

Making NMR Routine: Automated qNMR Workflows for Modern Dietary Supplements

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Why qNMR can be a powerful tool

Accuracy

Absolute quantification, high linearity, direct traceability to reference standards

Reproducibility

Highly reproducible technique, consistent physical measurement inter-laboratory

Rich Information

Rich chemical information and simultaneous analysis of multiple compounds

Robustness

Robust analytical platform, non-destructive with minimal sample preparation

Scalability

Scalable for high throughput, fast acquisition and suitable for routine testing



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Real practical challenges

~~Accuracy~~

Operator-dependent processing, manual peak integration, baseline correction.

~~Reproducibility~~

SOP adherence and local workflows may vary, leading to different results

~~Rich Information~~

Spectral complexity, peak overlaps, large number of different analytes / samples

~~Robustness~~

Managing method versions and maintaining method consistency over time

~~Scalability~~

Multi-site deployment is challenging, reporting burden for high-throughput testing



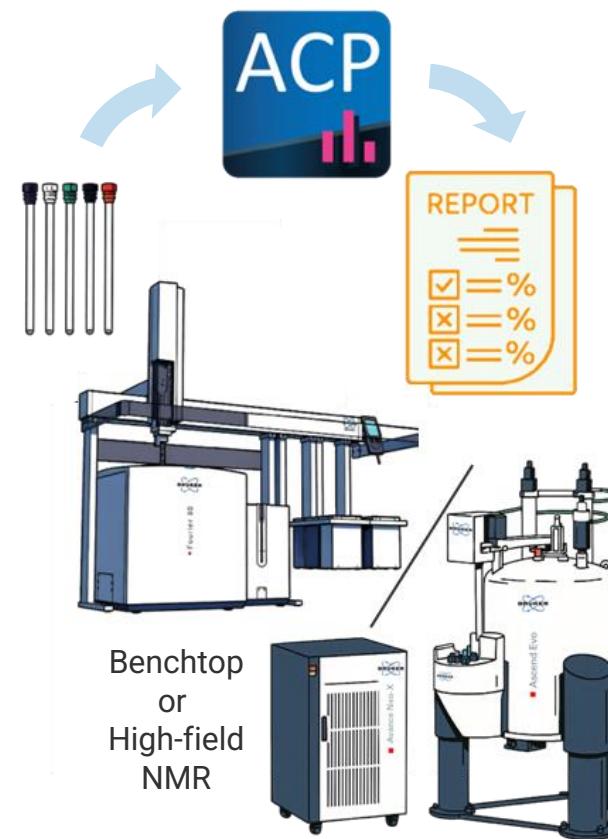
Advanced Chemical Profiling 2.0



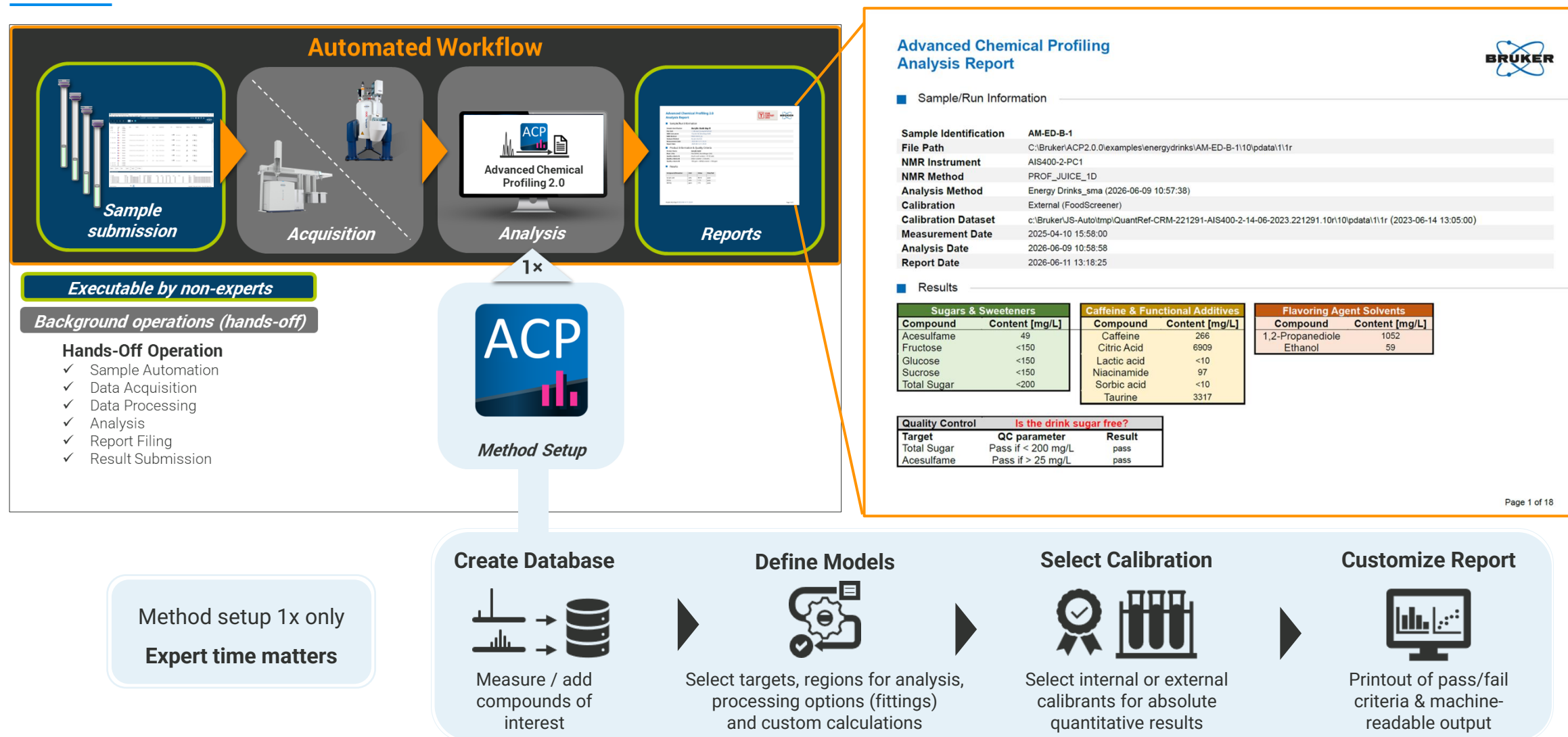
Automated qNMR Workflows

- Creation of databases and standardized quantification methods
- Advanced algorithms for automated analysis of complex and overlapping signals in multicomponent mixtures
- Batch processing and method sharing capabilities
- Customizable PDF reports with optional printout of user-defined pass/fail decision criteria
- Traceability and digital workflow integration via machine-readable output (LIMS)

From Sample to Report

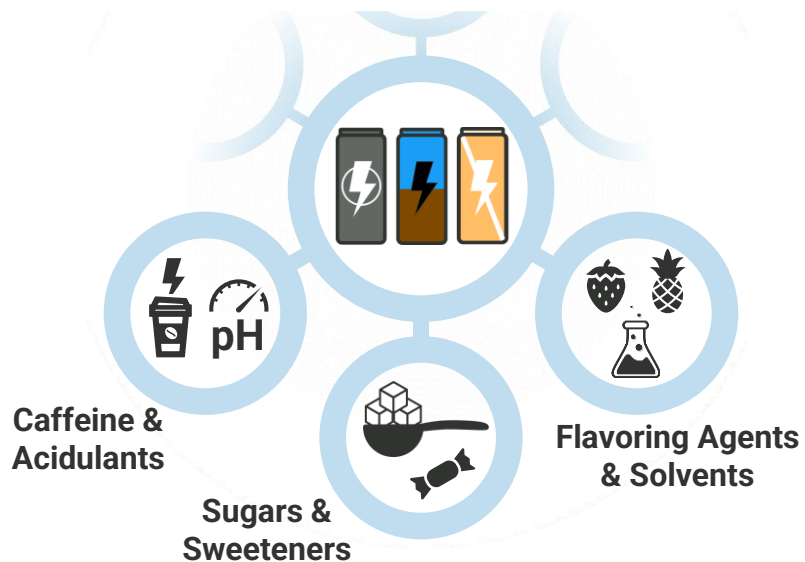


Advanced Chemical Profiling 2.0 – Setup Workflow



Advanced Chemical Profiling 2.0

Quality Control of Energy Drinks

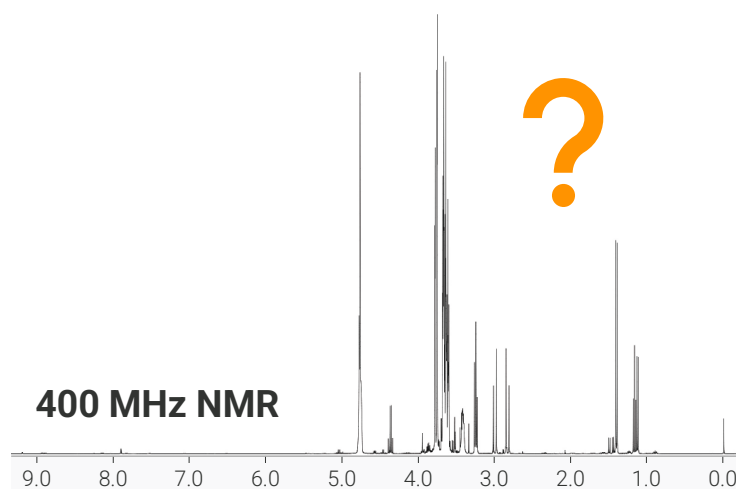


Background:

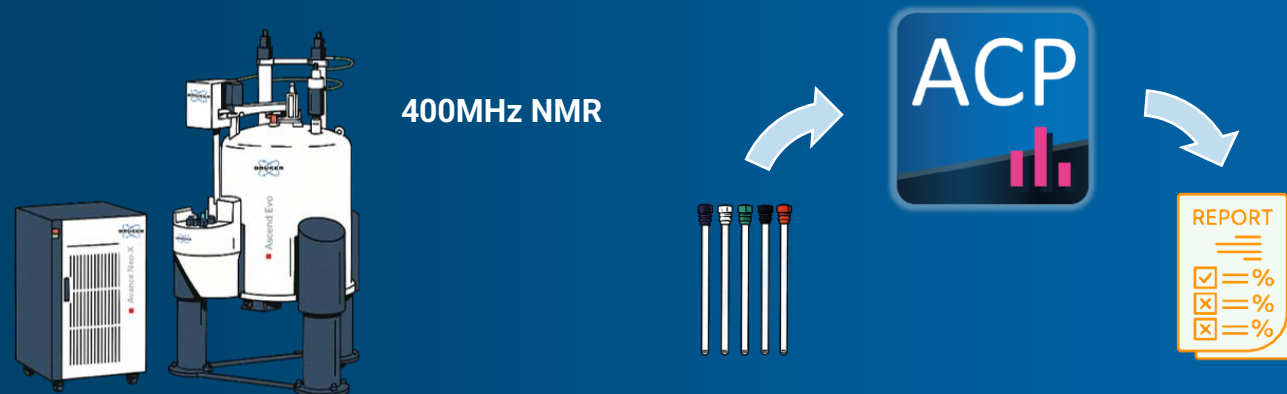
- Energy drinks are compositionally complex beverages
- Sugars, amino acids, vitamins, stimulants like caffeine, a variety of acidulants, flavor compounds, functional additives, among others.

Problem:

- Wide chemical diversity creates significant analytical challenges during formulation, quality control, and batch to batch consistency evaluation



Solution: NMR + Advanced Chemical Profiling 2.0



Advanced Chemical Profiling 2.0

Quality Control of Energy Drinks

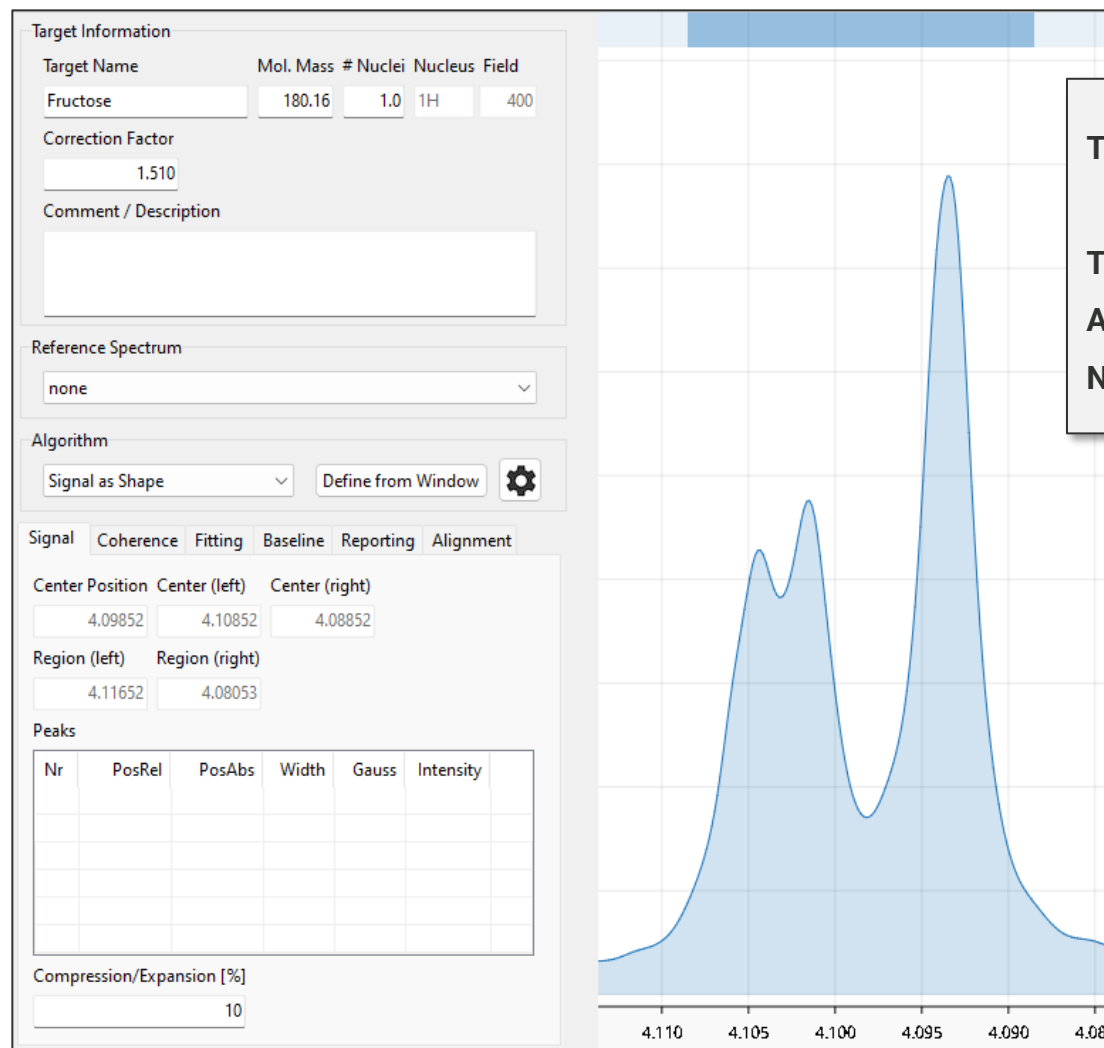
Setup:

1. Choose compounds (create database):

- Measure pure compounds of interest

2. Customize the method:

- Choose fitting algorithms** from peak fitting, shape fitting or simple region integration
- Apply baseline fitting** if necessary
- Define Pass/Fail criteria** and reporting details
- Use custom calculation tool to analyze derivative values** (e.g., automatically check the limits of glucose and sucrose against the defined limit in sugar-free drinks)



Target setup example:

Target: Fructose

Algorithm: Signal as Shape

Note: complex signal pattern

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Quality Control of Energy Drinks

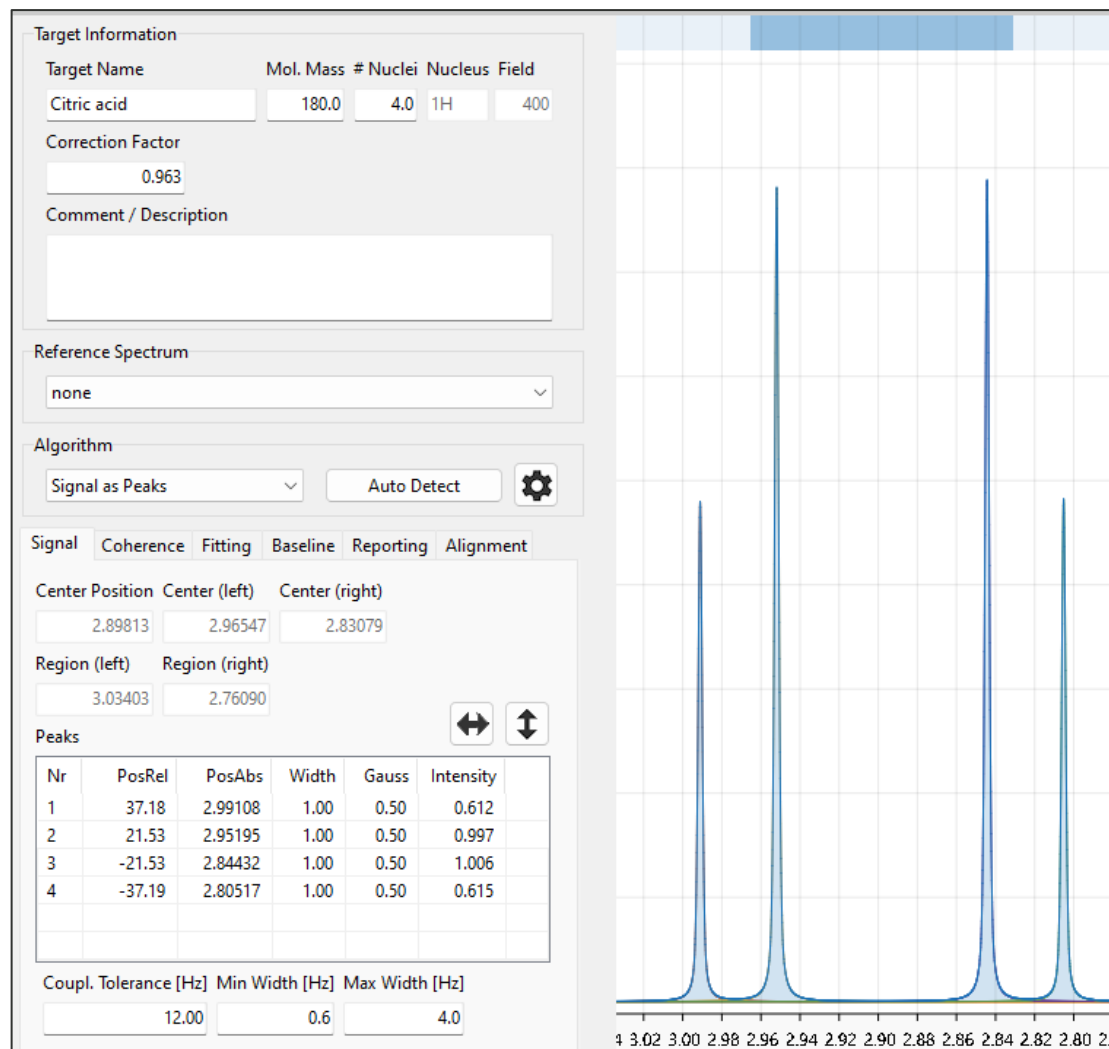
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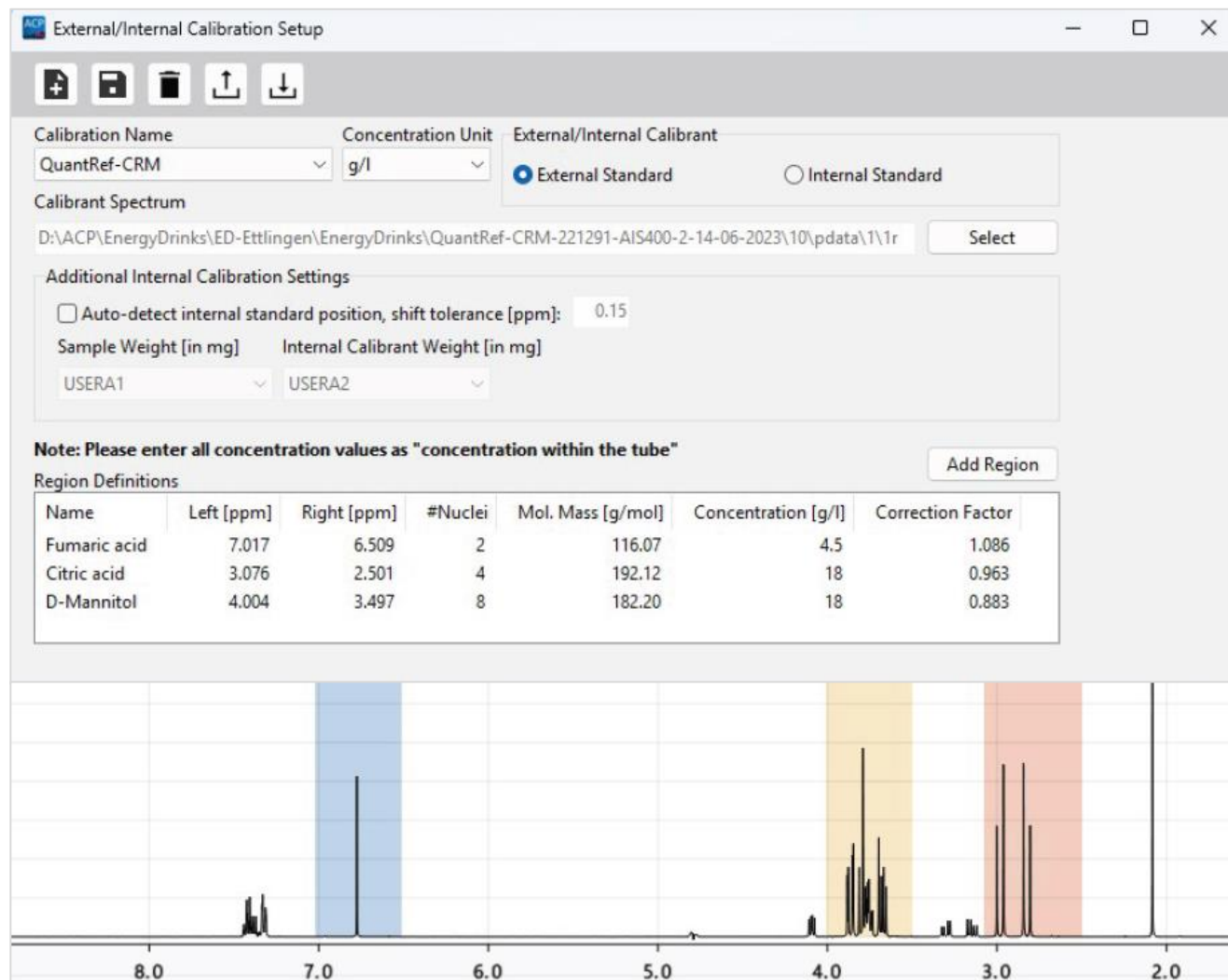
Target: Citric Acid

Algorithm: Signal as Peaks

Note: simple splitting pattern. Each peak of the multiplet gets defined and tabulated individually.

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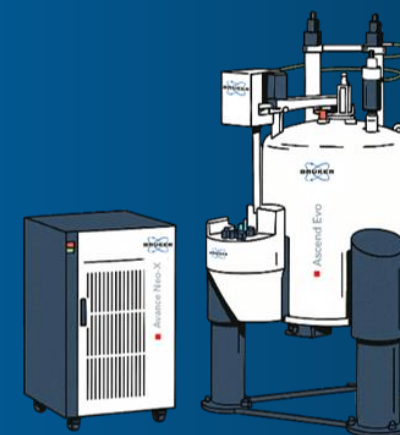
Quality Control of Energy Drinks



Sample Prep:

- Commercially available energy drinks in the EU.
- 900 μ L of degassed sample mixed with 100 μ L of phosphate buffer (pH 3.1)
- QuantRef-CRM **external calibrant** (fumaric acid, citric acid, and D-mannitol)

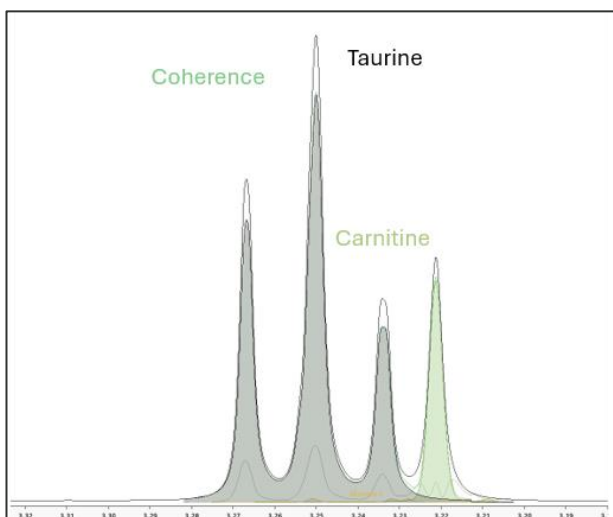
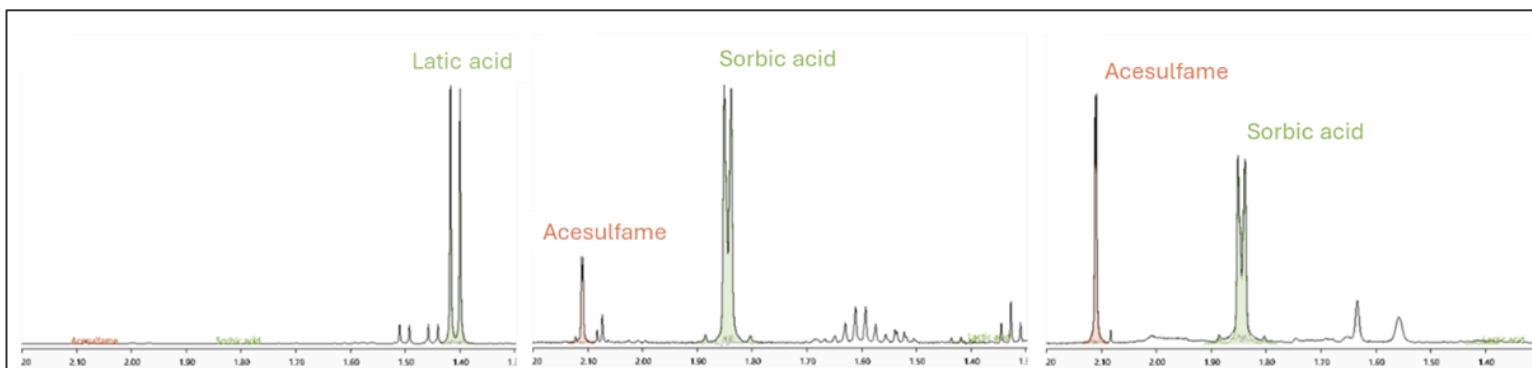
Instrument: 400MHz NMR



Advanced Chemical Profiling 2.0

Quality Control of Energy Drinks

- Results:** target compounds (12 in total) are automatically identified and quantified



Samples / Compounds	Caffeine (mg/L)	Taurine (mg/L)	Sorbic Acid (mg/L)	Citric Acid (mg/L)
Brand 1, Variety A	266	3317	n/a	6909
Brand 2, Variety A	280	3993	n/a	7727
Brand 2, Variety B	272	3876	n/a	2524
Brand 3, Variety A	244	3646	217	6579
Brand 3, Variety B	248	3475	226	6581

Sample Prep:

- Commercially available energy drinks in the EU.
- 900 μ L of degassed sample mixed with 100 μ L of phosphate buffer (pH 3.1)
- QuantRef-CRM external calibrant (fumaric acid, citric acid, and D-mannitol)

Instrument: 400MHz NMR

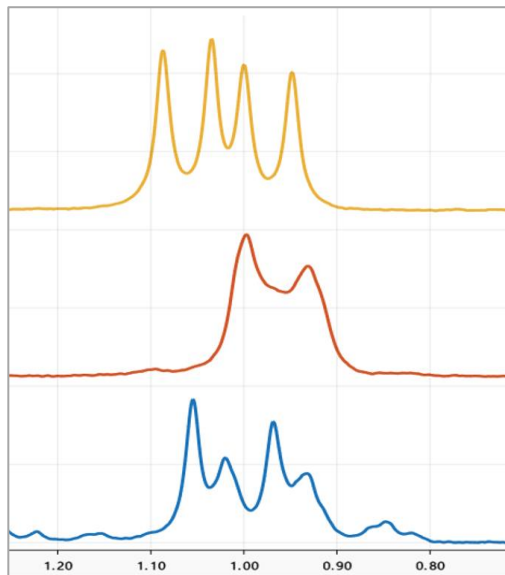
Full App Note



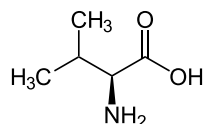
Advanced Chemical Profiling 2.0

Analysis of Branched-Chain Amino Acids

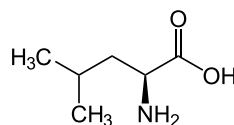
80 MHz Benchtop NMR



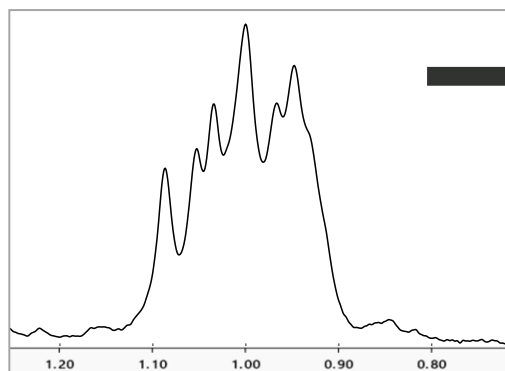
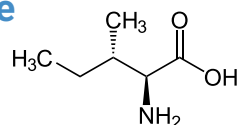
L-Valine



L-Leucine



L-Isoleucine



BCAA Sample

?? w% L-Valine

?? w% L-Leucine

?? w% L-Isoleucine

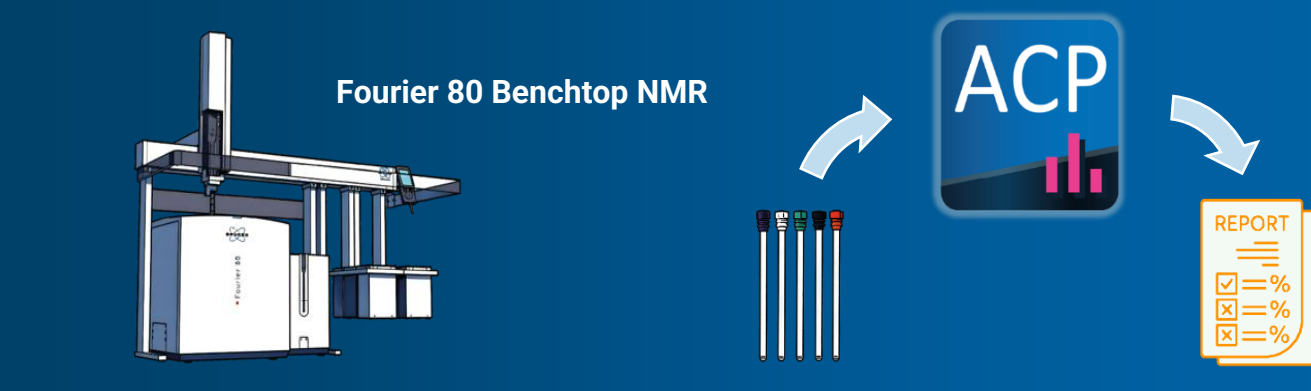
Background:

- Branched-Chain Amino Acid (BCAA) products represent one of the fastest growing segments in sports nutrition and wellness driven by rising interest in muscle recovery, healthy aging, and functional supplementation.

Problem:

- Formulation and product release require precise analysis of the product's composition and amino acid ratios. How to achieve an accurate and reproducible analytical workflow for global deployment?

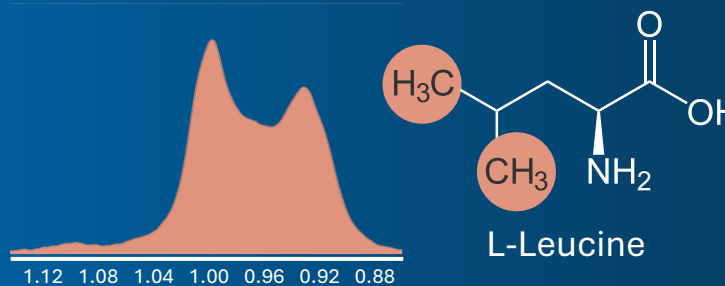
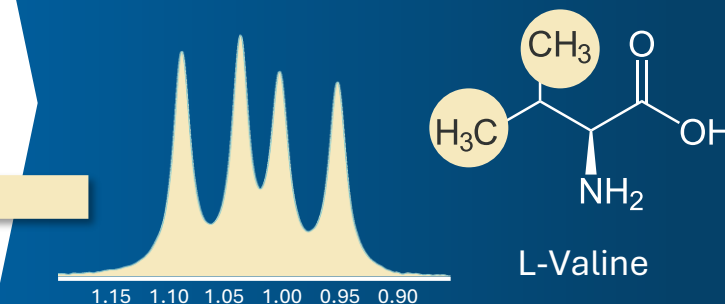
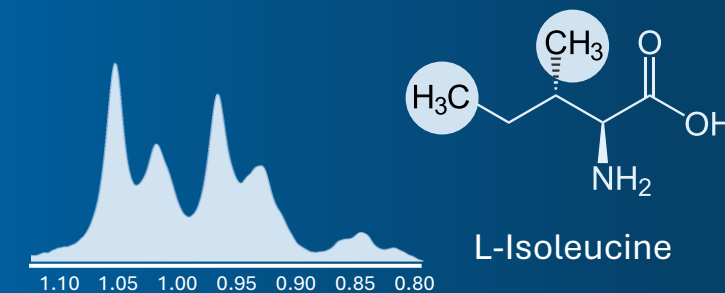
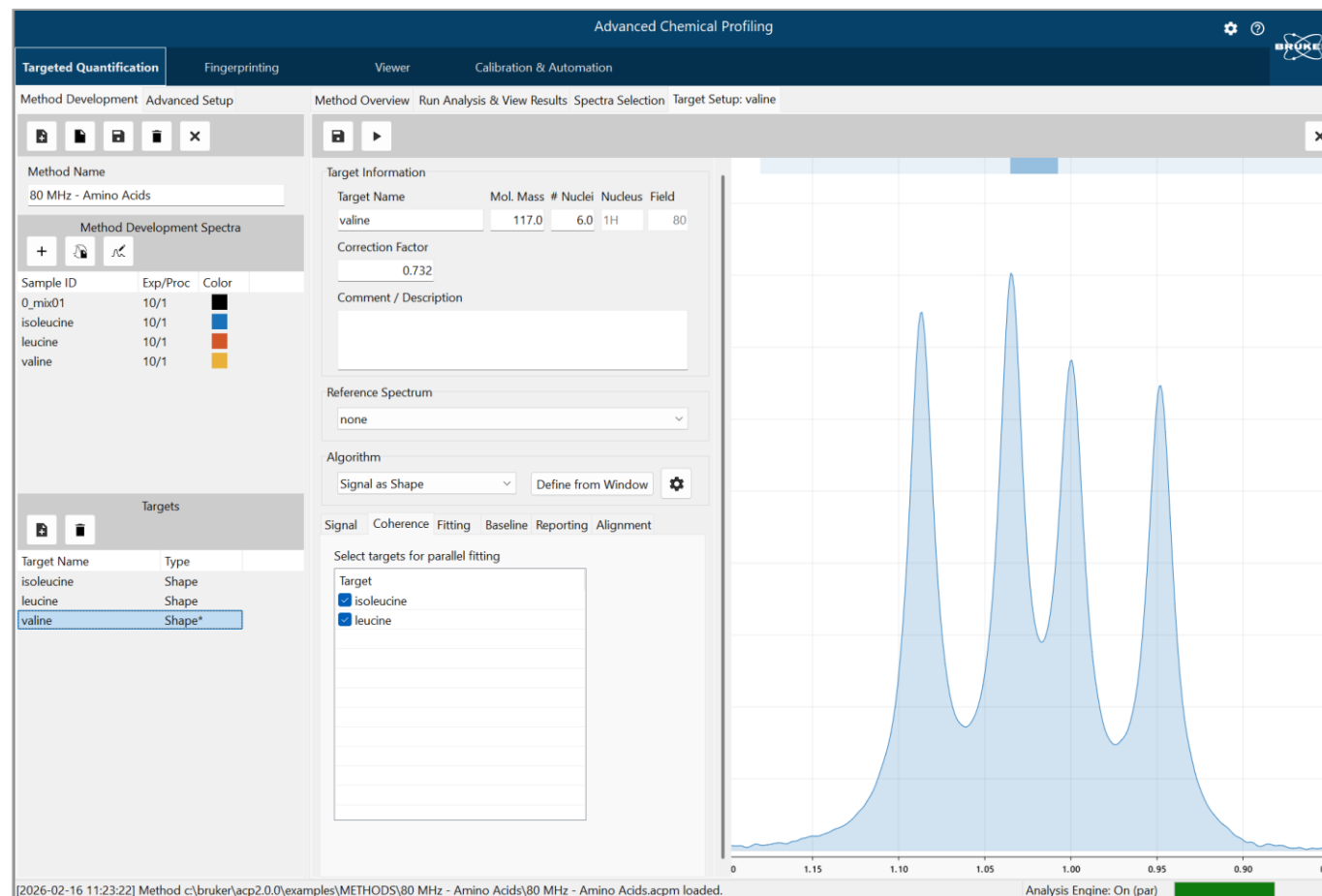
Solution: NMR + Advanced Chemical Profiling 2.0



Advanced Chemical Profiling 2.0

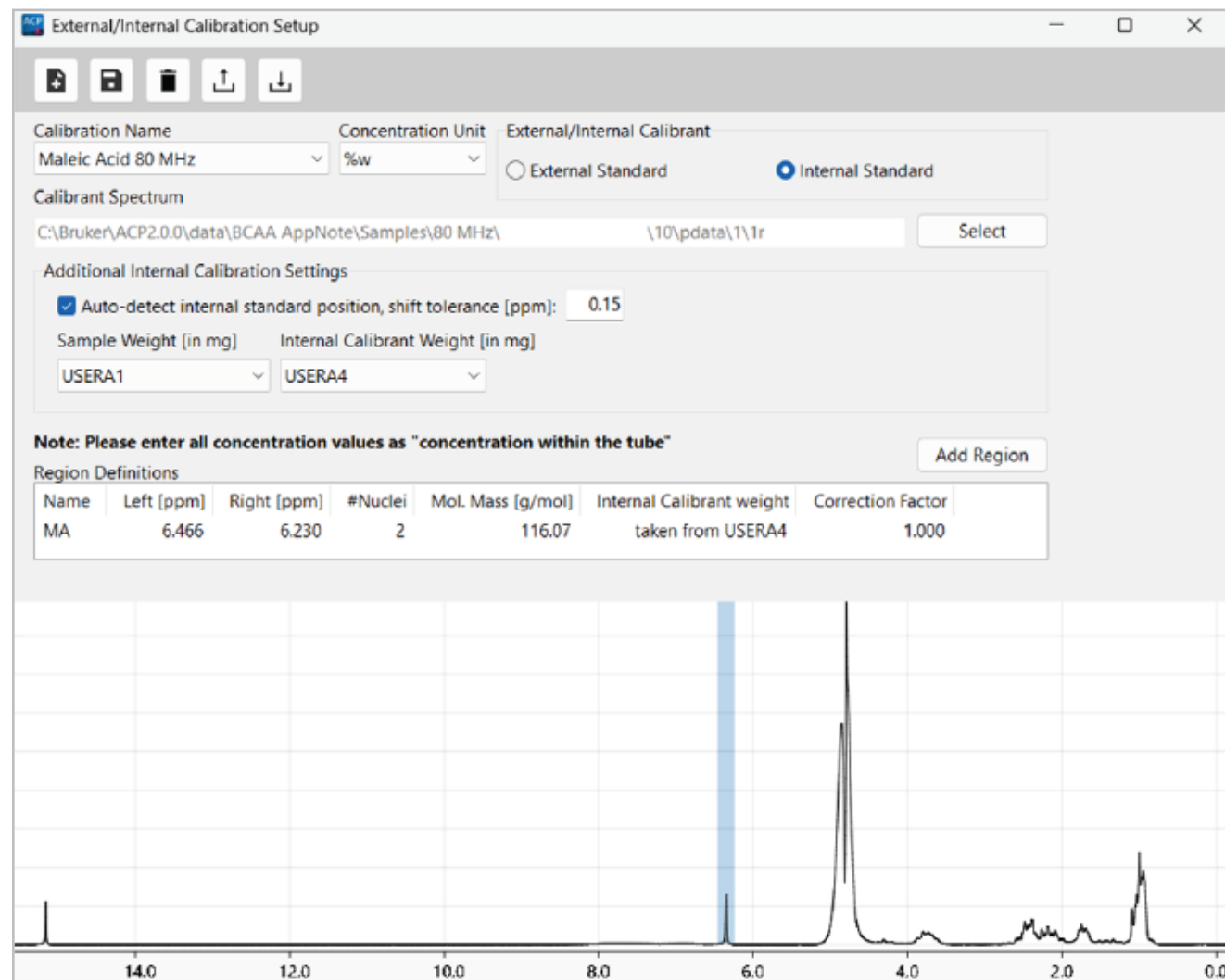
Analysis of Branched-Chain Amino Acids

- **Defining targets:** fitting algorithm set as “signal as shape” for all 3 compounds



Advanced Chemical Profiling 2.0

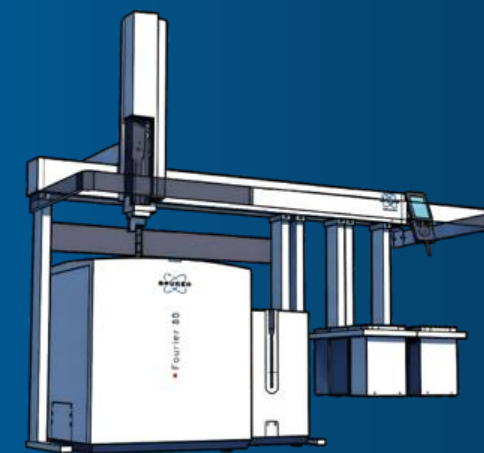
Analysis of Branched-Chain Amino Acids



Sample Prep:

- 1425 mg of BCCA sample + 160 mg of maleic acid (**internal calibrant**) were dissolved in 200 ml of tap water

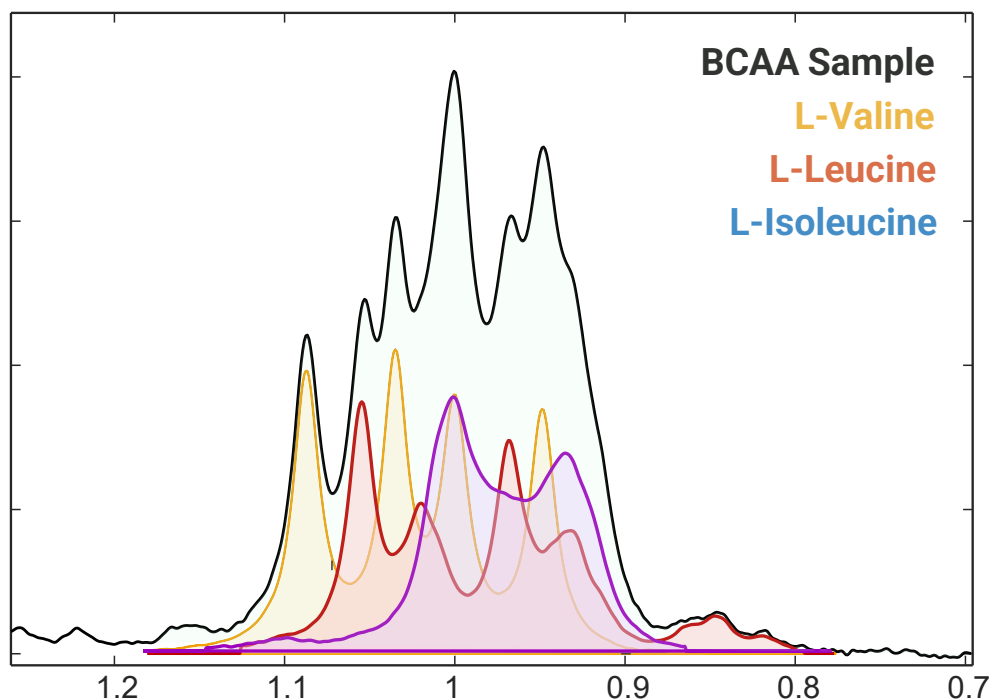
Instrument: Fourier 80 Benchtop NMR



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Analysis of Branched-Chain Amino Acids

- Results:** automated fit of the BCAA sample spectrum and calculation of the individual concentration of the 3 respective targets.



Target	Valine [%w]	Leucine [%w]	Isoleucine [%w]
Result	10.4	20.7	10.5

Sample Prep:

- 1425 mg of BCCA sample + 160 mg of maleic acid (internal calibrant) were dissolved in 200 ml of tap water

Instrument: Fourier 80 Benchtop NMR

Full App Note



Target Information

Target Name	Mol. Mass	# Nuclei	Nucleus	Field
LEU/ILE-ratio	1	1	1H	80

Correction Factor
1.000

Comment / Description

Reference Spectrum

none

Algorithm

Formula Auto Detect

Formula

Reporting

Formula

```
result = [leucine.wtp] / [isoleucine.wtp]
```

Unit

a.u.




Target Information

Target Name	Mol. Mass	# Nuclei	Nucleus	Field
LEU/ILE-ratio	1	1	1H	80

Correction Factor
1.000

Comment / Description

Reference Spectrum

none

Algorithm

Formula Auto Detect 

Formula

Reporting

Pass-Fail Options

Unit

☒ Fail, result lower (<) than
 ☒ Fail, result higher (>) than

1.9 2.1

Reporting Options

☒ Show in Report

Unit Digits LOQ

1 0

- ## Advanced Chemical Profiling Analysis Report



■ Sample/Run Information

Sample Identification	BCAA sample – Batch A9F8ADK
File Path	[File path to spectrum]
NMR Instrument	AIF80-4
NMR Method	PROF_PLASMA_NOESY_f
Analysis Method	BCAA_AppNote_80MHz (2026-02-16 14:41:20)
Calibration	Internal (Maleic Acid 80 MHz)
Calibration Dataset	[File path to calibration dataset] (2025-12-01 12:46:20)
Measurement Date	2025-12-01 14:09:46
Analysis Date	2026-02-16 14:42:01
Report Date	2026-02-16 14:42:09

■ Results

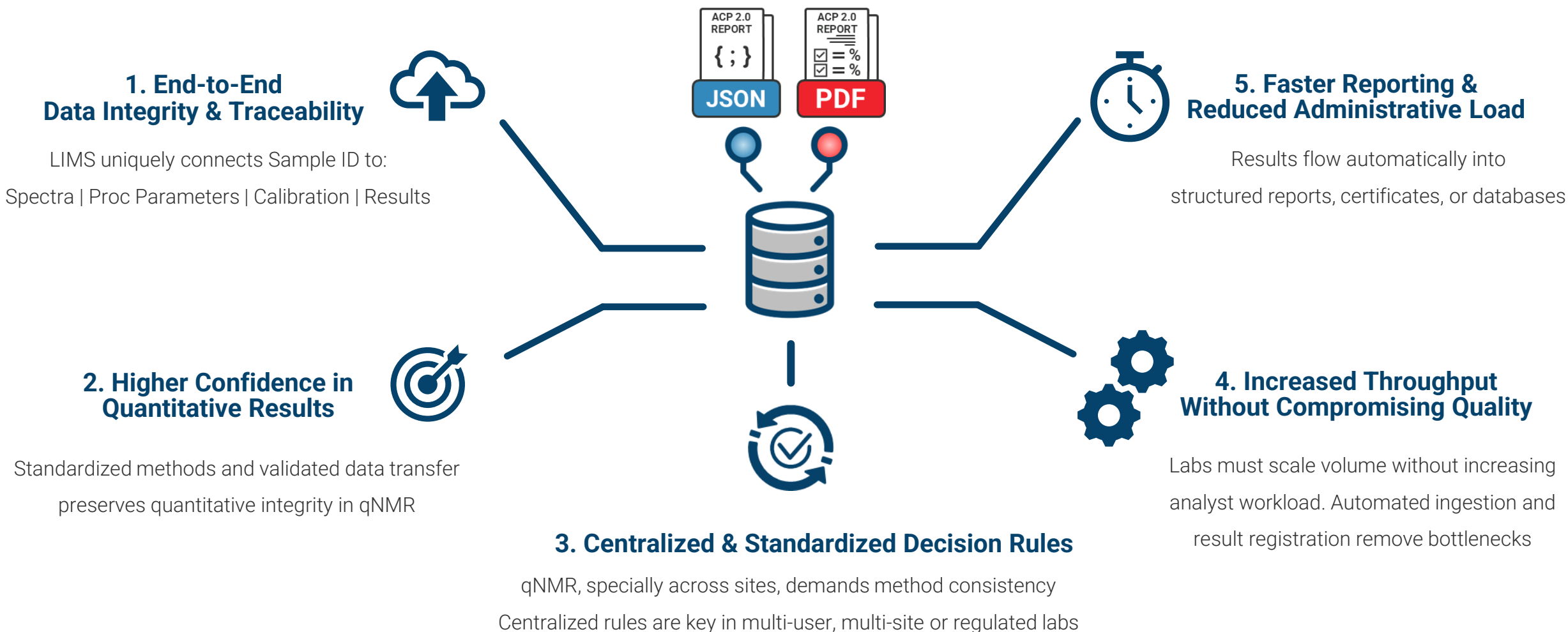
Amino Acid	Content
Leucine	20.7 wt%
Valine	10.4 wt%
Isoleucine	10.5 wt%
Total	41.6 wt%

Release batch only if ratio tests are passed!

Ratio	Result	Pass / Fail	Pass if
Leucine : Valine	2.0	pass	$1.9 \leq x \leq 2.1$
Leucine : Isoleucine	2.0	pass	$1.9 \leq x \leq 2.1$

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Digitalization & Connected Workflows



Advanced Chemical Profiling 2.0

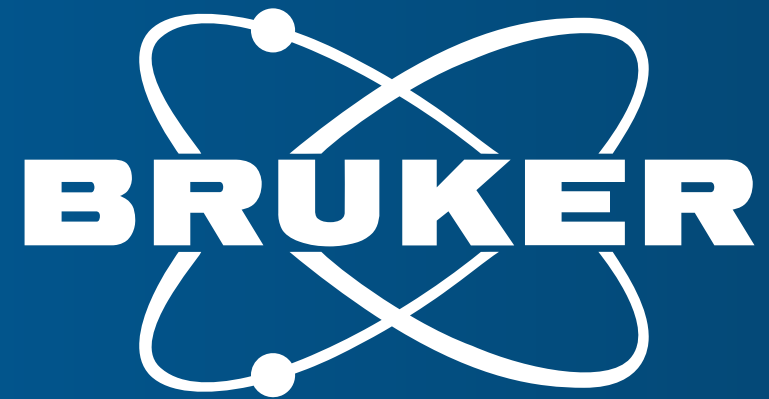
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- ✓ Install without administrator privileges
- ✓ Example datasets included to showcase ACP 2.0 tools
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