

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.



Built-in AI Assistant

Troubleshoot with AI
that knows your
instruments.



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.

3 Calibration

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

5 Review & Approve

Inspect calculation results, approve or reject runs. Historical models preserved for re-calculation at any time.

2 Method Configuration

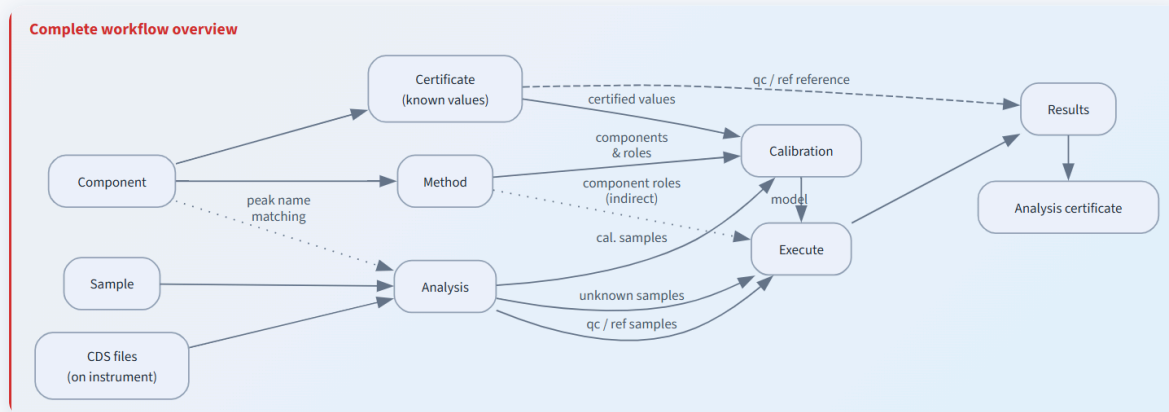
Define analytical methods with component roles: direct (calibrated), indirect (via RRF), or fixed (certified value).

4 Execute & Calculate

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

6 Certificates

Generate analysis certificates. Import external reference certificates from PDF (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 is reproducible 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 is built in. Physical-property calculation is available through optional modules* covering the full family of standards laboratories rely on.

PURPOSE	STANDARD FAMILY
Composition measurement	ISO / EN / DIN / BS 6974
Heating value, Wobbe index, density	ISO / EN / DIN / BS 6976
Compressibility factor Z	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, CO₂ emission factor and hydrogen-admixture coverage. * Planned — not yet implemented in the current 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 — no training required
- ✓ AI assistant answers questions on the fly
- ✓ 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 re-runs
- ✓ ISO 6974 built-in; ISO 6976 / 12213 / AGA 8 / 10 as modules*
- ✓ PDF certificate import with OCR for external references
- ✓ Role-based user management and alert notifications

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: one-time licence + optional modules

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 — just a predictable one-time licence supplemented with optional physical-property modules when your customers ask for them.

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, retraining the lab or renegotiating the licence. 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.



AI Assistant

Gemini, Claude or
OpenRouter.



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.

④ CDS file contents

☐ Highlight duplicate component names

In...	ISO-code	component_n...	CDS na...	Detector	AVG_PEAK	STD (RSD%)	MIN_PEAK	MAX_PEAK	Rep	Unit
☒	1	methane	Methane	TCD2 B, Back...	56690.5	33.42 (0.1%)	56658.9 (-1.0a/-0.1%)	56725.5 (+1.0a/+0.1%)	3	µV Sec
☒	2	ethane	Ethane	TCD2 B, Back...	3907.1	0.65 (0.0%)	3906.4 (-1.1a/-0.0%)	3907.7 (+0.9a/+0.0%)	3	µV Sec
☒	3	propane	Propane	FID1 A, Front SI...	120203.8	287.86 (0.2%)	119911.5 (-1.0a/-0.2%)	120487.0 (+1.0a/+0.2%)	3	µV Sec
☒	4	n-butane	n-Butane	FID1 A, Front SI...	29142.5	233.04 (0.8%)	28873.7 (-1.2a/-0.9%)	29287.2 (+0.6a/+0.5%)	3	µV Sec
☒	5	2-methylpropane	2-Methylpr...	FID1 A, Front SI...	24486.1	137.92 (0.6%)	24328.5 (-1.1a/-0.6%)	24584.6 (+0.7a/+0.4%)	3	µV Sec
☒	6	n-pentane	n-Pentane	FID1 A, Front SI...	10043.1	274.92 (2.7%)	9726.4 (-1.2a/-3.2%)	10220.3 (+0.6a/+1.8%)	3	µV Sec
☒	7	2-methylbutane	2-Methylbu...	FID1 A, Front SI...	9801.6	203.21 (2.1%)	9567.1 (-1.2a/-2.4%)	9925.1 (+0.6a/+1.3%)	3	µV Sec

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.

② Component roles

Method Name:
NGA_default_ISO6974

Description:
Default ISO6974 analyse

Select	ISO_code	component_id	role	created_at	is_current
☐	1	methane	direct	2026-03-10 17:40:05	☒
☐	2	ethane	direct	2026-03-12 07:23:32	☒
☐	3	propane	direct	2026-03-12 07:25:02	☒
☐	4	n-butane	direct	2026-03-12 07:26:10	☒
☐	5	2-methylpropane	direct	2026-03-12 07:25:27	☒
☐	6	n-pentane	indirect	2026-03-12 08:31:44	☒
☐	7	2-methylbutane	indirect	2026-03-12 08:31:44	☒

Pending: +0 / -0 / -0

Component roles: direct / indirect / fixed

③ RRF rules

Select	indirect_componen...	reference_componen...	rrf_mode	rrf_value	uncertainty	notes	created_at	is_current
☐	n-pentane	propane	calculated	1.67	0.17		2026-03-10 17:12:02	☒
☐	2-methylbutane	propane	calculated	1.67	0.17		2026-03-10 17:12:02	☒
☐	2,2-dimethylpropane	propane	calculated	1.67	0.17		2026-03-24 14:59:41	☒
☐	n-hexane	propane	calculated	2.00	0.20		2026-03-10 17:12:02	☒
☐	n-heptane	propane	calculated	2.33	0.23		2026-03-12 09:10:31	☒
☐	n-octane	propane	calculated	2.67	0.27		2026-03-12 09:10:50	☒
☐	n-nonane	propane	calculated	3.00	0.30		2026-03-12 09:49:36	☒

Pending: +0 / -0 / -0

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 fifth 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.

④ Calibration input data

Calibration model:

TESTCAL

Instrument:

TEST_GC

Method:

NGA_default_ISO6974

Cal. samples:

7

Filter on component

methane

Filter on sample

All

↑ ↓	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 against the configurable GOF threshold; 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.

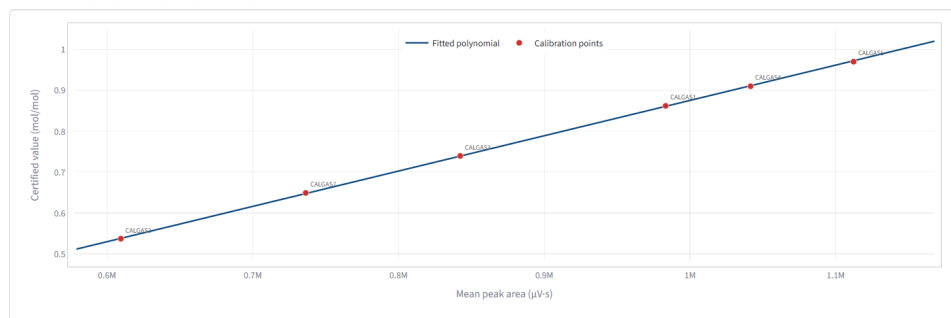
Full statistics

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

Interactive plots

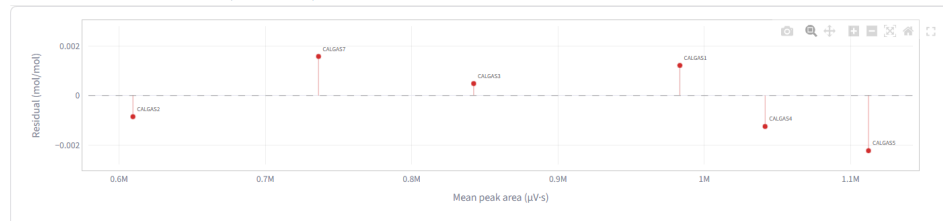
Hover on any point for peak area, certified value and each point's error contribution. Clear visual confirmation of the fit.

Calibration curve: methane



Calibration curve with hover tooltip

Residual: concentration (mol/mol)



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 re-runs

Calibration models are versioned with an is_current flag. Historical models remain available to reproduce past results 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.

* Optional calculation modules are planned — not yet implemented in the current 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

N₂, CO₂, C1–C5, C6+ via GC

- ISO 6974-5, EN ISO 6974-5

He, H₂, O₂, N₂, CO₂, C1–C8 via GC

- ISO 6974-6

Calorific value & bulk properties

Gross calorific value (GCV / H_g)

- ISO 6976, EN ISO 6976, ASTM D3588

Net calorific value (NCV / H_n)

- 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 (H₂S)

- 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 / H₂ in natural gas

- ISO 6974, EN 16726, ISO 17507-1/-2 (methane number for H₂ blends)

Supporting technical reports

ISO/TR 29922

- Supplementary guidance on the use of reference gas mixtures for calibration

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.

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