Juice-Profiling 4.0

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19.02.2024

Product Vision

- Solution for the **authenticity analysis** and **quality control** of fruit and vegetable juices
- Authenticity check combines:
  - ✓ Quantitative analysis of juice constituents
  - ✓ Statistical comparison of the NMR profile to reference groups

Streamline fruit juice analysis thanks to NMR, by allowing the simultaneous and fast analysis of a large number of parameters, with easy, inexpensive sample preparation and without the use of solvents.

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Value proposition of NMR

Parameter	Conventional method	Check for	Approx. Costs (€)
Ethanol	IFU 02 (GC) or enzymatic	Spoilage	50,-
Lactic acid	IFU 53 (enzymatic)	Spoilage	50,-
HMF	IFU 69 (HPLC)	Heat mistreatment	75,-
Fumaric acid	IFU 72 (HPLC)	Spoilage	75,-
Glucose	IFU 55 (enzymatic) or IC	Quality / sugar addition	55,-
Fructose	IFU 55 (enzymatic) or IC	Quality / sugar addition	
Sucrose	IFU 56 (enzymatic) or IFU 67 (HPLC)	Quality / sugar addition	
Malic acid	IFU 21 (enzymatic)	Quality	55,-
Citric acid	IFU 22 (enzymatic)	Quality / acid addition	55,-
Arbutin	*Lab. Internal (HPLC)*	Carry-over foreign fruit	100,-
Phlorin	*Lab. Internal (HPLC)*	Overextraction *Citrus*	100,-
Alanine	IFU 57 (column chromatography), Amino Acid Analyser	Quality	50,-
Galacturonic acid	IFU 78 (HPAEC-PAD)	Quality / excessive enzymation (use of pectinase)	75,-

Quantitative parameters considered for IFU NMR-based method

- In conventional analysis, different target parameters require their own methods (exception: glucose, fructose, sucrose and amino acids).
- The preparative effort and the duration of the analysis are very time-consuming in some cases.
- Quantitative ^{1}H-NMR thus represents an **enormous time and cost saving**.
- Quantitative 1H-NMR will become an IFU method for these parameters
- Besides these parameters, 1H-NMR allows to quantify additional parameters in the same analysis

IFU = International Fruit and Vegetable Juice Association

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Unique value proposition

- **Time and cost saving: replaces many conventional methods within one analytical run**
  - ✓ Simultaneous quantitative analysis of parameters pertaining to authenticity
  - ✓ Additional confirmation thanks to the statistical comparison of the NMR profile
  - ✓ < 20mn measurement time
- **Powerful method**
  - ✓ Robust quantification
  - ✓ Comprehensive and powerful for the detection of adulterations
  - ✓ On the way to be IFU recognized (for quantification parameters)
- **Ease of use**
  - ✓ Minimal sample preparation with no hazardous substances required
  - ✓ Fully automated workflow from sample to report
  - ✓ No NMR knowledge required for daily operation, very simple to use in routine analysis

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FoodScreener Platform

FoodScreener

- Floor standing 400MHz NMR Platform
- Compatible with Food Modules for Juice, Wine, Honey, and Olive Oil
- Configuration:
  - BBI 5mm FoodScreener-specific
  - 2 channels console (1H, X BB nuclei)
  - BOSS 3 shimsystem
  - Gimbal vibration dampers
  - Sample Case 60 with barcode reader
  - BCU I
  - SampleTrack and 2nd computer
  - Barcode printer and labels
  - Reference NMR tubes for calibration
  - AMIX

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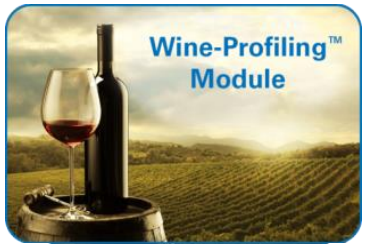
FoodScreener™ Module Portfolio



	Juice Version 4.0 Release 14 Feb 2024	Wine Version 4.0	Honey Version 3.1 Released Jan 2023	Olive Oil (80/400 MHz) Version 2.0
Database Size	~ 50k	~ 25k	~ 30k	~ 5k (400 MHz) ~ 3k (80 MHz)
Quantified Substances	41	55	36	20
Statistical Models included	~ 90	~ 70	34	4
Covering Reference values	> 100.000	> 2.000	> 70.000	> 40.000

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Workflow

Sample Preparation

Addition of 10% of a buffer solution

Note: for some type of samples, a dilution and/or centrifugation step may be required

NMR transfer

Transfer of 600 µl of sample in 5mm NMR tube and identification with barcode

Acquisition of NMR spectra

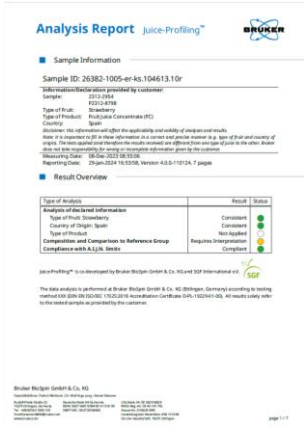
Automated measurement in SampleTrack according to the Juice-Profiling parameter set

< 20mn

Data Analysis

Transfer of the encrypted NMR data to the Data Analysis Server of Bruker

Results



Reception of analysis report (in SampleTrack) +

XML file of results (in data folder)

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What is new with Juice-Profiling 4.0 ?

Quantitative Analysis

- Improved quantitative analysis for IFU*-relevant parameters :

  Alanine, Arbutin, Citric Acid, Ethanol, Fructose, Fumaric Acid, Galacturonic Acid, Glucose, HMF, Lactic Acid, Malic Acid, Phlorin and Sucrose.

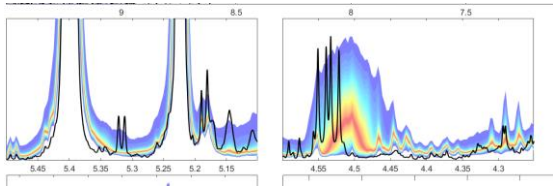
- Implementation of formol number quantification.

Statistical Analysis

- Database expansion by a factor of 3: > 49,200 reference juice samples from all over the world.
- Update of all existing models (v 3.0).
- 27 **fruit type** models.
- 17 new **country models**, to check the country of origin of the juices.
- Doubling of the number of models to differentiate **not from concentrate vs from concentrate** juices.
- New fruit content models.

Results reporting

- Update of the AIJN (European Fruit Juice Association) reference guidelines for the quantitative analysis.
- Indication of possible molecules in cause of deviations, in case of the detection of atypical profiles.
- Updated analysis report.
- Quantile plots provided with the results.



* IFU = International Fruit and Vegetable Juice Association

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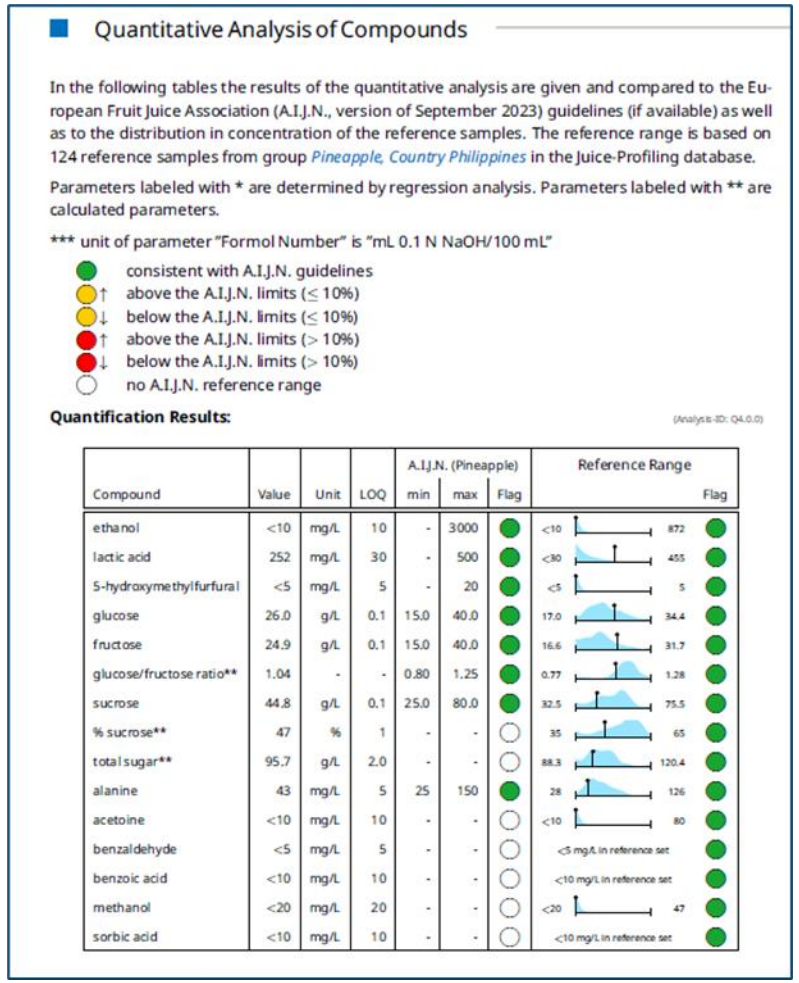
Updates of the quantitative analysis



Quantitative Analysis of Compounds

In the following tables the results of the quantitative analysis are given and compared to the European Fruit Juice Association (A.I.J.N., version of September 2023) guidelines (if available) as well as to the distribution in concentration of the reference samples. The reference range is based on 124 reference samples from group *Pineapple, Country Philippines* in the Juice-Profiling database.

Parameters labeled with * are determined by regression analysis. Parameters labeled with ** are calculated parameters.

*** unit of parameter "Formol Number" is "mL 0.1 N NaOH/100 mL"

- consistent with A.I.J.N. guidelines
- ↑ above the A.I.J.N. limits (≤ 10%)
- ↓ below the A.I.J.N. limits (≤ 10%)
- ↑ above the A.I.J.N. limits (> 10%)
- ↓ below the A.I.J.N. limits (> 10%)
- no A.I.J.N. reference range

Quantification Results:

(Analysis-ID: Q4.0.0)

Compound	Value	Unit	LOQ	A.I.J.N. (Pineapple) min	A.I.J.N. (Pineapple) max	Flag	Reference Range	Flag
ethanol	<10	mg/L	10	-	3000		<10 872	
lactic acid	252	mg/L	30	-	500		<30 455	
5-hydroxymethylfurfural	<5	mg/L	5	-	20		<5 5	
glucose	26.0	g/L	0.1	15.0	40.0		17.0 34.4	
fructose	24.9	g/L	0.1	15.0	40.0		16.6 31.7	
glucose/fructose ratio**	1.04	-	-	0.80	1.25		0.77 1.28	
sucrose	44.8	g/L	0.1	25.0	80.0		32.5 75.5	
% sucrose**	47	%	1	-	-		35 65	
total sugar**	95.7	g/L	2.0	-	-		88.3 120.4	
alanine	43	mg/L	5	25	150		28 126	
acetoine	<10	mg/L	10	-	-		<10 80	
benzaldehyde	<5	mg/L	5	-	-		<5 mg/L in reference set	
benzoic acid	<10	mg/L	10	-	-		<10 mg/L in reference set	
methanol	<20	mg/L	20	-	-		<20 47	
sorbic acid	<10	mg/L	10	-	-		<10 mg/L in reference set	

- Improved quantitative analysis for IFU*-relevant parameters :

  Alanine, Arbutin, Citric Acid, Ethanol, Fructose, Fumaric Acid, Galacturonic Acid, Glucose, HMF, Lactic Acid, Malic Acid, Phlorin and Sucrose.

- Implementation of formol number quantification.
- Update of the AIJN (European Fruit Juice Association) reference guidelines for the quantitative analysis.

* IFU = International Fruit and Vegetable Juice Association

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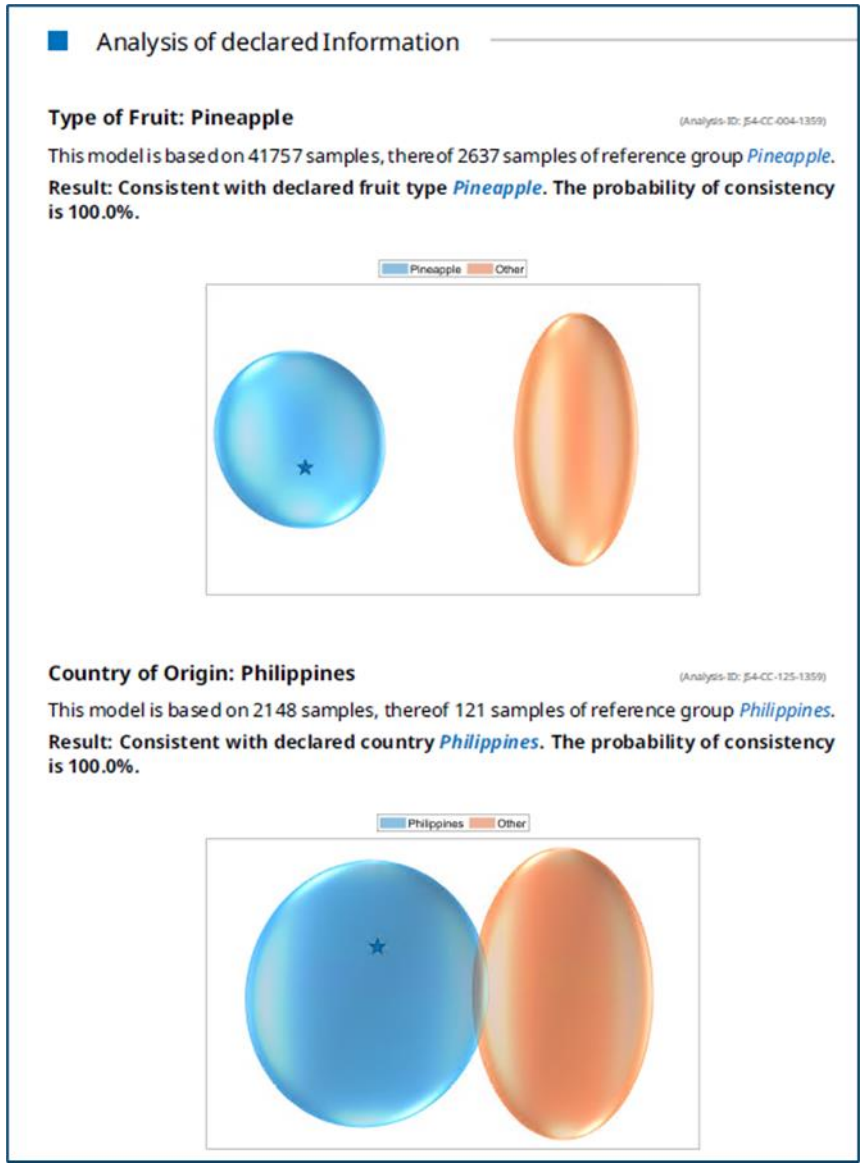
Updates of the classification models



- The declared fruit type or country of origin is compared to the group of „others“ which contains all other fruits or countries.
- Result given as probability of consistency

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Updates of the classification models

- **New Fruit type models**
  - ✓ Carrot, Acerola, Lime, Aronia, Elderberry, Cranberry, Tomato
- **New Country models**
  - ✓ All models are now single country models (exception for Apple: Germany/Poland)
  - ✓ Orange (Italy), Pineapple (Costa Rica, Philippines, Thailand), Mango (Columbia, Peru), Grape (Spain), Grapefruit (Cuba, South Africa), Passion Fruit (Ecuador, Peru), Peach (Greece, Turkey), Banana (Guatemala, Ecuador), Strawberry (Poland, Spain)
- **New Product type (FC/NFC*) models**
  - ✓ Grape, Grapefruit, Passion Fruit, Sour Cherry, Black Currant
- **Fruit content models**
  - ✓ Acerola, Lime

* FC = From Concentrate. NFC = Not From Concentrate

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Updates of the univariate analysis

Statistical Comparison with the Reference Group

The models are based on 159 samples of group *Strawberry, Country Spain*.

Univariate Verification (Verification, Analysis ID: JS4-NTV-144-111252)

Result: Deviating signals were found at following chemical shifts:

4.313^{high}

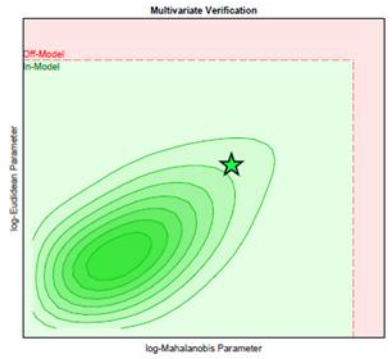
The suffix *high* indicates that the intensity is higher than in the reference group, the suffix *low* indicates that the intensity is lower than in the reference group.

Possible molecules: gluconic acid, lactic acid

This list gives indication about possible molecules responsible for deviations.

Multivariate Verification (Verification, Analysis ID: JS4-NTV-144-111252)

Result: No deviation was detected in multivariate verification (In-Model).



When the univariate analysis detects signals that deviate from the reference group, a list of the possible molecules in cause is given in the report

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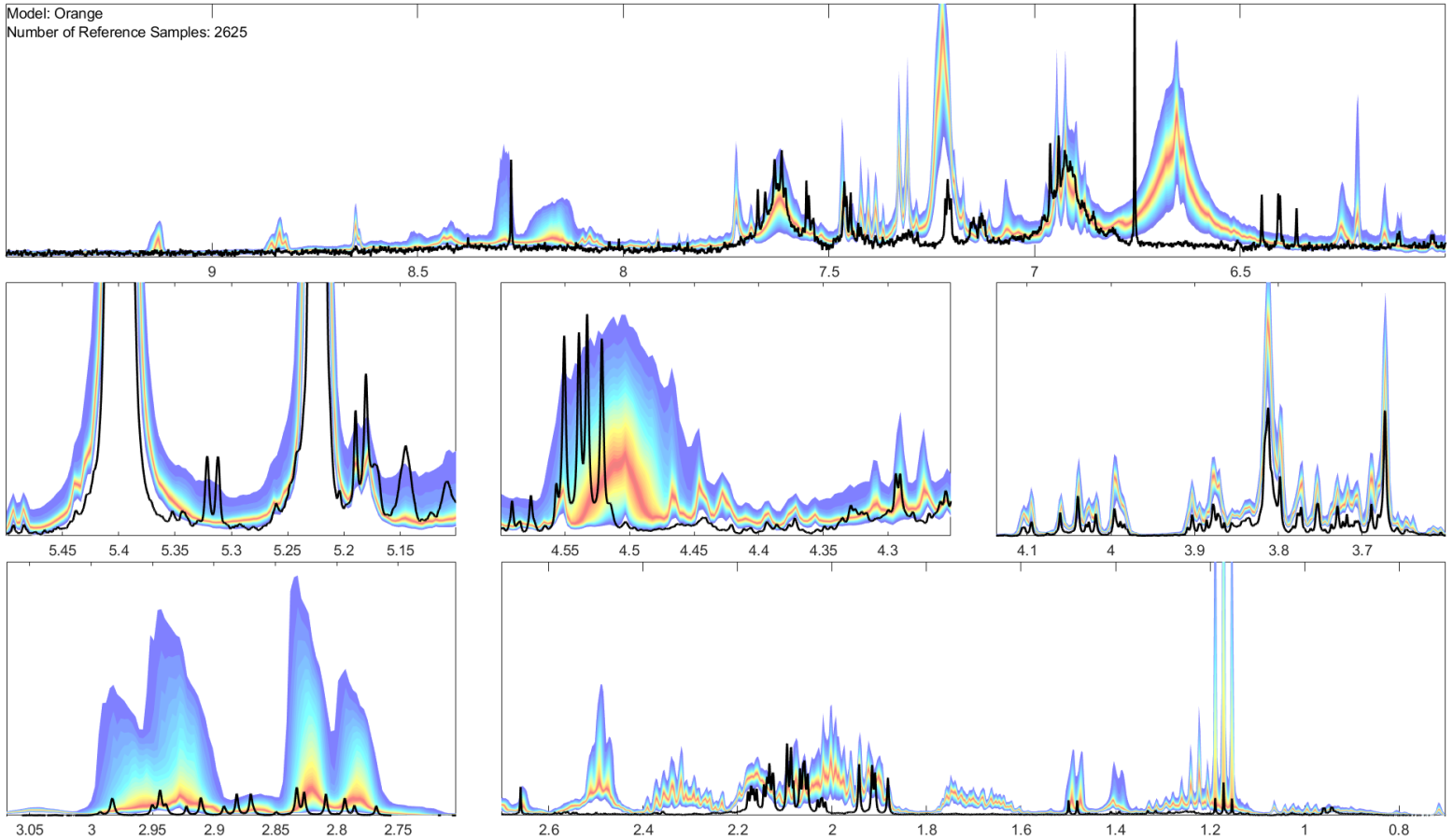
Quantile Plots



Quantile plots provided with the results.

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Customer Testimonials

Markus Jungen, SGF International e.V. about the Juice Profiling Solution

For a span of a decade, our collaborative efforts with Bruker have been pivotal in advancing the Juice-Profiling database. This noteworthy upgrade represents a significant stride in reinforcing the role of Nuclear Magnetic Resonance (NMR) as both an alternative and supplementary analytical technique, presenting a swift and comparatively cost-effective approach in the realm of juice analysis.

The Juice-Profiling methodology, a robust tool, not only expedites the evaluation of authenticity in fruit juices but also extends its reach to encompass vegetable juices. By harmonizing quantitative scrutiny of constituent elements and intricate statistical analyses of profiles, including provenance, this method offers a comprehensive and efficient means of discerning the authenticity of both fruit and vegetable juices.

Markus Jungen
Technical Manager, SGF International e.V.

André Platzek, Tentamus Chelab GmbH about the Juice Profiling Solution

The updated juice profiling method is a formidable tool for the authenticity analysis of fruit juices. It allows time-efficient and versatile scanning of a wide array of parameters helping us to meet our individual customer's needs. Simultaneous analysis of selected parameters provides a significant increase in efficiency with PCA analysis yielding valuable information on the authenticity of the fruit juices with special regard to purity and geographical origin of specific fruits.

André Platzek
Head of NMR Analytic Department, Tentamus Chelab G

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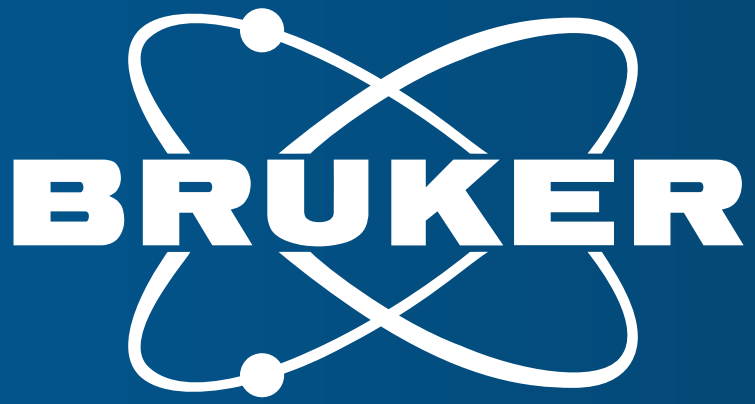
Thank you!



Innovation with Integrity