

NMR SOFTWARE

Advanced Chemical Profiling 2.0

Bruker's Next-Generation Solution for Quantitative
NMR Workflow Automation

Innovation with Integrity

Advanced Chemical Profiling 2.0: One Software Platform for Quantitative NMR Workflows at any Field Strength

Advanced Chemical Profiling (ACP) 2.0 software empowers laboratories to harmonize analytical methods across research, development, manufacturing and quality control with a fully automated, end-to-end NMR workflow. This harmonization results in increased throughput, enhanced efficiency, and reduced cost through standardized, GMP-ready, operator-independent analysis from sample to report.

Automated End-to-End Workflow

Delivers fully automated NMR analysis from sample to report, ensuring consistent, expert level results across any lab.

Standardized Decision Making

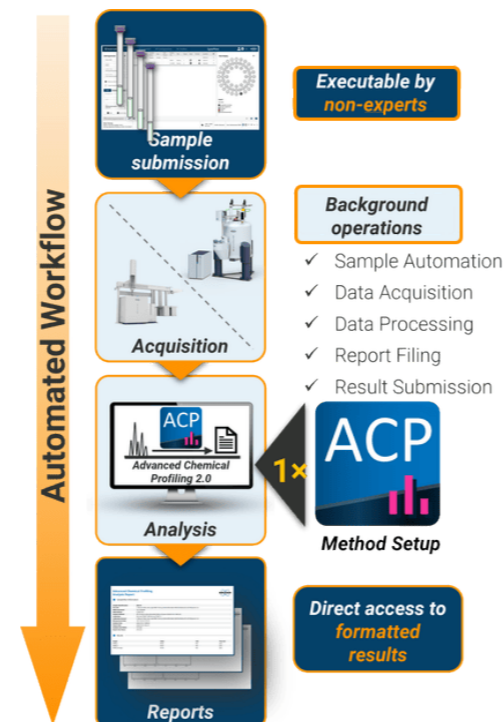
Embeds reliable pass/fail logic into workflows, eliminating subjective interpretation and ensuring harmonized global decision making.

High Throughput Analysis

Accelerates complex workflows with on the fly or batch processing, boosting productivity and reducing time to decision.

Precision Through High-Performance Algorithms

Applies advanced fitting and deconvolution methods to deliver accurate, reliable quantification across even the most complex spectra.



ACP 2.0 addresses the tasks of data processing, interpretation, and report filing for any quantitative NMR workflow. This enables the streamlined analysis of incoming goods, process intermediates, and final product formulations to improve both quality and efficiency in R&D lab-scale, pilot, and volume production processes. Once setup, analyses can be executed at the push-of-a-button, even in NMR novice environments.

Hands-Off Workflow Automation for Anything from Simple Tasks to the Most Complex Analyses

ACP 1.0 successfully redefined automated qNMR workflows with a database-driven identification & quantification algorithm; it enabled sample-to-report capabilities for the analysis of neat compounds or simple mixture. ACP 2.0 takes a bold leap forward. ACP 2.0 enables the **automation of any qNMR workflow**, from simple tasks such as routine purity determinations or relative quantifications, to deciphering complex and overlapping signals in multicomponent mixtures. ACP 2.0 can even be applied in the presence of strong background signals leveraging new, ground-breaking fitting capabilities.

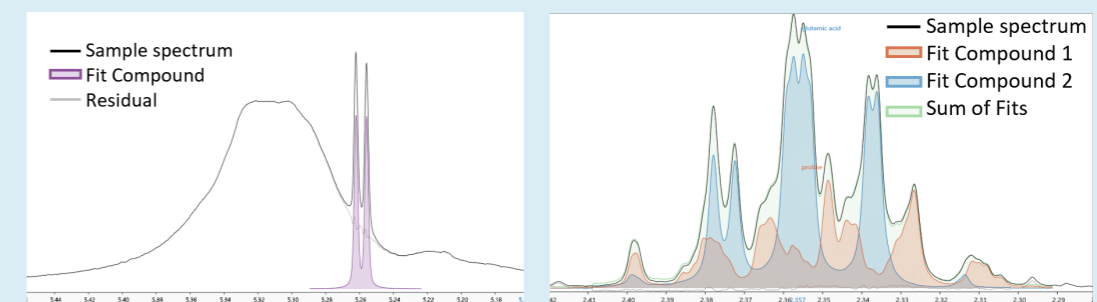


Figure 1: Fit in the presence of background signals

Figure 2: Fit strongly overlapping signals

Different algorithms are now available to suit each case and challenge to ensure robust and accurate quantification:

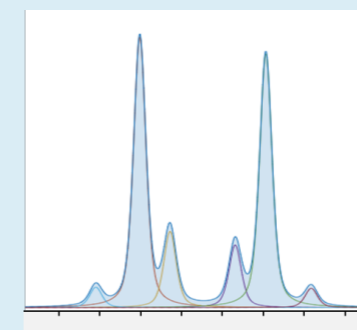


Figure 3: Peak Fitting

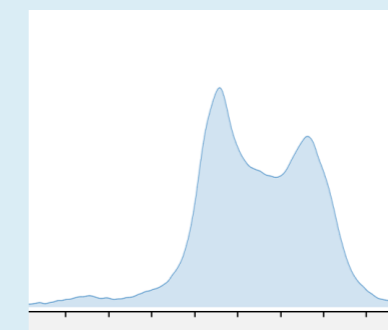


Figure 4: Shape Fitting

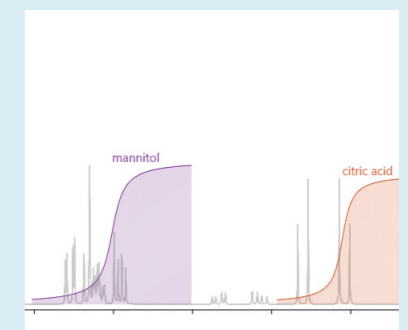


Figure 5: Region Integration

Clear, Actionable Results at Scale

Results can be expressed and formatted exactly as required using the new powerful custom equation setup, avoiding any additional data processing steps. Results can be viewed directly in ACP 2.0, exported to an Excel file or printed into a highly customizable report. As ACP 2.0 also features a custom-set pass/fail decision option, you can even print out the test result in an easily comprehensible way without having to interpret the detailed data printed in the report.

Each method can be set up with few clicks and can be shared between sites to achieve a harmonized analyses throughout your organization.

Once set up, the method can be either applied to hundreds of spectra in one go, or for routine and on-the-fly analysis: directly link the method to the acquisition parameters for fully automated analysis execution after data acquisition. It enables robust deployment of sophisticated NMR-based analysis in NMR novice environments such as manufacturing and QC labs, including into regulated environment thanks to built-in GMP compliance support.

Advanced Chemical Profiling Analysis Report
Product: Acrylic Acid
Sample/Run Information

Sample Identification	Data
File Path	C:\temp\80 MHz - Relative Quantification - Acrylic Acid QC\Data18\pdata111r
NMR Instrument	F80-HD-13C
NMR Method	PROC13DEC_64
Analysis Method	80 MHz - Relative Quantification - Acrylic Acid QC (2025-11-28 11:32:11)
Measurement Date	2025-06-05 15:28:16
Analysis Date	2025-11-28 11:33:52
Report Date	2025-11-28 11:34:17

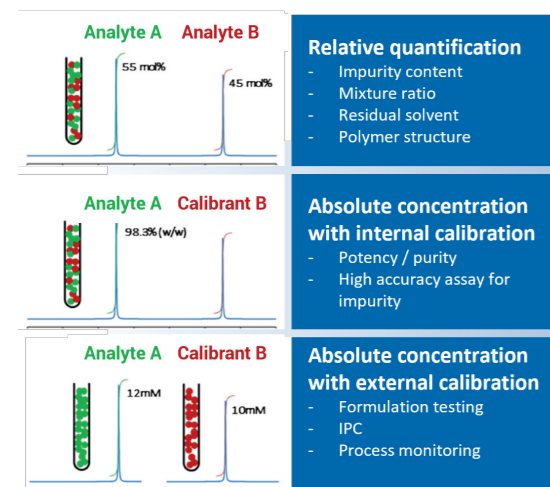
Results

Check Spectral Quality first! Results only valid if all spectral quality tests pass.

Target	Value	Result	QC criteria
Acrylic Acid	97.9 wt%	pass	> 97.50 wt%
Dimer	2.1 wt%	pass	< 2.50 wt%
MEHQ (inhibitor)	182 ppm	pass	150 ppm > x < 250 ppm

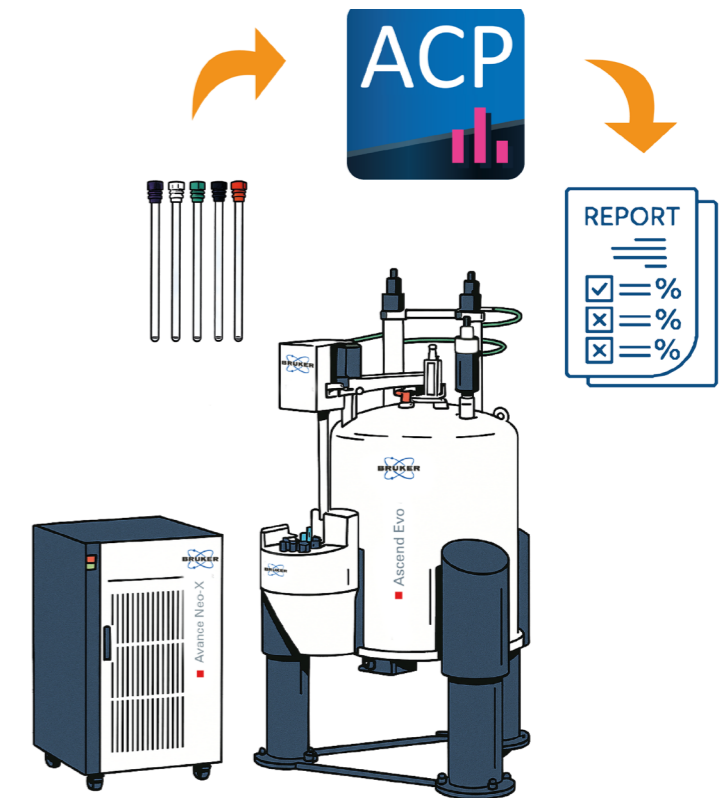
Spectral Quality Parameter	Value	Result	Criteria
FWHM Check	1.69 Hz	pass	Pass ≤ 2 Hz
Shim/Phase check	0.127	pass	Pass ≤ 0.2

Page 1 of 6



Get the Most Out of Your Instrument, Data and Time

- Automation for any quantitative NMR workflow from simple purity determination to analyzing highly complex mixtures
- No need to perform repetitive tasks: Ensure you can **focus on valuable tasks only**
- Multiple fitting options:** Signal deconvolution and peak fitting, shape fitting (e.g. polymers or low fields)
- Setup **multi-region-integration workflows in minutes with few clicks**
- Include **custom calculations** based on spectroscopic data including print-out on the report for **quick decision making**
- Machine readable output** can be directly fed into LIMS system
- No mixture spectra too complex** to analyze with the elaborate algorithms of ACP 2.0
- TopSpin only needed for sample-to-report automation; re-processing of existing data through ACP 2.0 possible as **standalone software**



Your Benefits

Automation & Accessibility

ACP 2.0 delivers fully automated, end-to-end NMR workflows that eliminate manual intervention, enabling consistent, high-quality analysis even in non-expert environments.

High Throughput & Efficiency

ACP 2.0 accelerates analytical workflows through on-the-fly analysis or batch processing as well as streamlined data handling, significantly increasing throughput and freeing up expert time.

Standardization & Decision Support

ACP 2.0 empowers standardized, data-driven decision-making by automating pass/fail assessments for critical control points in chemical production.

Knowledge Sharing & Harmonization

ACP 2.0 facilitates seamless sharing of analytical methods across teams and sites, driving harmonization and collaboration in global organizations.

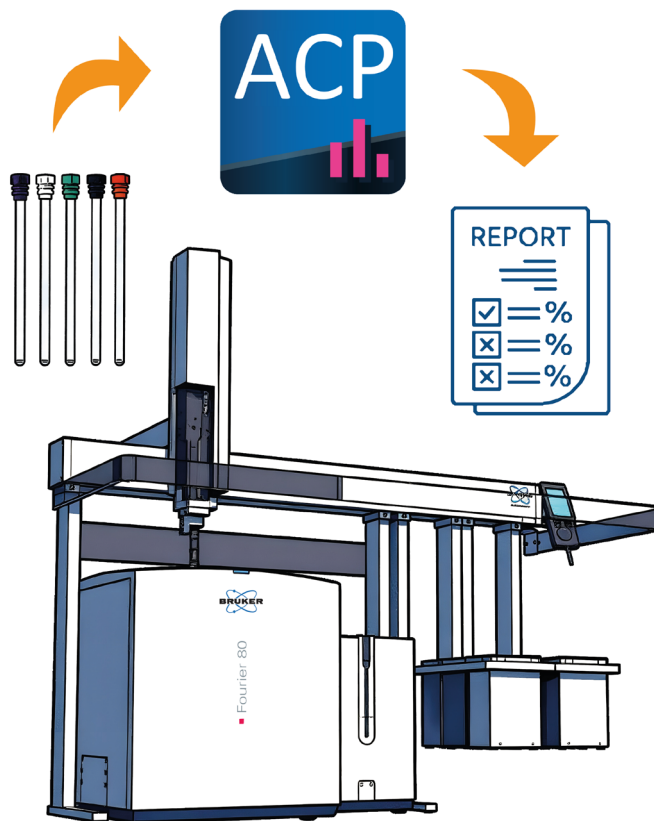
Usability & User Experience

ACP 2.0 combines powerful analytical capabilities with an intuitive interface, enabling users to set up sophisticated NMR workflows with just a few clicks.

- Unified solution for all qNMR workflows
- User-friendly interface for method setup - no script, no external files
- User-selectable algorithms for each target to adapt to each product and matrix, including complex baseline and overlapped signals
- Highly customizable, with direct pass/fail decision capabilities, tailored calculation methods, and flexible reporting options

Harmonization Through Automation

- **Share methods** between laboratories and sites globally
- **Deploy sophisticated NMR analysis**, developed with ACP 2.0, as push-button solutions in volume manufacturing or quality control environments
- Receive **fully customized report with pass / fail decision print-out**, that is easy to read and does not require knowledge of NMR spectra interpretation
- Use inherently quantitative NMR spectroscopy with automated data analysis and reporting for **operator- and site-independent global harmonization of analysis** with high result consistency and comparability with **auditable workflows**
- Accelerate time-to-money: New product innovation often relies on NMR spectroscopy. Why look for alternatives when it comes to scale-up and plant introduction when you can stay with NMR enabled by **ACP 2.0's sample-to-report push-button operation**
- Stay in control: Real-time access to NMR data and results with optional **LIMS integration**



Download now
and try the
new software
for free!



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Customer Support
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