassCDS (.DATA)

OTHER CDS VIA EXPORT

Thermo Fisher Chromeleon • InterScience • Shimadzu — and any CDS exporting its peak table as CSV, Excel or text

Results export as CSV and certificates as PDF, for your LIMS or ERP | One unified workflow regardless of instrument brand or CDS

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Beyond Composition — Physical Properties and Benefits on Demand

Aligned with ISO, EN, DIN, BS, ASTM and AGA — extensible for the calculations your customers ask for next.

Built on International Standards

ISO 6974 composition analysis and the ISO 6976:2016 physical properties — calorific value, density, relative density, Wobbe index and compression factor, each with its Annex B uncertainty — are built in. Further physical-property calculations are available as optional modules.*

PURPOSE	STANDARD FAMILY
Composition measurement	ISO / EN / DIN / BS 6974
Heating value, Wobbe index, density, compression factor at reference conditions	ISO / EN / DIN / BS 6976 (2016)
Compressibility factor Z at line conditions*	ISO / EN 12213-1 · 12213-2 (AGA 8-DC92) · 12213-3 (SGERG-88)
Speed of sound*	ISO 20765-1 / -2 · AGA Report No. 10
Methane number*	ISO / EN 17507 · ISO/TR 22302 · ASTM D8221
Water content / water dew point*	ISO / EN 18453 · ISO 6327
Hydrocarbon dew point*	ISO / EN 23874
Gas quality & interchangeability*	ISO / EN 13686 · EN 16726

*Full quantity-by-quantity reference index on the next page, including sulphur / odorants, CO_2 emission factor and hydrogen-admixture coverage. * Optional module — not included in the standard version.*

NexChrom serves three audiences at once in a single tool. The **analyst** spends most of the working day in it and needs a workflow that flows from sample to certificate without friction. The **lab manager** is answerable for quality, traceability and audit-readiness. The **finance officer** decides whether the investment earns its keep. Below is the short version of what each of them gets from NexChrom.

For the Analyst

- ✓ Intuitive step-by-step workflow
- ✓ Native Agilent and Scion import; other CDS via CSV export
- ✓ Side-by-side peak tables per detector / signal
- ✓ Every result traceable to its source CDS file

For the Lab Manager

- ✓ Full audit trail: sample → method → CDS file → result
- ✓ Versioned calibrations and methods, reproducible runs
- ✓ ISO 6974 and ISO 6976 built in; ISO 12213 / AGA 8 / 10 as optional modules*
- ✓ PDF certificate import with OCR for external references
- ✓ Role-based user management and alert notifications
- ✓ Optional Aura2 sensor: live lab T, p and RH

For the Finance Officer

- ✓ No cloud subscription — runs on existing hardware
- ✓ No vendor lock-in — works across your instrument park
- ✓ Single licence covers the complete lab workflow
- ✓ Zero IT overhead: Python + SQLite, no server or DBA
- ✓ Predictable TCO: installation and instruction, then one annual fee

Whether you are evaluating NexChrom for a single-operator benchtop GC or for a multi-instrument custody-transfer lab, the same licence covers the full scope of your workflow. No per-seat upgrade fees, no pay-per-calculation, no cloud-usage surprises: one laboratory licence that starts with two days of installation and instruction, includes a year of remote service, and continues for one predictable annual fee that keeps the updates and the remote service coming.

Today you may only need composition and heating value. Tomorrow a new customer asks for compressibility, speed of sound or a methane number; next year a hydrogen-admixture report lands on your desk. NexChrom's modular architecture lets you add those calculations without switching platform or retraining the lab. The core application stays the same: new modules slot into the same workflow, the same audit trail and the same certificate engine, so what your analysts already know stays valuable as the reporting scope grows.

Python 3.13
Modern, maintainable, easy to extend.

Streamlit UI
Browser-based. No client install.

SQLite
File-based database. Zero-admin.

Works Offline
No network needed. No cloud service.

Multi-Vendor
Agilent, Scion native; other CDS via export.

Ready to modernize your gas chromatography lab?

Ask for a demo or a tailored quotation — including physical-property add-on modules.

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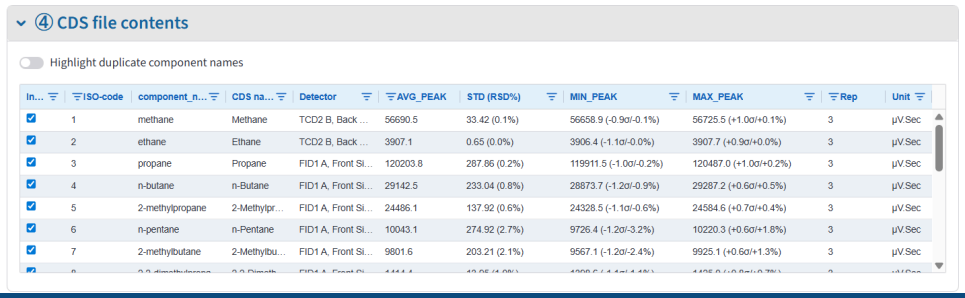
Analysis & Method Setup

From CDS peak table to quantified components — every step traceable and reproducible.

NexChrom reads chromatographic measurement data directly from the vendor's Chromatography Data System (CDS) file — natively from Agilent ChemStation `.D` folders and Scion / Bruker CompassCDS `.DATA` files, and from Thermo Fisher, InterScience, Shimadzu and other systems through CSV, Excel or text exports — without re-integration. Each file is parsed into peak tables per detector and per signal, the original uncertainty estimate is preserved where the instrument provides one, and component names are matched through an alias table so that vendor-specific and local naming conventions converge on a single identity.

A **Method** then decides how each component is quantified. **Direct** components are calibrated against an external reference certificate; **indirect** components are derived from another component through a configurable **Relative Response Factor (RRF)** rule with its own uncertainty contribution; **fixed** components take their value straight from a certified source. This role-based model lets one analytical run cover trace species, main constituents and balance gases together, with every result traceable back to the CDS file, the method, and the certificate that backed the calibration.



CDS file contents — per detector / per signal

CDS import

Agilent ChemStation and Scion / Bruker CompassCDS read natively, straight from the vendor file, no re-integration; Thermo Fisher, InterScience, Shimadzu and other CDS via CSV, Excel or text export.

Per-detector inspection

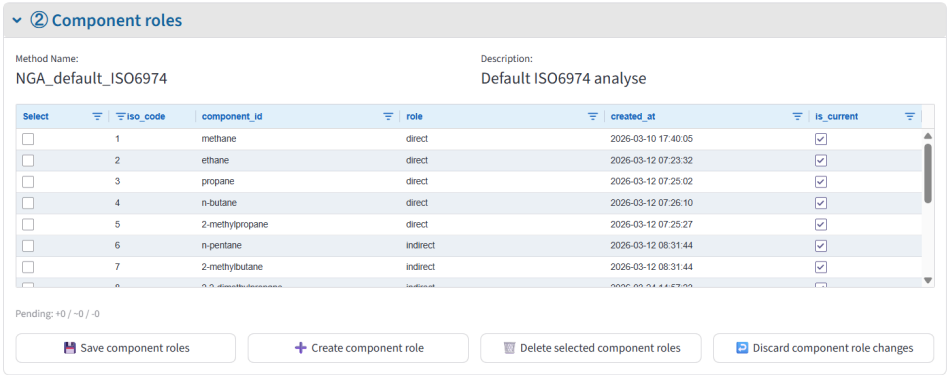
See every peak per channel before import. Toggle UNKNOWN peaks, highlight duplicate names, sanity-check the integration.

Three component roles

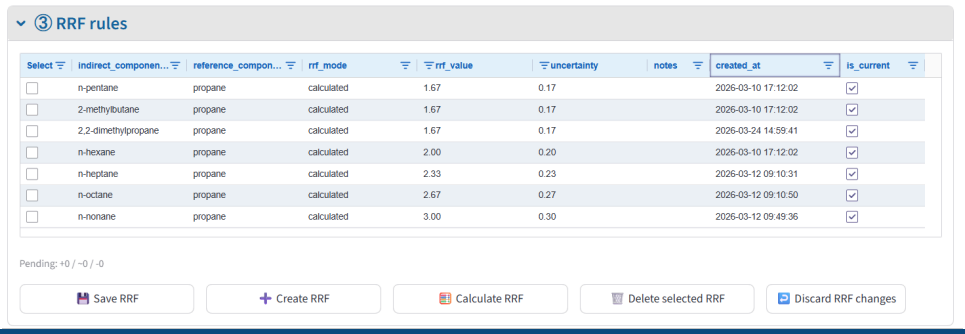
Direct (calibrated), indirect (via RRF) and fixed (certified) roles cover trace, main and balance components in one method.

Component aliases

Vendor-specific and local peak-name spellings resolve to a single component via a user-editable alias table.



Component roles: direct / indirect / fixed



RRF rules for derived components

RRF rules

A Relative Response Factor turns one measured component into a group of derived results — useful for C6+ fractions and trace hydrocarbons.

End-to-end traceability

Every result links back to the source CDS file, the method, the calibration model and the certificate that backed it.

In practice this role-based model means a single analytical run can cover a natural-gas sample with a main methane content, a balance-nitrogen component and a handful of trace hydrocarbons at ppm level — without a special configuration per customer. The analyst sees one method, one calibration and one result sheet; under the hood NexChrom routes every component through the right calculation path and keeps a full audit trail for the lab manager to hand over at audit time.

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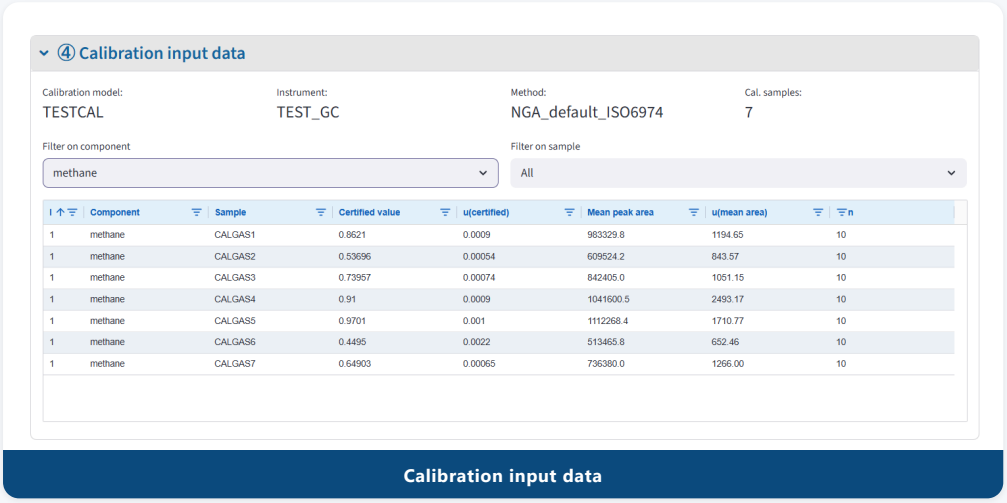
Calibration & Regression

Choose the right model for your data — with full statistics, not just a fitted line.

ISO 6974 recommends regression by the **ISO 6143 error-in-both-variables** method, which accounts for uncertainty in *both* the peak response and the certified reference value. NexChrom implements this alongside three classical alternatives — **OLS** (ordinary least squares), **WOLS** (weighted least squares) and **GLM** (generalised linear model). The analyst is free to pick whichever method matches the data, the detector response behaviour and the applicable regulatory or accreditation framework.

For every run, NexChrom fits several polynomial orders at once — from a straight line up to third degree — and suggests the order that best matches the data. The analyst can override that choice from the results grid whenever a different fit makes more sense. The quality figures that really matter — how each calibration point deviates from the fit, the range the calibration covers, the largest remaining deviation and the uncertainty on the fitted parameters — all appear directly on the plots and in the grid, so every calibration can be checked at a glance instead of taken on trust.



I	Component	Sample	Certified value	u(certified)	Mean peak area	u(mean area)	n
1	methane	CALGAS1	0.8621	0.0009	983329.8	1194.65	10
1	methane	CALGAS2	0.53696	0.00054	609524.2	843.57	10
1	methane	CALGAS3	0.73957	0.00074	842405.0	1051.15	10
1	methane	CALGAS4	0.91	0.0009	1041600.5	2493.17	10
1	methane	CALGAS5	0.9701	0.001	1112268.4	1710.77	10
1	methane	CALGAS6	0.4495	0.0022	513465.8	652.46	10
1	methane	CALGAS7	0.64903	0.00065	736380.0	1266.00	10

Calibration input data

Four regression methods

EIV (ISO 6143 via crvftw) pre-selected, OLS, WOLS and GLM selectable — all orders computed in one run, optimal order auto-picked per component on the goodness-of-fit limit of ISO 6143 (GOF ≤ 2), for every method; every fit shows a Pass / Fail fit test, and every result is checked against the calibrated concentration range.

Per-component control

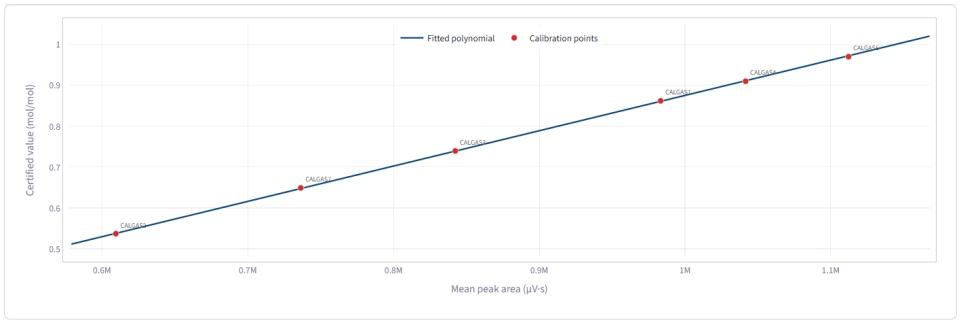
Override the automatic order per component from a single grid; calibration range and quality metrics update instantly.

Full statistics

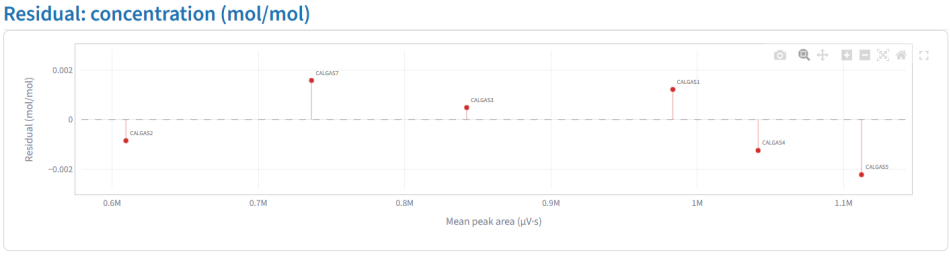
Calibration range, max calibration error and at-sample concentration per component; parameter uncertainties included.

Interactive plots

Hover on any point for peak area, certified value and each point's error contribution. Clear visual confirmation of the fit.



Calibration curve with hover tooltip



Residuals per calibration point (relative %)

ISO 6143 via crvftw

The error-in-both-variables regression recommended by ISO 6974; honours response *and* reference uncertainties in the fit.

Reproducible results

Calibration models are versioned and kept when archived. Every run keeps its model, method and k, so a past result can be re-inspected at any time.

A calibration model in NexChrom is not a black box that the analyst has to defend with a spreadsheet on the side. Curves, residuals and statistics sit next to the method and certificate that produced them, the chosen regression order is recorded per component, and every historical model is retained under an is_current flag. When an auditor asks how last quarter's certificate was produced, you can simply open the run that generated it and show the fit that was used at the time.

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Extended Reference Index

Physical quantities and the standards that govern them — the complete landscape NexChrom maps to.

Every physical quantity a gas-quality lab reports is pinned to a specific standard or technical report, and customers increasingly expect to see those references on the certificate. The index below lists the quantities NexChrom can derive today — directly or via an optional calculation module* — and the normative documents that govern each one. Use it as a quick check when matching a new customer requirement to what the application already covers.

*ISO 6974 and ISO 6976 quantities are built in. * Optional module — not in the standard version.*

Composition

Molar composition of natural gas
- ISO 6974, EN ISO 6974 (NEN / BS / DIN)

Mol fraction + uncertainty from GC analysis
- ISO 6974-1, ISO 6974-2, ISO 6974-3

N_2, CO_2, C1–C5, C6+ via GC
- ISO 6974-5, EN ISO 6974-5

He, H_2, O_2, N_2, CO_2, C1–C8 via GC
- ISO 6974-6

Calorific value & bulk properties

Gross calorific value (GCV / H_s)
- ISO 6976, EN ISO 6976, ASTM D3588

Net calorific value (NCV / H_i)
- ISO 6976, EN ISO 6976, ASTM D3588

Gross Wobbe index
- ISO 6976, EN ISO 6976 (BS / DIN)

Net Wobbe index
- ISO 6976, EN ISO 6976

Density at reference conditions
- ISO 6976, EN ISO 6976, ASTM D3588

Relative density / specific gravity
- ISO 6976, EN ISO 6976, ASTM D3588

Molar mass
- Derived from ISO 6974 composition; applied in ISO 6976 context

Compressibility & thermodynamics*

Compressibility factor Z — detailed method
- ISO 12213-2 / EN ISO 12213-2 (AGA 8-DC92)

Compressibility factor Z — simplified / SGERG
- ISO 12213-3 / EN ISO 12213-3 (SGERG-88)

Supercompressibility / gas deviation factor
- AGA Report No. 8, ISO 12213-1

Speed of sound
- ISO 20765-2 (GERG-2008), AGA Report No. 10

Enthalpy, entropy, isentropic exponent
- ISO 20765-2 (GERG-2008), AGA Report No. 10, AGA 8

Critical flow / sonic-nozzle coefficient C*
- AGA Report No. 10

Water & dew points*

Water content
- ISO 18453, EN ISO 18453, ASTM D1142, ASTM D5454

Water dew point
- ISO 18453, EN ISO 18453, ISO 6327

Hydrocarbon dew point
- ISO 23874, EN ISO 23874 (BS / DIN)

Sulphur & odorants

Hydrogen sulphide (H_2S)
- ISO 6326 series, ISO 19739, ASTM D5504

Total sulphur
- ISO 6326 series, ASTM D6667, ASTM D5504

Mercaptans / thiols / sulphides / THT
- ISO 19739, ISO 6326 series, ASTM D5504

Individual components

Oxygen
- ISO 6974, ASTM D1945

Hydrogen
- ISO 6974, ASTM D1945

Helium
- ISO 6974, ASTM D1945

C1–C5 hydrocarbons
- ISO 6974, ASTM D1945

C6+ fraction
- ISO 6974, ASTM D1945

Methane number*

Methane number / MN
- ISO 17507-1, ISO 17507-2, EN ISO 17507-1/-2, ISO/TR 22302, ASTM D8221

Gas quality & interchangeability

Gas quality specification
- ISO 13686, EN ISO 13686, EN 16726

H-group / European gas quality
- EN 16726 (DIN / BS)

Interchangeability
- EN 16726, ISO 13686, Wobbe via ISO 6976

Condensation behaviour / phase envelope*
- ISO 23874, ISO 20765-3 (GERG-2008), AGA 8 context

Hydrogen admixture / H_2 in natural gas
- ISO 6974, EN 16726, ISO 17507-1/-2 (methane number for H_2 blends)

Supporting technical reports

ISO/TR 29922
- Supporting information on the ISO 6976 calculations

ISO/TR 24094
- Validation methods for gaseous reference materials

Together these references form the map that keeps NexChrom results defensible in audits, certifications and customer acceptance. When a new norm is published or an existing one is revised, NexChrom's calculation modules are updated so that your lab stays aligned — without changing the way the analyst works day-to-day. Ask us for an up-to-date traceability statement whenever you need one for a tender or a quality review.