

WEBINAR 2021

New Software Functionality: How next generation software results in better performance and time-efficient operation

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How next generation software results in better performance and time-efficient operation



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Ph D, Analytical Chemistry, Hamburg

2001 Method Development Bruker AXS

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Ph D, Geoscience, Hannover

2019 Product Management Bruker AXS

Product Management XRF

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Outline

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Introduction to XRF

02

What a Software needs

03

How to calibrate your Spectrometer

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Routine Operations without PC

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Q&A

When to use X-ray Fluorescence (XRF) Analysis?



Elemental compositions often define the properties or quality of a compound, material or product.

- XRF is used for fast and accurate analysis of elemental compositions in various materials
- XRF is an established analytical tool for process and quality control in the industry
- XRF allows to meet changing quality requirements based on excellent data quality
- XRF analysis can be used, e.g., to define material value based on grade control (mining)
- XRF analysis adds value and can often determine the suitability of a product for specific applications (high tech functional material)

Mature Technology in XRF?

Are there any Changes to Address Future Requirements



Applications are getting more demanding for higher accuracy, better precision, better detection of traces

New legislation is enforcing extended analysis – more elements, lower detection limits, closer monitoring

Examples:

- **Sand/Quartz:** Construction, playgrounds, glass or solar cells, semicon wafers (Fe content)
- **Coal:** heating, power generation, electrodes for aluminium, electrodes for batteries (S, Cl, trace elements)
- **Pt/Rh** – jewelry, car catalysts, electrodes in fuel cells (Traces, thickness)
- **Additives in lubricants and polymers** – use the expensive additives sparsely while meeting the desired performance

XRF X-ray Fluorescence Analysis

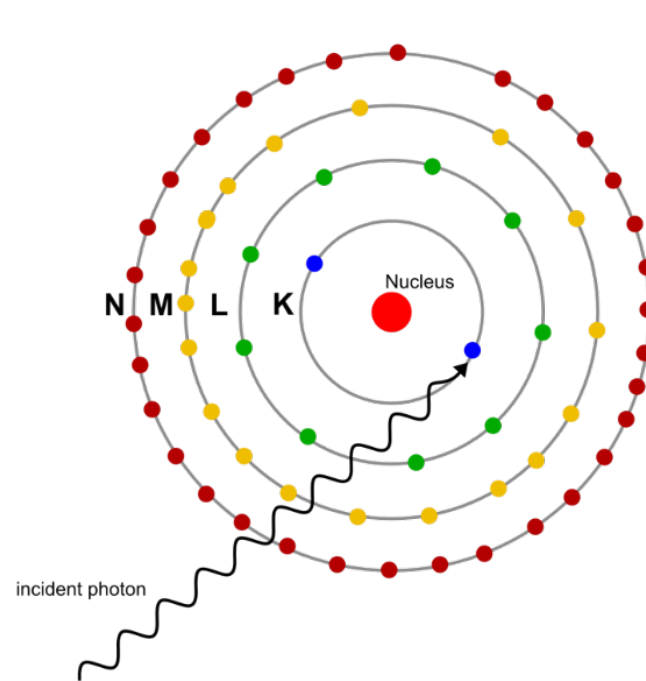
X-ray Spectrometry

- ... is the method to do qualitative and quantitative analysis of elemental composition by excitation of atoms and detection of their characteristic
- X-rays: one form of "Electromagnetic Radiation"

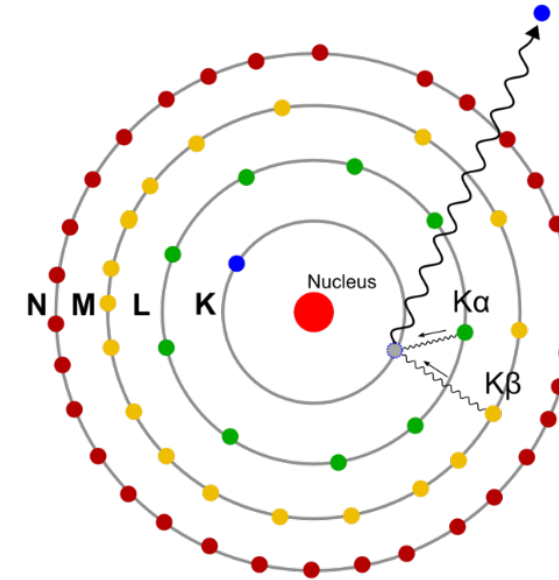
Energy [keV]	Wavelength	Description
$< 10^{-7}$	cm to km	Radio waves
$< 10^{-3}$	μm to cm	Microwaves
$< 10^{-3}$	μm to mm	Infrared light
0.0017 - 0.0033	380 to 750 nm	Visible light
0.0033 - 0.1	10 to 380 nm	Ultraviolet light
0.1 - 100	0.01 to 10 nm	X-rays
10 - 5000	0.0002 to 0.12 nm	Gamma radiation

X-ray Fluorescence Analysis (XRF)

Principle – Photoelectric Effect



- Sample excited with an X-ray beam causing fluorescence
- Electron ejected from an inner shell of its atom
- Electron from a shell farther out falls into the vacancy



- Energy difference is emitted as an X-ray photon
- Discrete energy or wavelength is characteristic for the emitting element / transition
- Intensity of characteristic radiation is proportional to concentration of the element in the sample

X-ray Fluorescence Analysis Capabilities

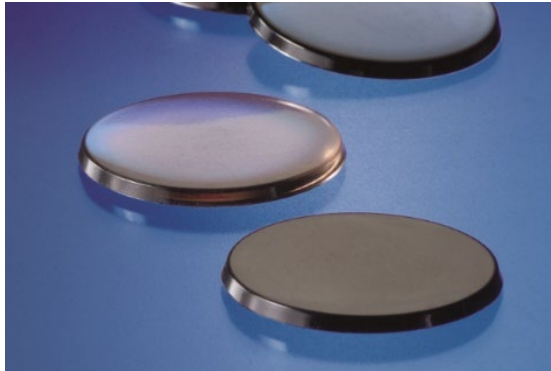


- Qualitative Analysis
 - Identification of elements
 - “What’s inside?”
- Quantitative Analysis
 - Determination of concentrations
 - “How much is inside?”
- Semi-Quantitative Analysis
 - Estimation of concentration
 - “About how much?”
- Solid and liquid samples can be analyzed directly:
- Little or no sample preparation required
- Analysis is non-destructive to the sample
- Sampling-to-analysis result time is relatively short
- Quantitative and qualitative analyses are possible
- Accuracy and long-term stability
- Elemental range: (Be) Na to U
- Linearity from ppm to 100%



Sample Preparation – Driven by Application

Fused beads – Best results for
Major Element QC



Powder – Fastest preparation,
less precise



Pressed Pellets – Simple, fast,
great for traces

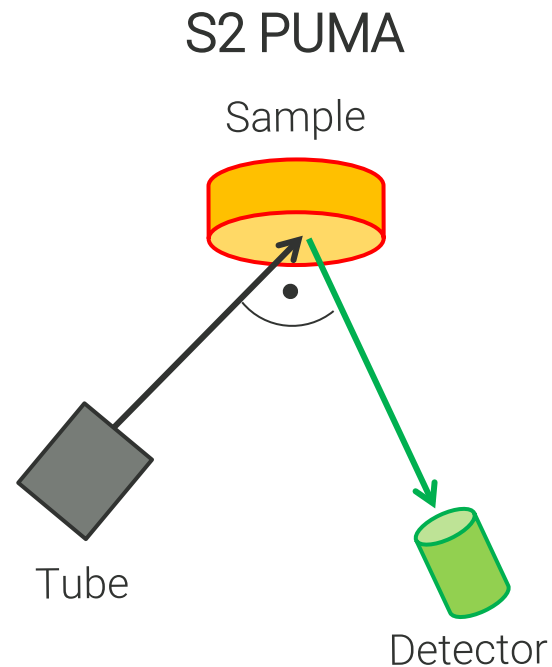


Liquid – Simple and
reproducible



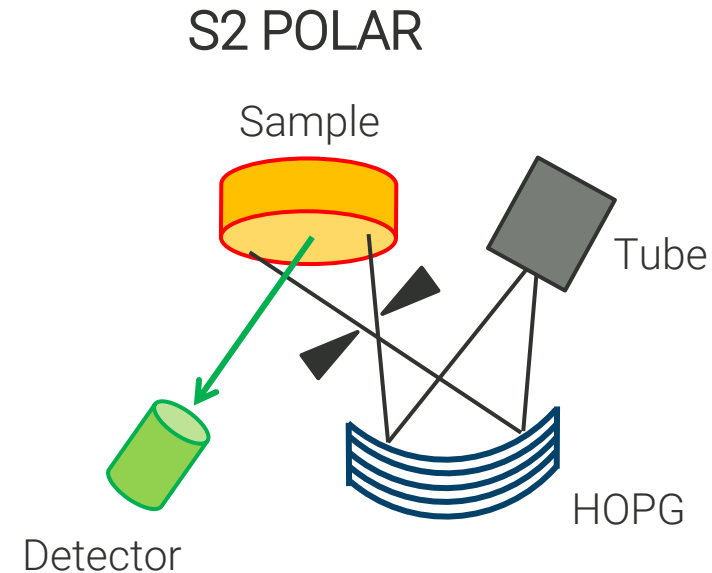
EDXRF Excitation Techniques

Direct Excitation vs. Polarized Excitation



Direct excitation:

- Leads to very high intensity
- But also to higher background intensity



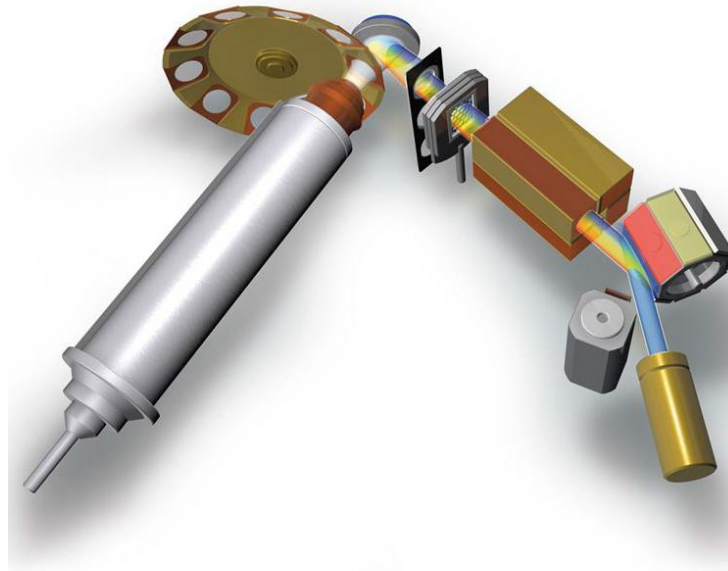
Polarized excitation:

- Reduced background due to polarization
- Improved signal to background ratio (better LLD)

Wavelength-Dispersive XRF (WDXRF)

Analytical flexibility and high performance for sub-ppm traces

- 4 kW excitation
20 – 60 kV
- 5 – 170 mA
- 10 beam filters
- 4 collimators
- 8 crystals
- 2 detectors



S8 TIGER WDXRF Beam path



Floorstanding WDXRF S8 TIGER
With 1, 3 or 4 kW

X-ray Fluorescence Analysis (XRF)

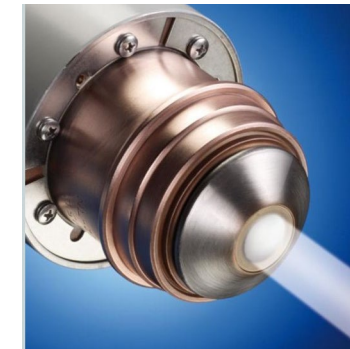
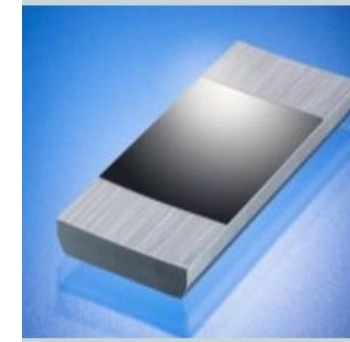
The Comparison of Energy and Wavelength Dispersive Spectrometers

EDXRF

- Mechanical simplicity
- Cheaper
- Sensitivities: down to the ppm level
- Records the entire spectrum
- Easy operation
- Smaller, "can be brought to the sample"

WDXRF

- High precision mechanics
- Higher capital
- Precision: <0.05%
- Higher resolution
- Sensitivities: down to the ppm level, but roughly one to two orders more sensitive
- Records the counts at a given wavelength
- Very fast analysis
- Highest sample throughput



What requirements for a modern spectrometer software?

- Intuitive user interface
- Full functionality
- Different user levels
- Short processing times
- High stability
- Flexible data management

Modern XRF software offers better analytical performance and **saves time!**

(training, operation, evaluation)



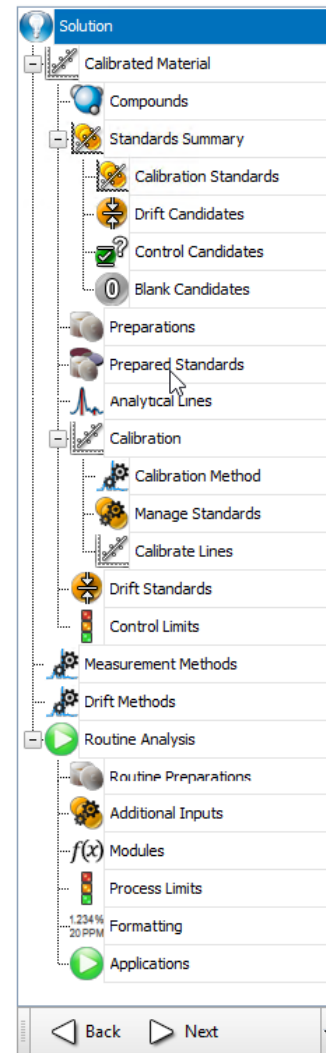
SPECTRA.ELEMENTS: Next Generation XRF Software Platform

NEW SOFTWARE FUNCTIONALITY

How to Calibrate

The WIZARD walks you smoothly through the calibration process

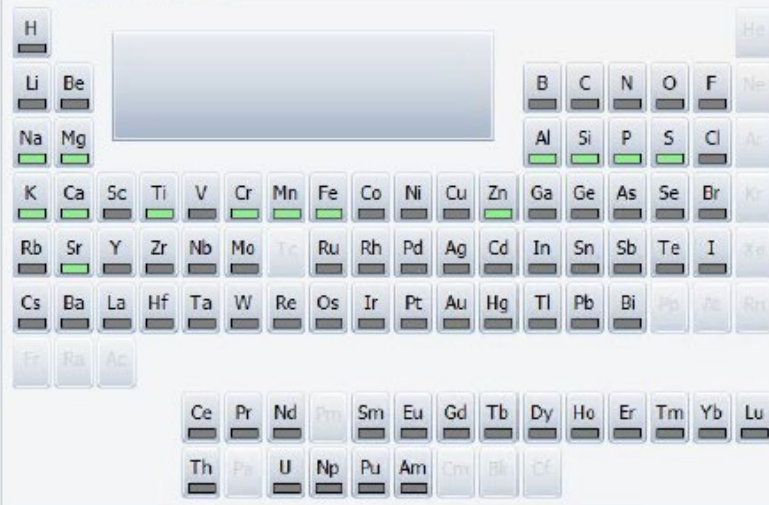
- The proven tree-structure guides the user through the calibration:
 - Define the compounds to be measured
 - Make use of a broad compound library or define your own “special” compound
 - Defined the matrix
 - Use Compton balance for Oxygen



Z	Name	Formula	Evaluation Mode	Value	Unit	Digits
11	Sodium Oxide	Na ₂ O	Measured (Calibration)		%	2
12	Magnesium Oxide	MgO	Measured (Calibration)		%	2
13	Aluminum Oxide	Al ₂ O ₃	Measured (Calibration)		%	2
14	Silicon Oxide	SiO ₂	Measured (Calibration)		%	2
15	Phosphorus Oxide	P ₂ O ₅	Measured (Calibration)		%	2
16	Sulfur Oxide	SO ₃	Measured (Calibration)		%	2
19	Potassium Oxide	K ₂ O	Measured (Calibration)		%	2
20	Calcium Oxide	CaO	Measured (Calibration)		%	2
22	Titanium Oxide	TiO ₂	Measured (Calibration)		%	2
24	Chromium Oxide	Cr ₂ O ₃	Measured (Calibration)		%	2
25	Manganese(III) Oxide	Mn ₂ O ₃	Measured (Calibration)		%	2
26	Iron Oxide	Fe ₂ O ₃	Measured (Calibration)		%	2
30	Zinc Oxide	ZnO	Measured (Calibration)		%	2
38	Strontium Oxide	SrO	Measured (Calibration)		%	2

Select or deselect using periodic table

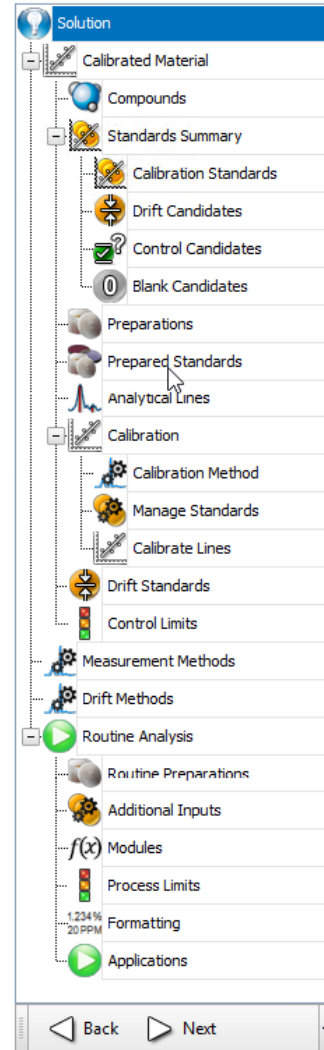
Selection mode:
☒ Element
☐ Oxide



Hide periodic table X Delete Compound Compound Library... Modification

The WIZARD walks you smoothly through the calibration process

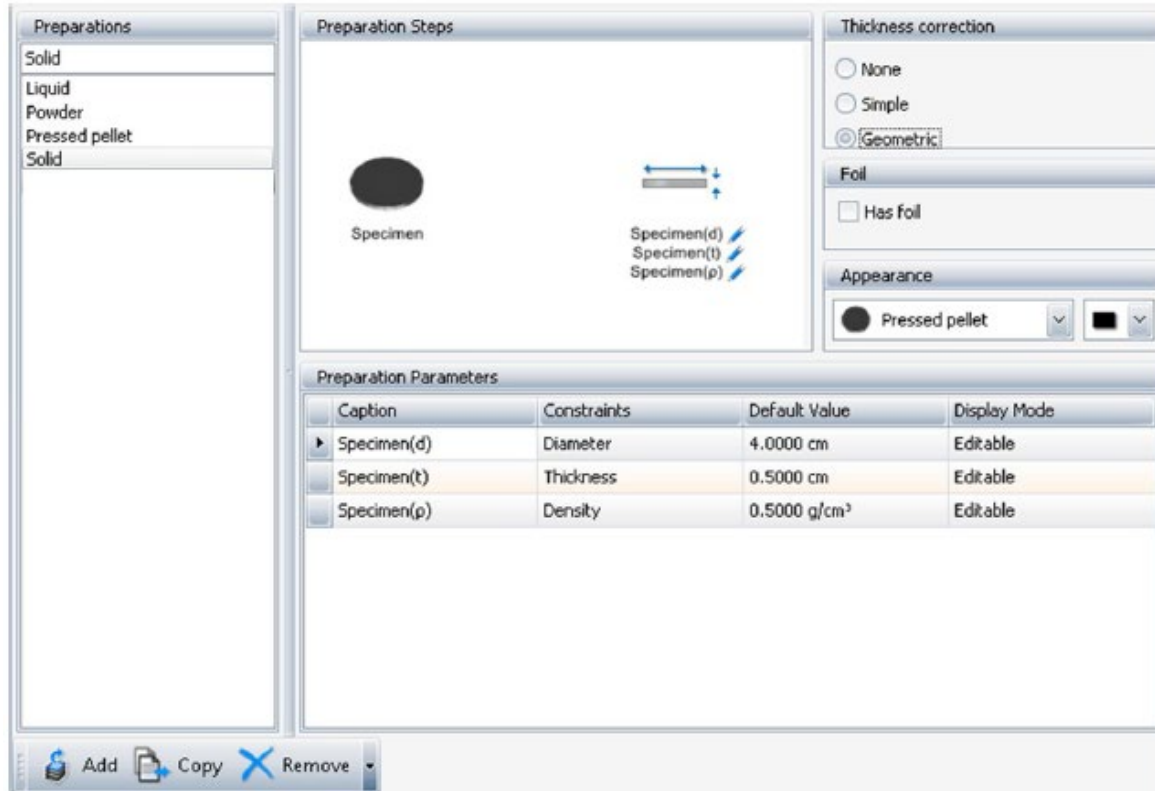
- The proven tree-structure guides the user through the calibration:
 - Copy & Paste compositions of the reference materials
 - Auto illustration of **high** and **low** contents
 - Select control standards, drift and blanks (or decide to add them later)



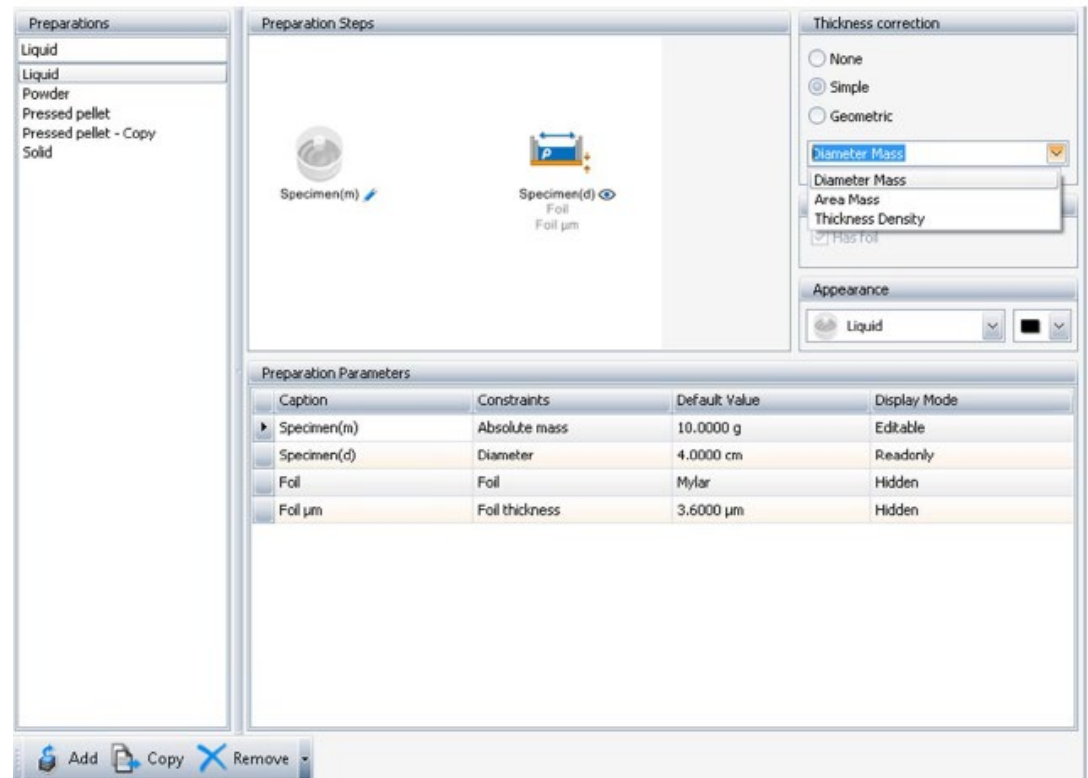
Used	Name	Path / Job ID	Measurement D...	State	SiO (%)	ZnO (%)	Fe2O3 (%)	Mn2O3 (%)	Cr2O3 (%)	TiO2 (%)	CaO (%)	K2O (%)	SO3 (%)	P2O5 (%)	SiO2 (%)	Al2O3 (%)	MgO (%)	Na2O (%)
<input checked="" type="checkbox"/>	GQB-01	Database ...	3/2/2018 10:49...	Found in dat...	0.00	0.02	0.85	0.17	0.00	0.01	57.52	0.05	0.00	0.02	0.50	0.20	40.36	0.00
<input checked="" type="checkbox"/>	GQB-02	Database ...	3/2/2018 11:09...	Found in dat...	0.00	0.01	2.01	0.02	0.00	0.09	0.79	5.02	0.00	0.00	76.15	12.15	0.05	3.38
<input checked="" type="checkbox"/>	GQB-03	Database ...	3/2/2018 11:28...	Found in dat...	0.00	0.00	0.79	0.87	0.00	0.39	31.20	0.38	1.44	0.00	39.00	6.20	18.90	0.24
<input checked="" type="checkbox"/>	GQB-04	Database ...	3/6/2018 11:13...	Found in dat...	0.07	0.00	3.74	0.04	0.00	0.58	23.57	3.19	0.00	7.36	47.09	4.93	8.64	0.17
<input checked="" type="checkbox"/>	GQB-05	Database ...	3/2/2018 12:06...	Found in dat...	0.07	0.00	1.18	0.00	0.05	3.77	0.24	0.44	0.00	0.13	8.19	85.32	0.21	0.08
<input checked="" type="checkbox"/>	GQB-06	Database ...	3/2/2018 12:25...	Found in dat...	0.05	0.00	0.02	0.00	0.00	0.02	1.08	0.21	0.00	0.01	67.88	19.95	0.00	10.74
<input checked="" type="checkbox"/>	GQB-07	Database ...	3/2/2018 12:44...	Found in dat...	0.03	0.00	0.08	0.02	0.00	0.02	96.22	0.04	0.03	0.01	1.24	0.21	0.27	0.03
<input type="checkbox"/>	GQB-08	Database (0)		Not found	0.00	0.00	1.18	0.00	0.02	1.23	0.19	2.53	0.00	0.08	58.07	35.91	0.34	0.39
<input checked="" type="checkbox"/>	GQB-09	Database ...	3/2/2018 1:03 PM	Found in dat...	0.00	0.00	100.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<input checked="" type="checkbox"/>	GQB-10	Database ...	3/2/2018 1:22 PM	Found in dat...	0.14	0.00	0.06	0.00	0.00	0.00	41.11	0.03	57.72	0.01	0.56	0.13	0.23	0.01
<input type="checkbox"/>	GQB-11	Database (0)		Not found	0.23	0.00	1.36	0.04	0.00	0.11	35.52	0.68	46.23	0.03	10.96	2.56	2.18	0.09
<input checked="" type="checkbox"/>	GQB-12	Database ...	3/5/2018 2:03 PM	Found in dat...	0.00	0.00	0.01	0.00	0.00	0.03	0.00	0.00	0.00	0.00	99.79	0.05	0.00	0.00
<input type="checkbox"/>	GQB-13	Database (0)		Not found	0.00	0.00	84.87	0.11	0.00	0.22	5.37	0.13	0.05	3.61	3.61	0.52	0.92	0.15
<input checked="" type="checkbox"/>	GQB-14	Database ...	3/5/2018 12:47...	Found in dat...	0.00	0.00	12.41	0.01	0.07	3.77	0.03	0.01	0.21	0.07	5.41	77.74	0.02	0.00
<input type="checkbox"/>	GQB-15	Database (0)		Not found	0.11	0.00	0.30	0.06	0.00	0.04	70.00	0.11	2.25	0.12	21.80	4.85	0.42	0.10
<input checked="" type="checkbox"/>	GQB-16	Database ...	3/5/2018 1:06 PM	Found in dat...	0.29	0.05	2.62	0.07	0.01	0.28	64.51	0.82	2.97	0.17	20.89	5.54	1.47	0.23
<input checked="" type="checkbox"/>	GQB-17	Database ...	3/5/2018 1:44 PM	Found in dat...	0.09	0.06	4.08	0.19	0.01	0.32	58.41	1.03	3.12	0.17	22.72	7.31	2.19	0.19
<input checked="" type="checkbox"/>	GQB-18	Database ...	3/5/2018 1:26 PM	Found in dat...	0.01	0.00	0.10	0.00	0.00	0.04	0.37	10.73	0.00	0.07	69.84	15.44	0.00	2.11
<input type="checkbox"/>	GQB-19	Database (0)		Not found	0.07	0.01	3.24	0.03	0.04	1.15	42.89	0.29	18.19	0.06	8.73	23.10	1.62	0.47
<input type="checkbox"/>	GQB-20	Database (0)		Not found	0.05	0.02	2.88	0.06	0.02	0.56	56.60	0.68	10.91	0.07	14.35	11.62	1.84	0.28
<input type="checkbox"/>	FLX-21				0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<input type="checkbox"/>	FLX-22				0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<input type="checkbox"/>	FLX-57				0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Sample preparation

- Select e.g., type, geometry, flux, using check boxes and drop-down menus.
- The WIZARD performs an **automatic thickness correction** using the density of the material



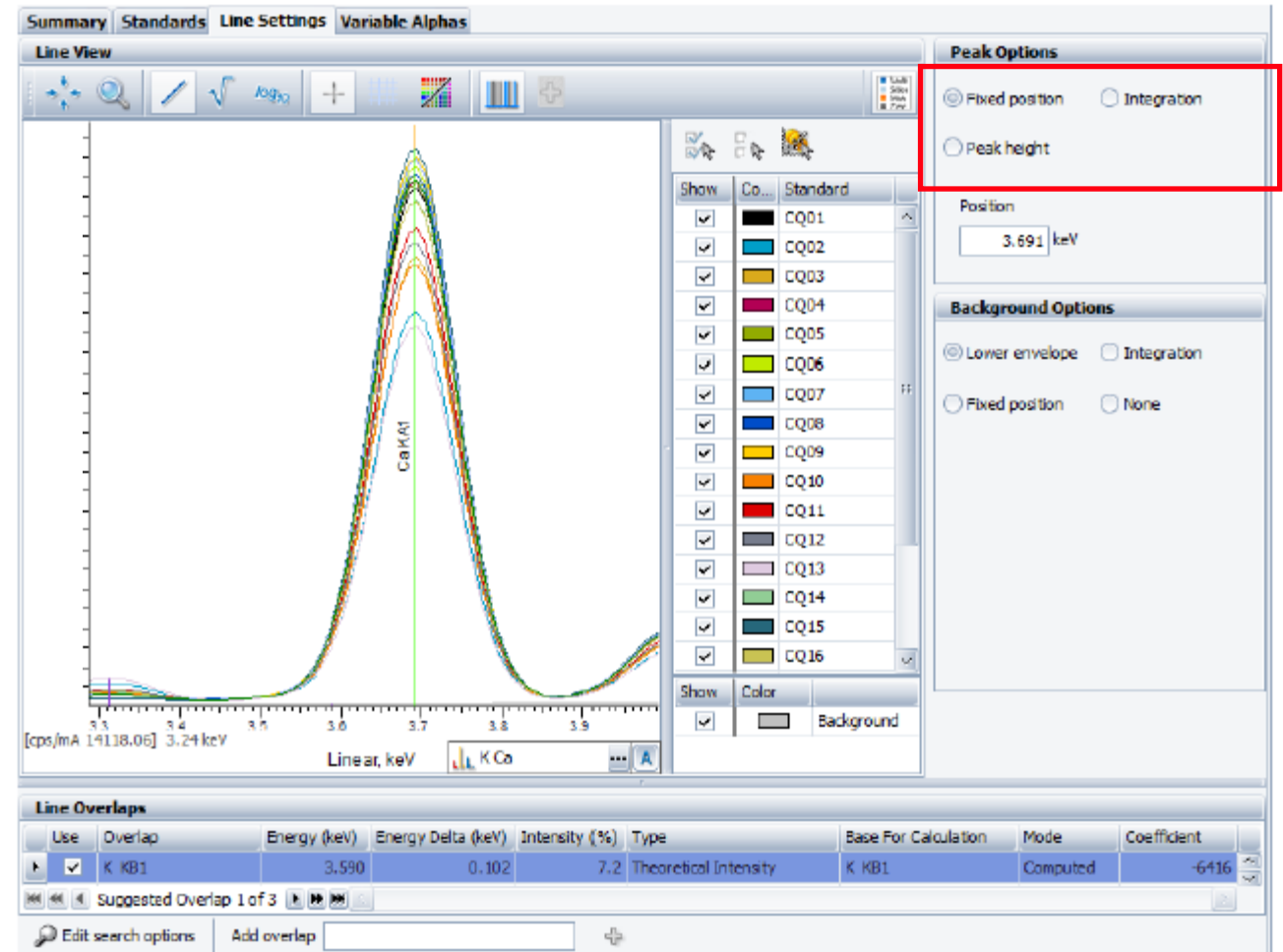
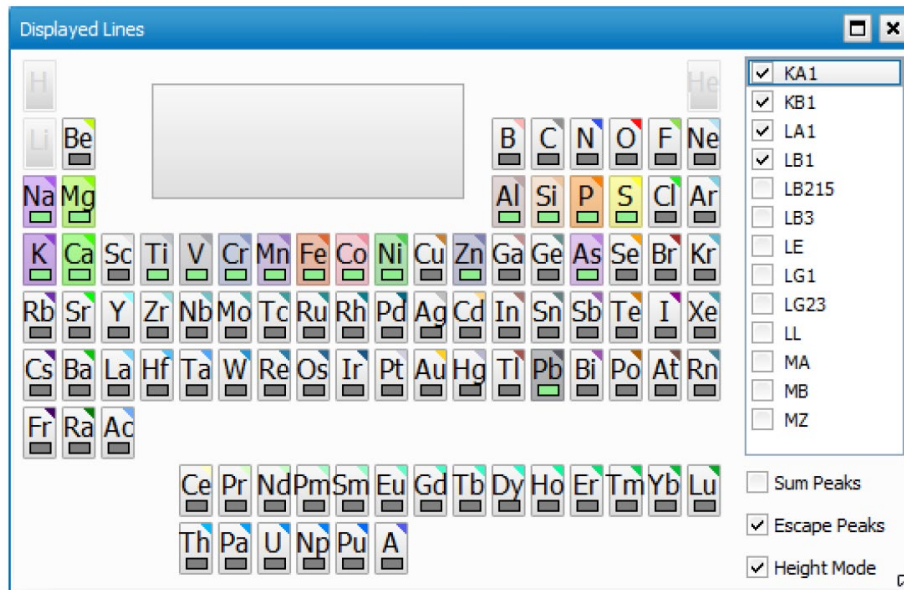
Caption	Constraints	Default Value	Display Mode
Specimen(d)	Diameter	4.0000 cm	Editable
Specimen(t)	Thickness	0.5000 cm	Editable
Specimen(ρ)	Density	0.5000 g/cm ³	Editable



Caption	Constraints	Default Value	Display Mode
Specimen(m)	Absolute mass	10.0000 g	Editable
Specimen(d)	Diameter	4.0000 cm	Readonly
Foil	Foil	Mylar	Hidden
Foil μm	Foil thickness	3.6000 μm	Hidden

The WIZARD walks you smoothly through the calibration process

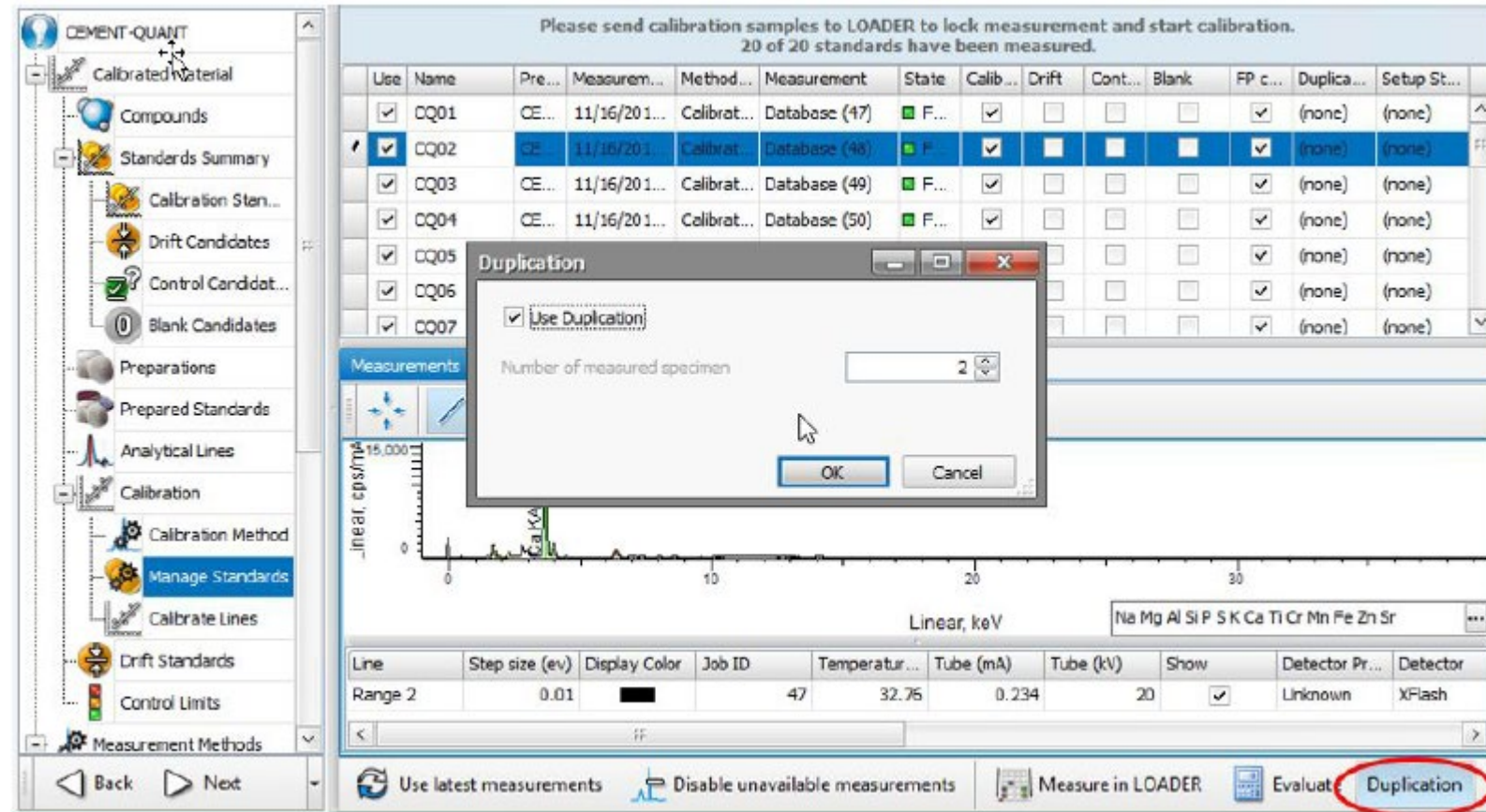
Once the standards are measured the software provides various options to optimize your calibration based on the properties of your samples



The WIZARD walks you smoothly through the calibration process

Some processes require duplicate standard measurement.

This can be setup easily in SPECTRA.ELEMENTS.



The screenshot displays the SPECTRA.ELEMENTS software interface during a calibration process. On the left, a tree view shows the 'CEMENT-QUANT' project with various sub-items like 'Calibrated Material', 'Compounds', 'Standards Summary', 'Calibration Sten...', 'Drift Candidates', 'Control Candidat...', 'Blank Candidates', 'Preparations', 'Prepared Standards', 'Analytical Lines', 'Calibration', 'Calibration Method', 'Manage Standards', 'Calibrate Lines', 'Drift Standards', and 'Control Units'. The 'Measurements' section is currently selected.

The main window shows a table of calibration standards with columns: Use, Name, Pre..., Measur..., Method..., Measurement, State, Calib..., Drift, Cont..., Blank, FP c..., Duplica..., and Setup St... The table lists standards CQ01 through CQ07, all marked as 'Use' and 'Calibrated'. A message at the top states: 'Please send calibration samples to LOADER to lock measurement and start calibration. 20 of 20 standards have been measured.'

A 'Duplication' dialog box is open in the center, with the 'Use Duplication' checkbox checked. It asks for the 'Number of measured specimen' (set to 2) and has 'OK' and 'Cancel' buttons.

Below the table, a spectrum plot shows 'Linear, cps/mV' vs 'Linear, keV'. The x-axis ranges from 0 to 30 keV, and the y-axis ranges from 0 to 15,000 cps/mV. A peak is visible around 4 keV, labeled 'Ca Kα'.

At the bottom, a table shows measurement parameters for 'Range 2':

Line	Step size (ev)	Display Color	Job ID	Temperatur...	Tube (mA)	Tube (kV)	Show	Detector Pr...	Detector
Range 2	0.01		47	32.75	0.234	20	<input checked="" type="checkbox"/>	Unknown	XFlash

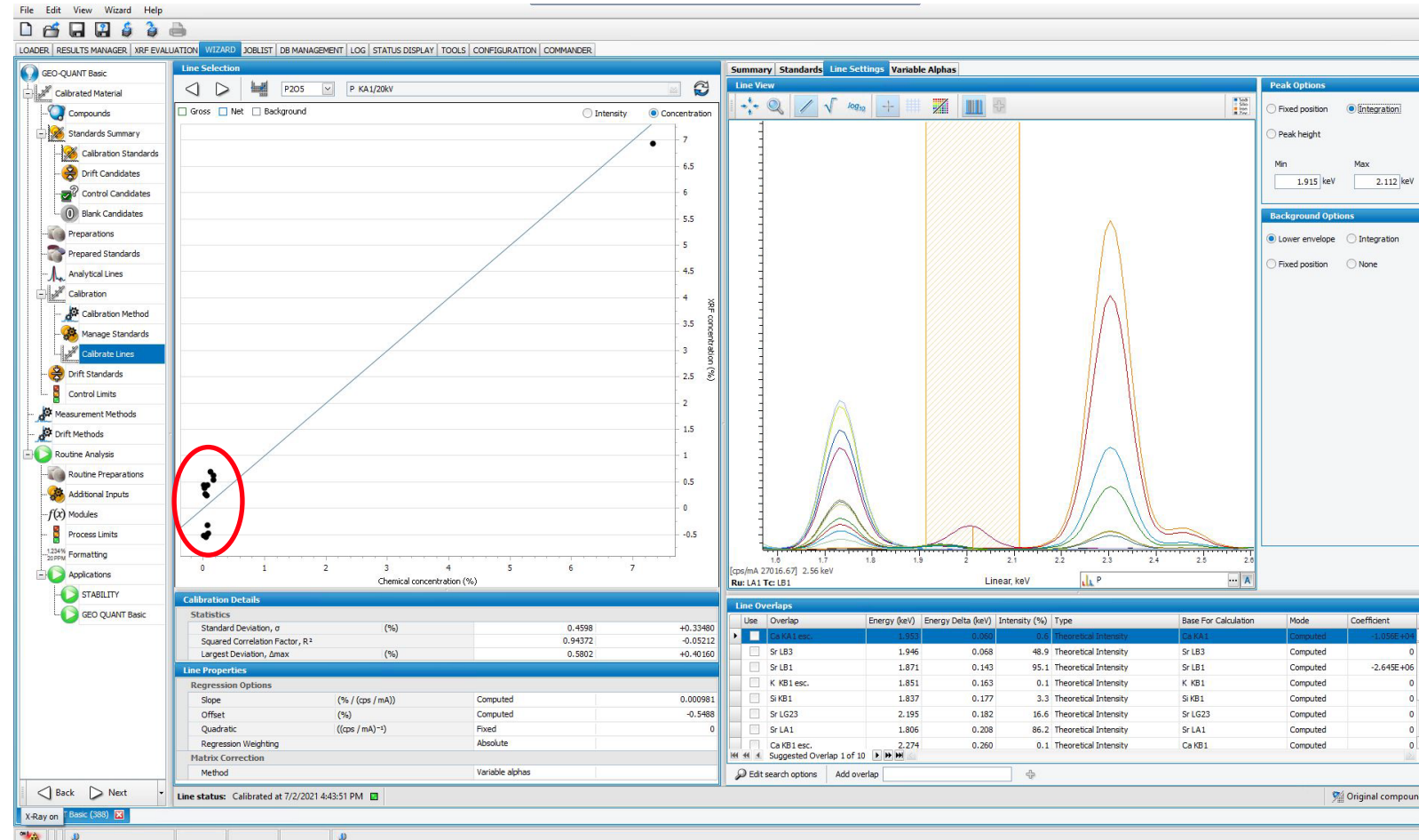
The bottom status bar includes buttons for 'Use latest measurements', 'Disable unavailable measurements', 'Measure in LOADER', 'Evaluate', and 'Duplication' (which is circled in red).

Calibration example

Smart overlap correction

Examples 1: P205 in geo-materials

- Poor correlation if all potential overlaps are unchecked ($R^2 = 0.944$)

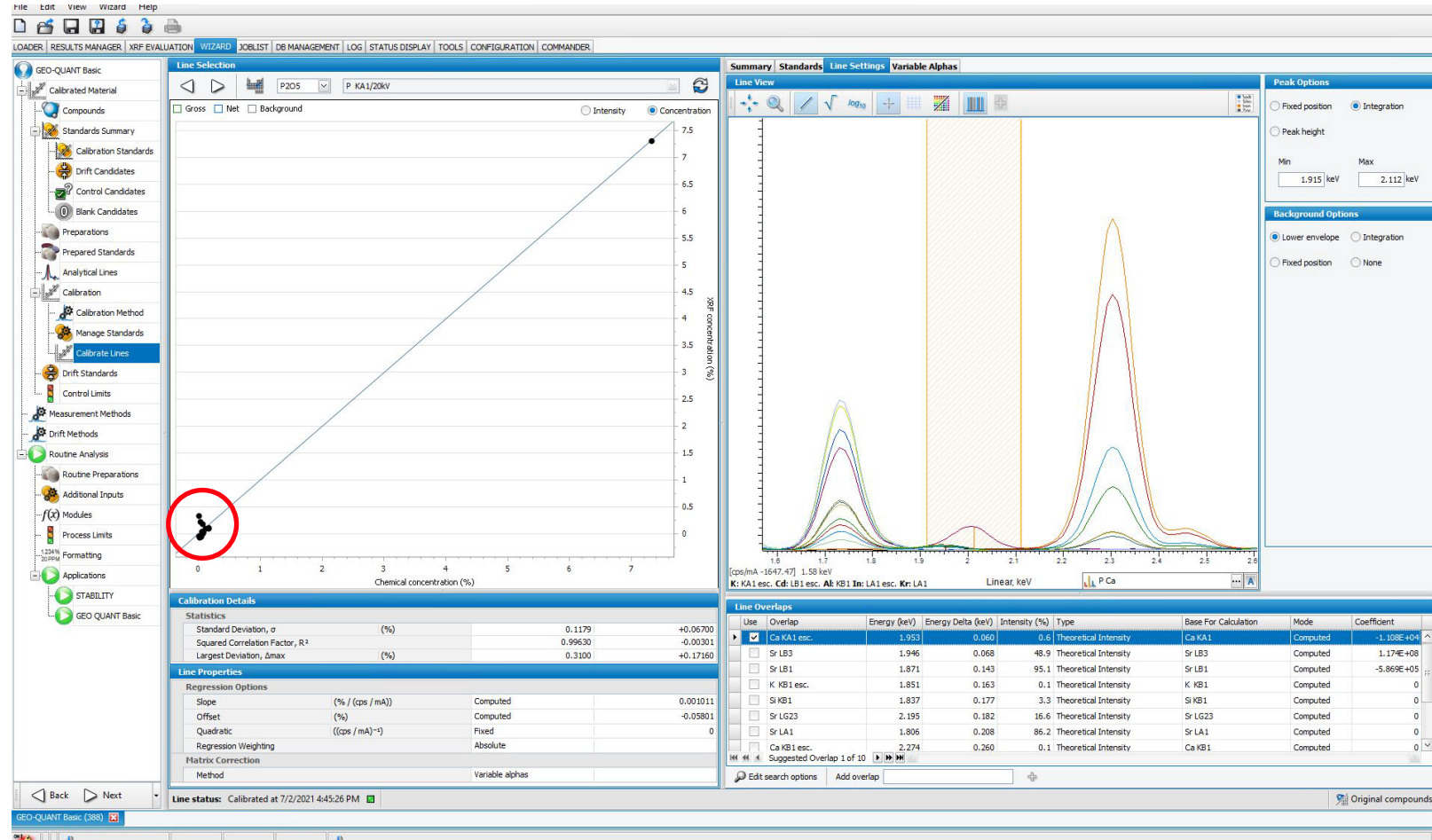


Calibration example

Smart overlap correction

Examples 1: P205 in geo-materials

- Poor correlation if all potential overlaps are unchecked ($R^2 = 0.944$)
- Significant improvement if Ca KA1 escape peak overlap correction is applied ($R^2 = 0.996$)

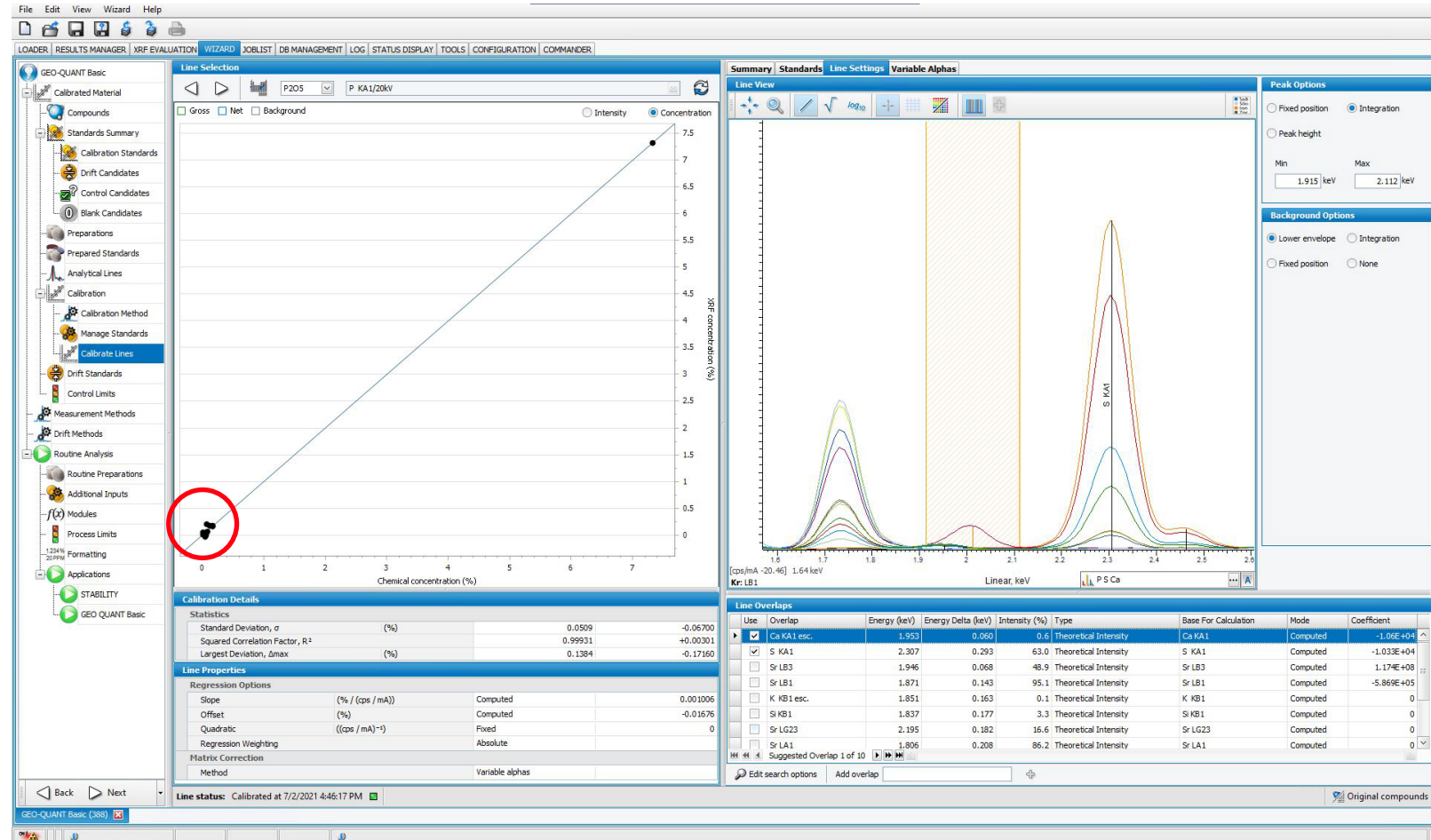


Calibration example

Smart overlap correction

Examples 1: P205 in geo-materials

- Poor correlation if all potential overlaps are unchecked ($R^2 = 0.944$)
- Significant improvement if Ca KA1 escape peak overlap correction is applied ($R^2 = 0.996$)
- Further improvement if S KA1 is considered ($R^2 = 0.999$)

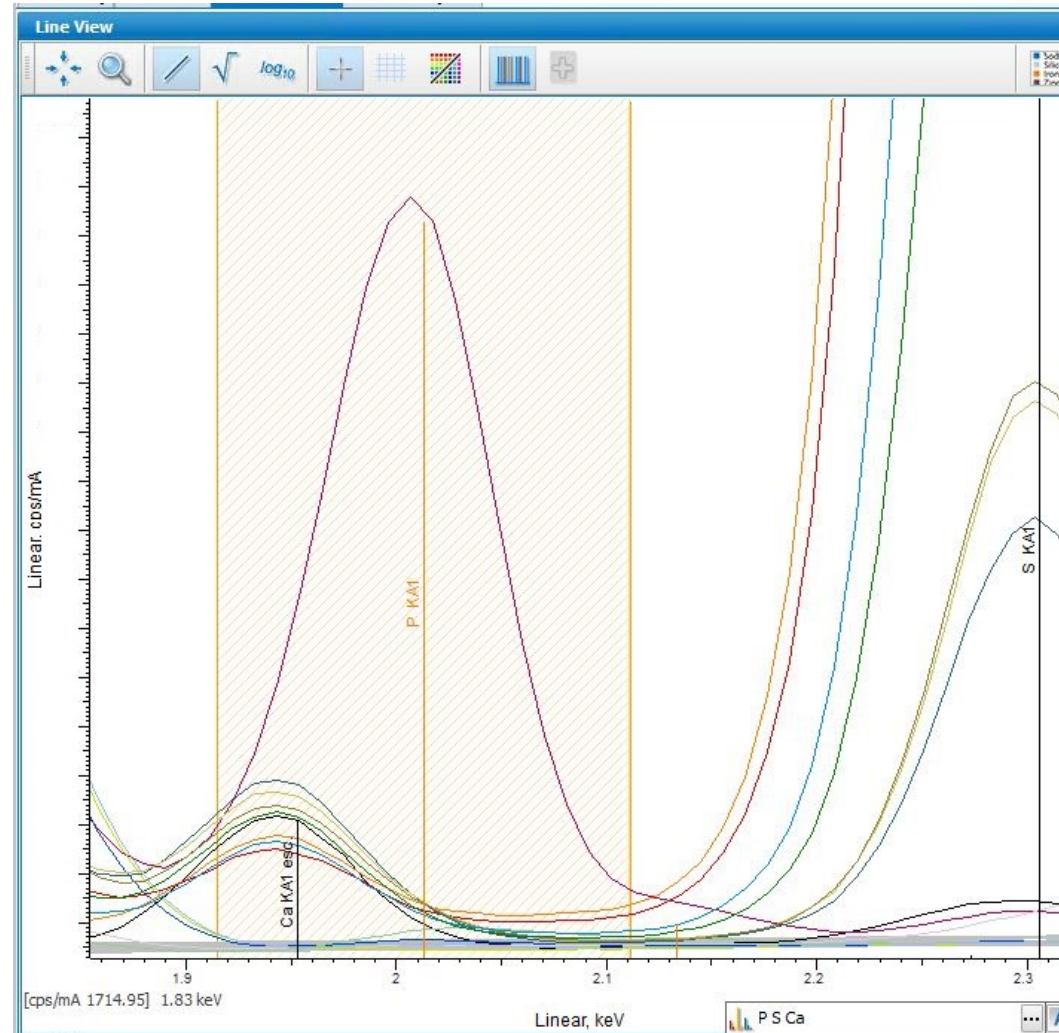


Calibration example

Smart overlap correction

Examples 1: P205 in geo-materials

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Setting Control Limits

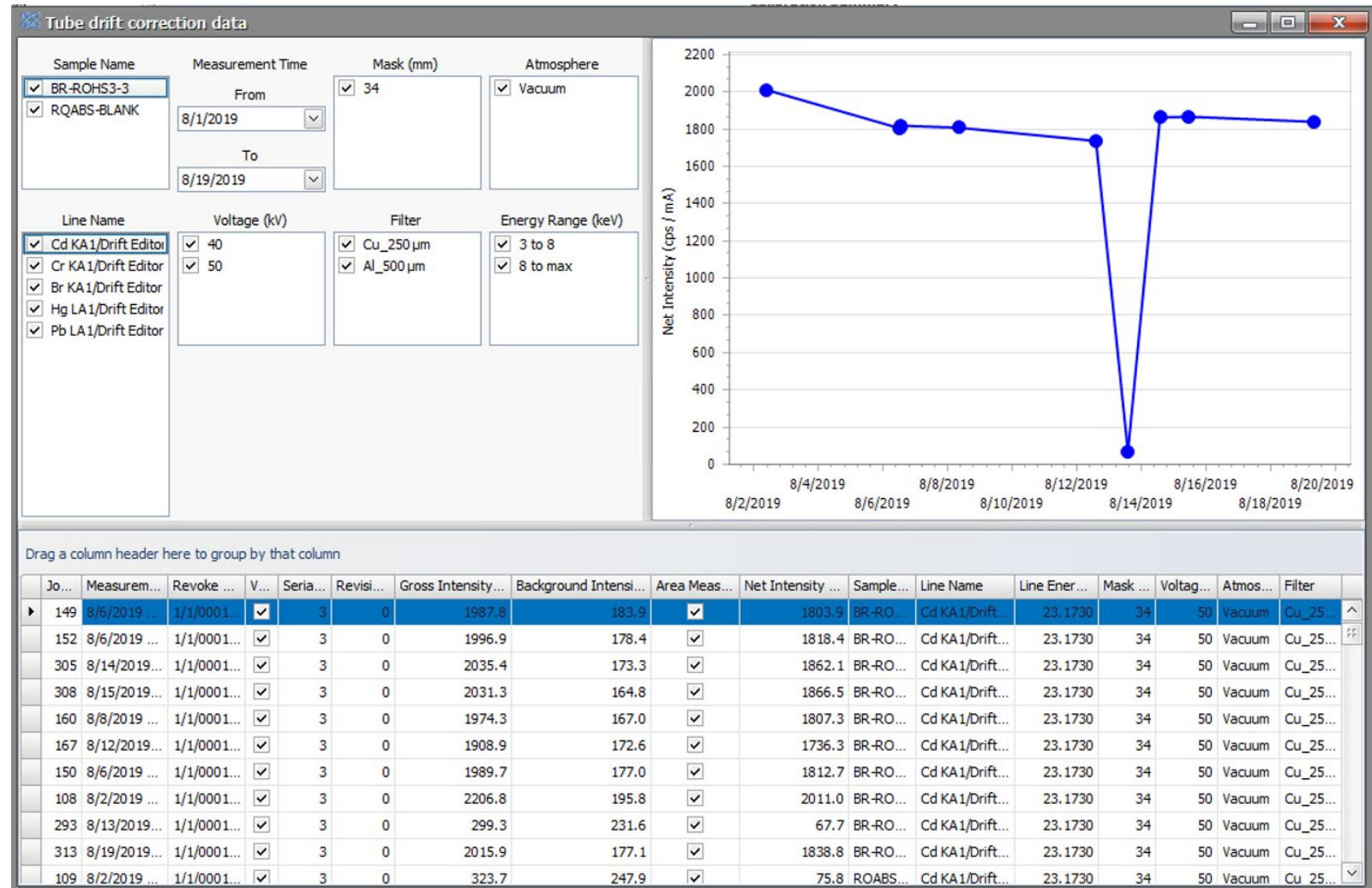
- Setup color-coded control limits for allow a quick decision during production, e.g.:
 - **Normal** → all good
 - **Warning** → production can continue but a closer look or re-analysis may be needed
 - **Alarm** → immediate production stop

Control Standards		Concentration Limits						
Use	Standard Name	Compound Name	Alarm Low	Warning Low	Nominal	Warning High	Alarm ...	Thresholds
<input checked="" type="checkbox"/>	Control sample	Silicon Oxide	25.41 %	26.22 %	26.75 %	27.29 %	28.09 %	<input type="text"/> <input type="text"/> Absolute Value
		Aluminum Oxide	6.62 %	6.83 %	6.97 %	7.11 %	7.32 %	<input type="text"/> <input type="text"/> Absolute Value
		Iron Oxide	1.97 %	2.03 %	2.07 %	2.11 %	2.17 %	<input type="text"/> <input type="text"/> Absolute Value
		Calcium Oxide	55.01 %	56.75 %	57.91 %	59.07 %	60.81 %	<input type="text"/> <input type="text"/> Absolute Value
		Magnesium Oxide	1.25 %	1.29 %	1.32 %	1.35 %	1.39 %	<input type="text"/> <input type="text"/> Absolute Value
		Sulfur Oxide	2.96 %	3.06 %	3.12 %	3.18 %	3.28 %	<input type="text"/> <input type="text"/> Absolute Value
		Sodium Oxide	0.45 %	0.46 %	0.47 %	0.48 %	0.49 %	<input type="text"/> <input type="text"/> Absolute Value
		Potassium Oxide	1.17 %	1.21 %	1.23 %	1.25 %	1.29 %	<input type="text"/> <input type="text"/> Absolute Value
		<input type="text"/>						<input type="text"/> <input type="text"/> Absolute Value

Create/Reset
 Set Limits ...
 Remove Values

New drift monitor

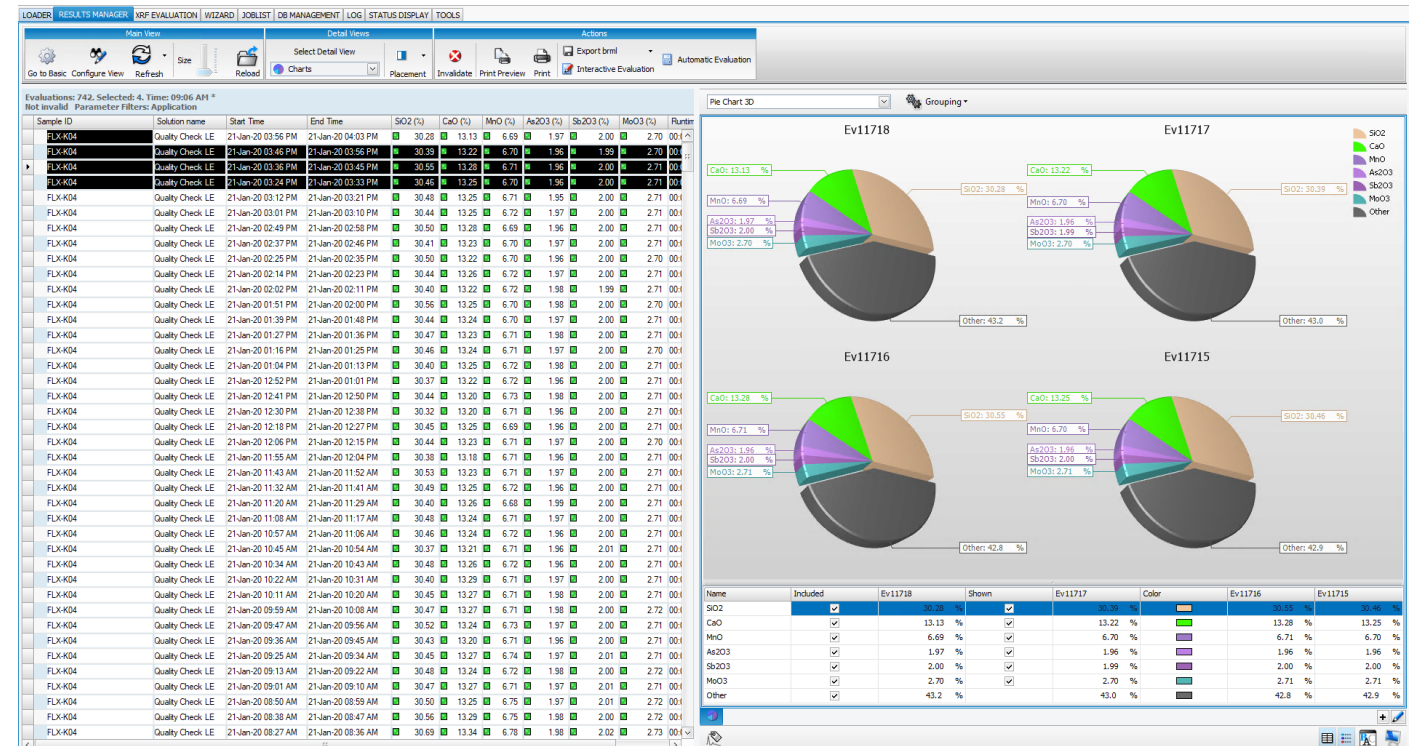
- Possible Reasons for a **Warning/Alarm**:
 - Material out of spec
 - Contamination
 - Check spectra for untypical features / element ratios
 - Broken sample
 - Check camera image / sample
 - Instrument drift
 - Use drift standards and the new **drift monitor** to quickly evaluate your system.



Customize your views and reports



- Basic and Advanced Mode allows you to focus on the key information during routine operation and switch quickly to the details of interest in case further evaluation is needed.



NEW SOFTWARE FUNCTIONALITY

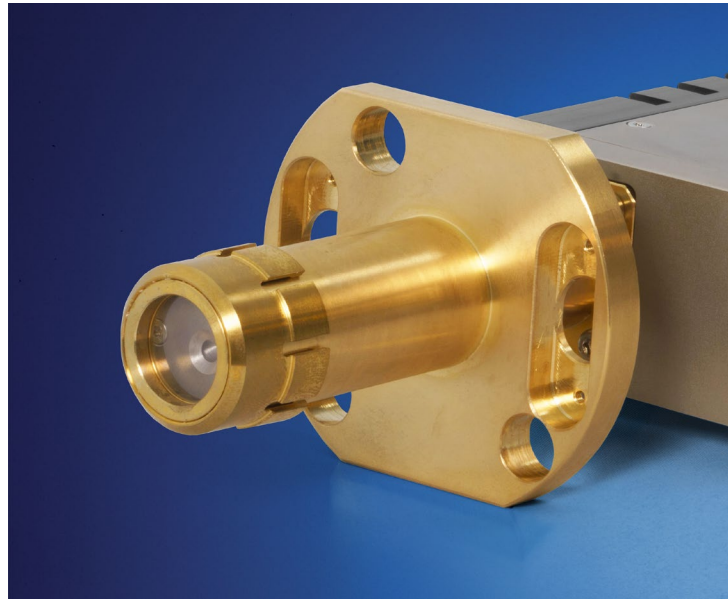
Latest Features

HighSense™ XP Detector

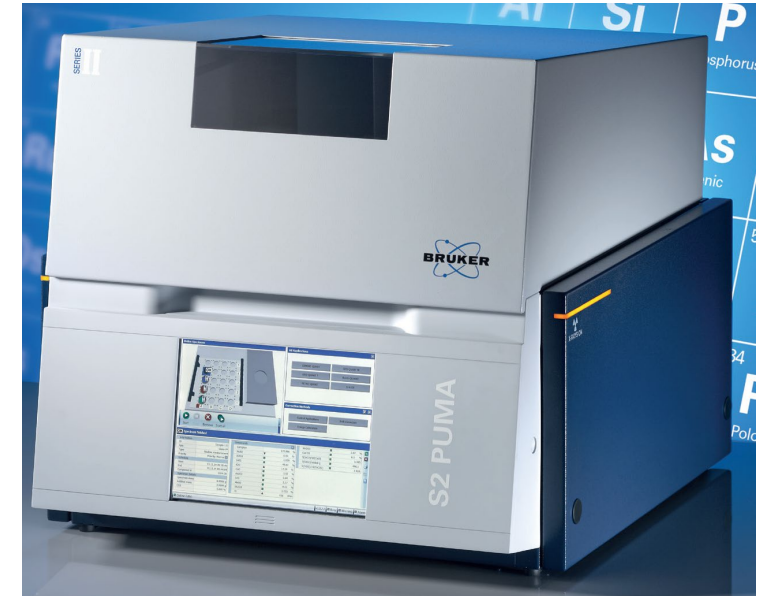
Now available for the S2 PUMA Series 2

State-of-the-Art Hardware & Next Generation Software

- New premium detector for all elements (C to Am)
- Robust, high transmission Graphene window (non-toxic)
- Bruker's detector chip technology
- Further enhanced cooling (Peltier) performance
- New SPECTRA.ELEMENTS with Dynamic Detector Profiling



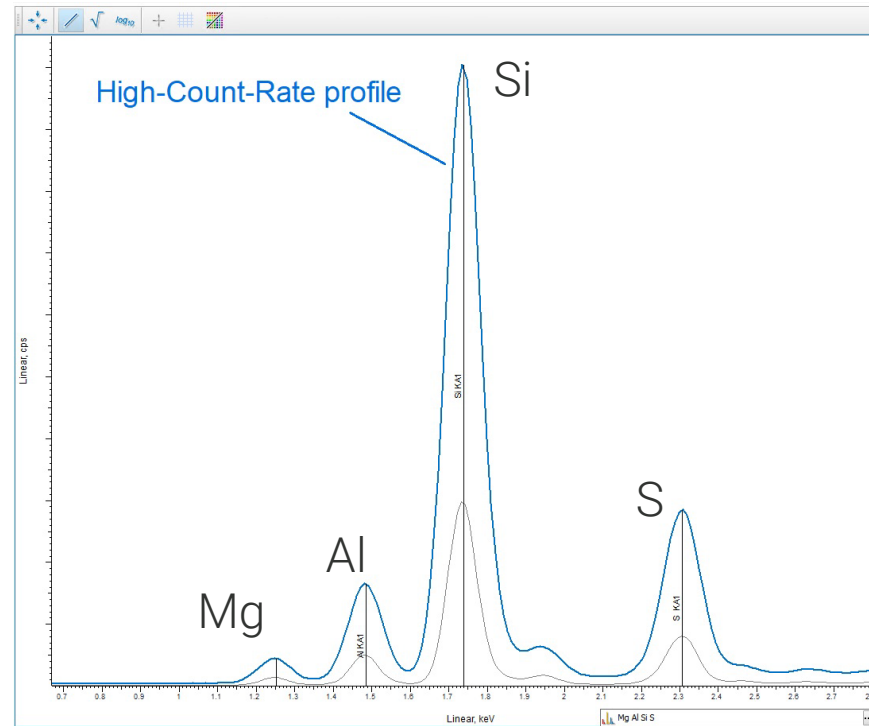
New HighSense XP Detector



S2 PUMA Series 2 with XY Autochanger

The Benefits of Detector Profiling

- New, fully integrated feature in SPECTRA.ELEMENTS
- Flexible: Make your selection each analytical range
 - **High Resolution** for optimal peak separation of neighboring elements
 - **High-Count-Rate** to boost the throughput or decrease LLD



SPECTRA.ELEMENTS

Easy. Fast. Smart. Powerful.

Achieve up to 4 x higher net intensity with the High-Count-Rate profile

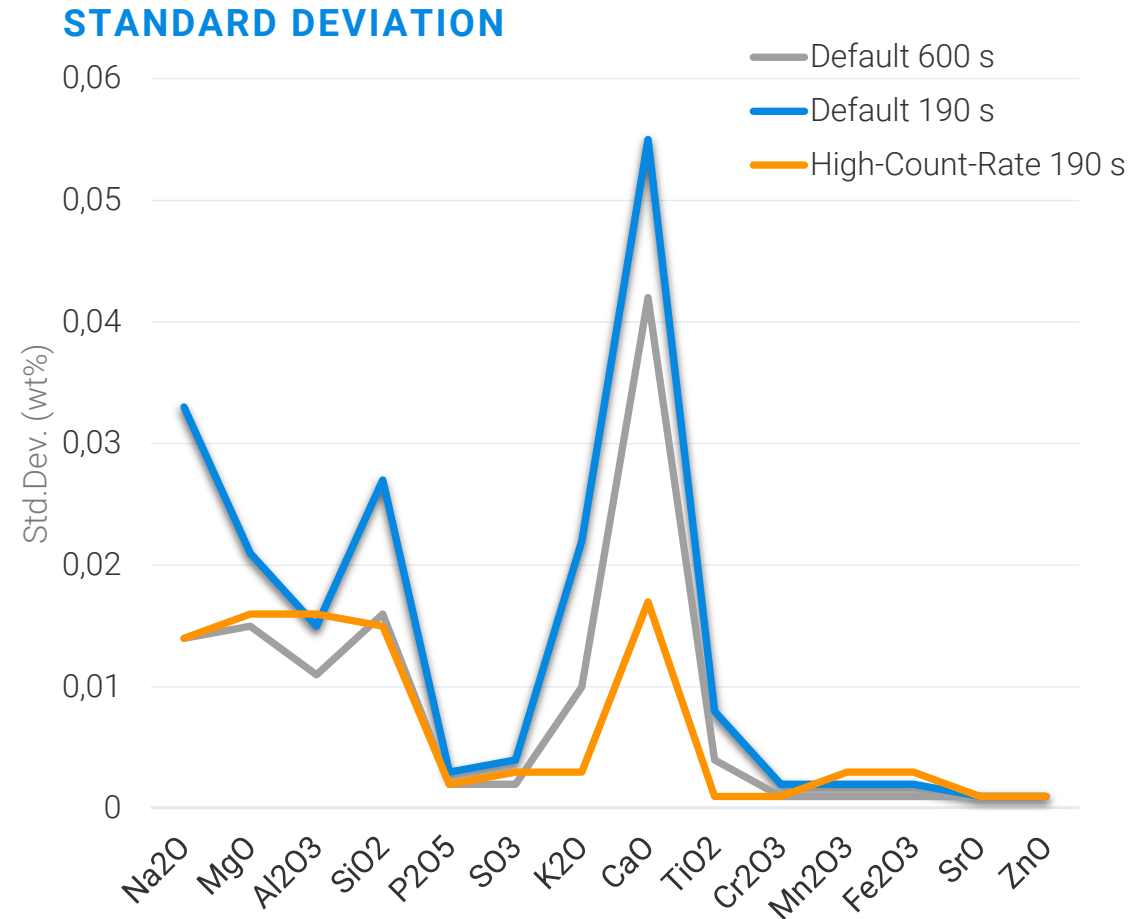
→ Enhance the performance for heavy trace elements in polymers

The Benefits of Detector Profiling

Precision Test

- Cement QC sample
- 3 ranges, 190 or 600 s total counting time, 25 repetitions

The [High-Count-Rate](#) setting allows to reduce the counting time factor of ~3

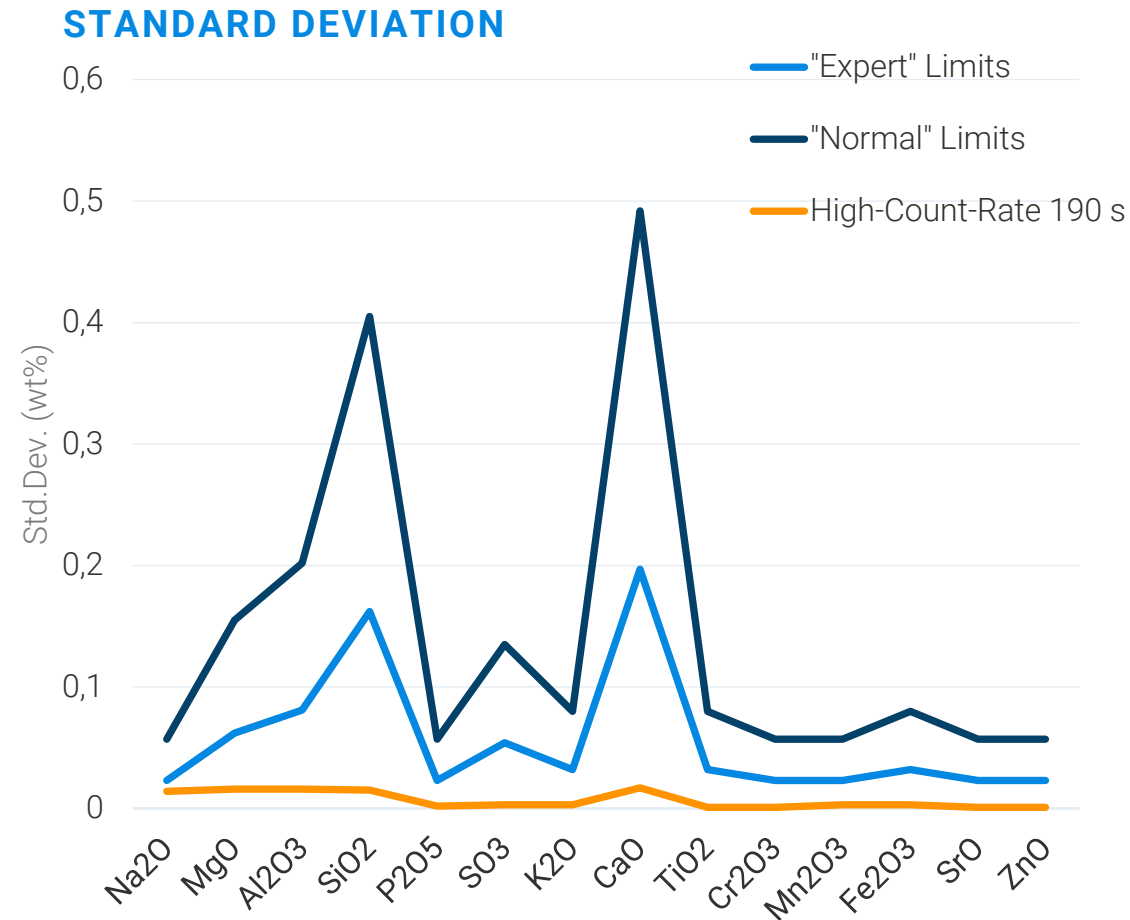


The Benefits of Detector Profiling

ISO 29581 / EN 196-2:

A Cement norm which defines two categories of precision (repeatability) :
“Normal” and “Expert”

- The S2 PUMA Series 2 with HighSense XP meets standard deviation limits easily.

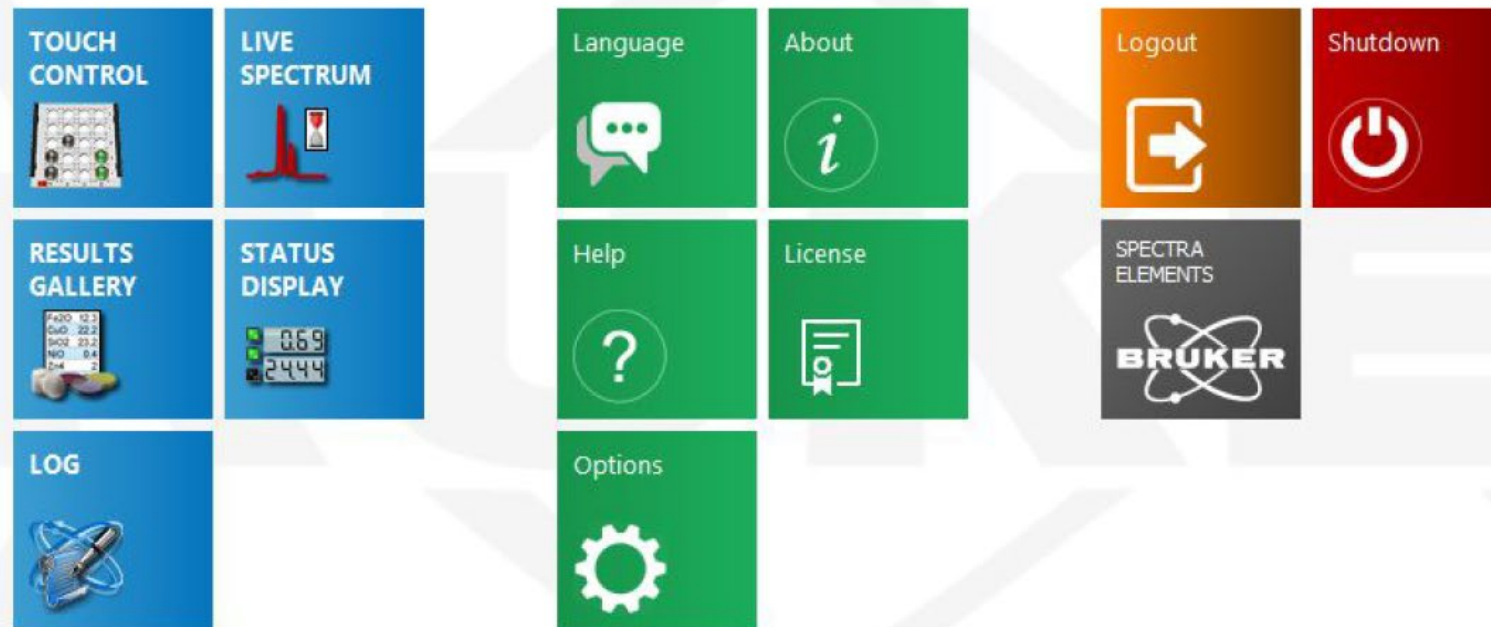


NEW SOFTWARE FUNCTIONALITY

Routine Analysis

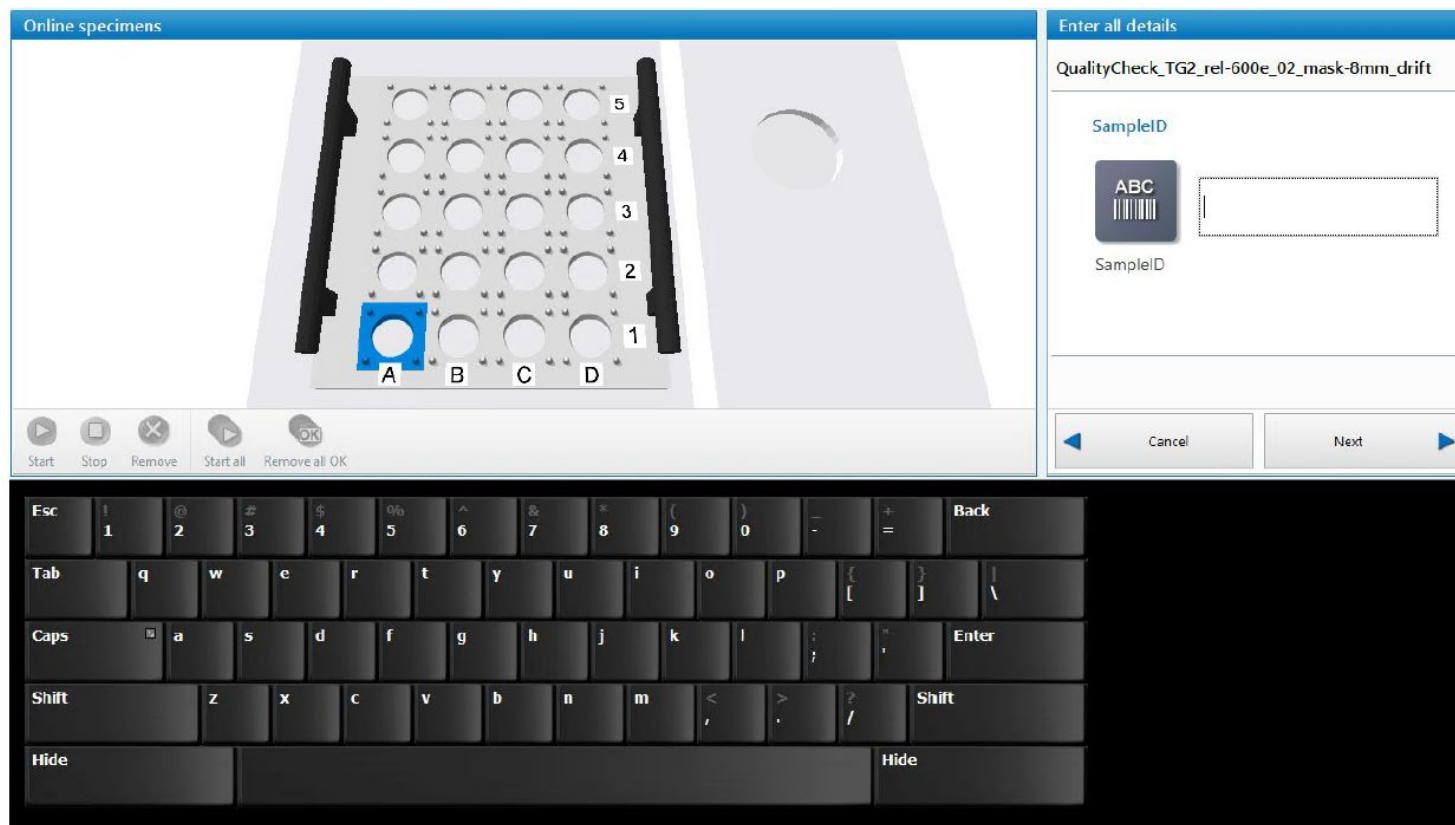
Daily Operation made easy!

TouchControl – Home Screen



Daily Operation made easy!

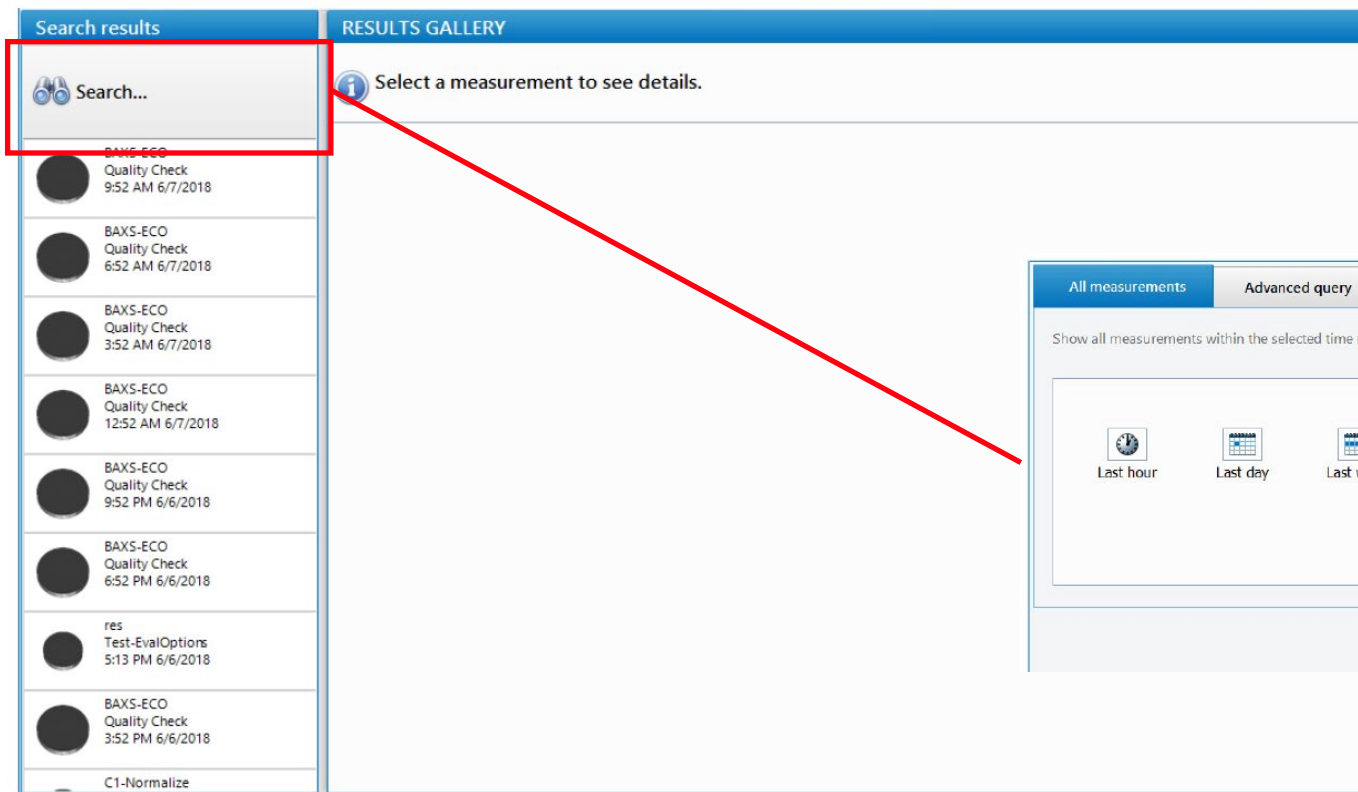
TouchControl – LOADER



- Select a position on the LOADER
- Select the method
- Enter the sample ID
- Enter method specific sample information (e.g., LOI)
- Hit start!
- Get the results within minutes!
- Remain fully flexible: Stop, modify, adjust priority ...

Daily Operation made easy!

Results Gallery



Search results

RESULTS GALLERY

Select a measurement to see details.

Search...

BAXS-ECO
Quality Check
9:52 AM 6/7/2018

BAXS-ECO
Quality Check
6:52 AM 6/7/2018

BAXS-ECO
Quality Check
3:52 AM 6/7/2018

BAXS-ECO
Quality Check
12:52 AM 6/7/2018

BAXS-ECO
Quality Check
9:52 PM 6/6/2018

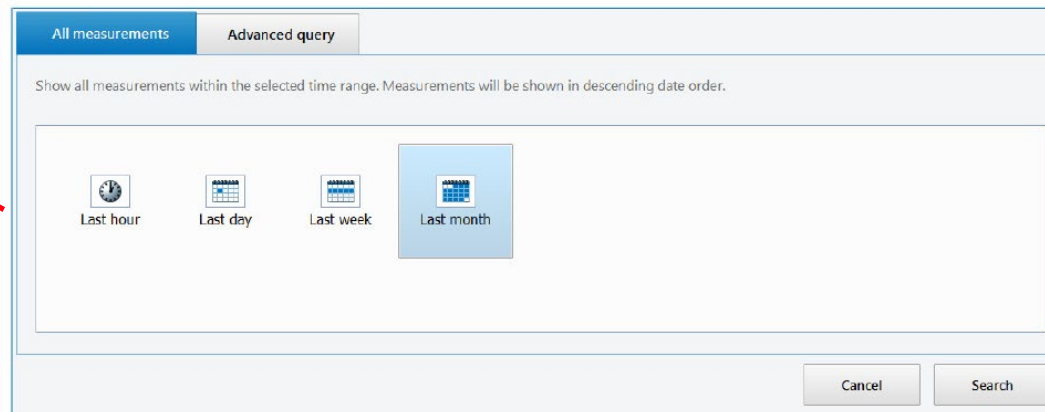
BAXS-ECO
Quality Check
6:52 PM 6/6/2018

res
Test-EvalOptions
5:13 PM 6/6/2018

BAXS-ECO
Quality Check
3:52 PM 6/6/2018

C1-Normalize

- Intuitive search functions provide easy and fast access to your database



All measurements | Advanced query

Show all measurements within the selected time range. Measurements will be shown in descending date order.

Last hour | Last day | Last week | Last month

Cancel | Search

Daily Operation made easy!

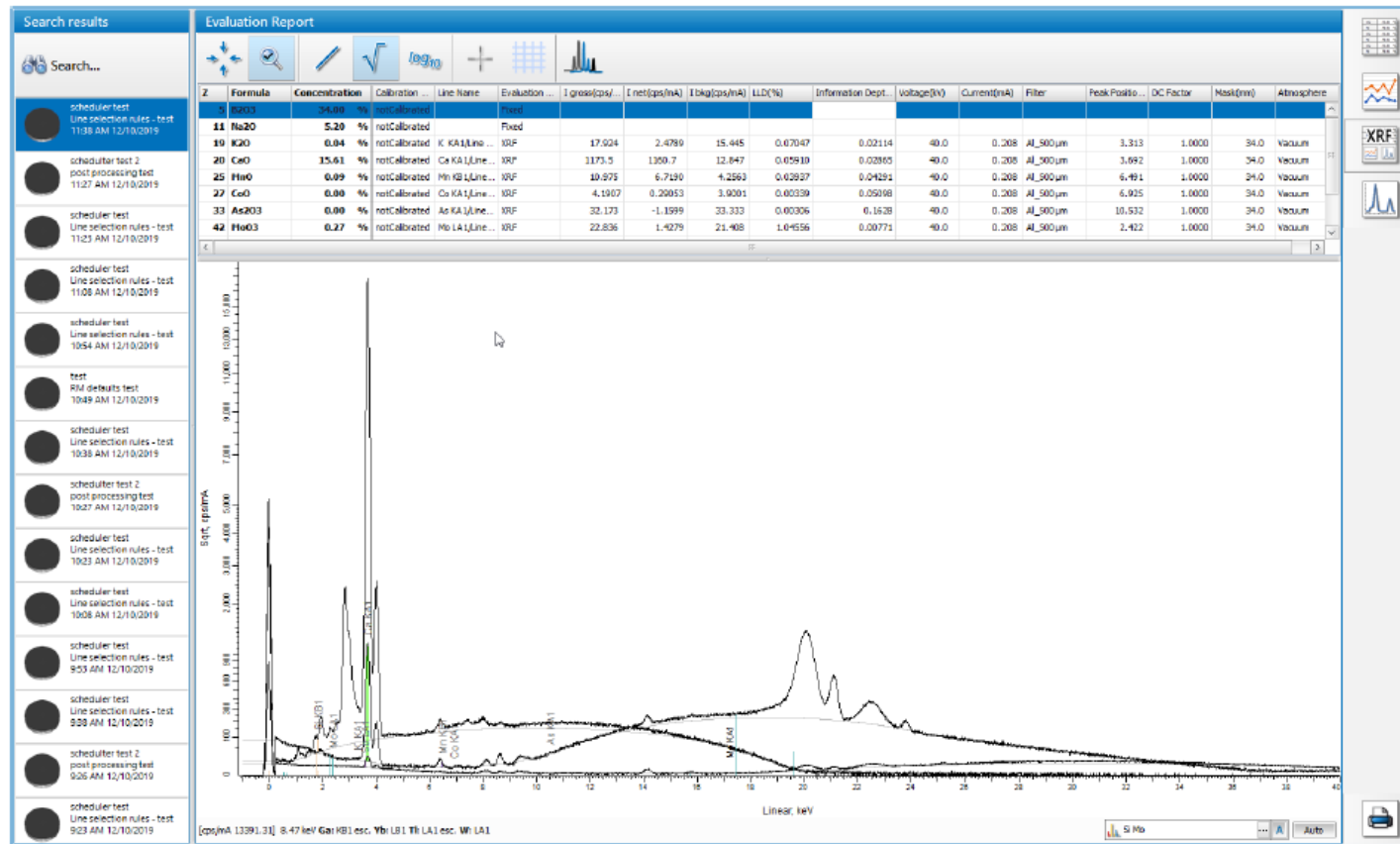
Results Gallery



- All information at your fingertips
- Quick access to statistics to monitor the production process
- Color coding based on customized concentration limits

Daily Operation made easy!

Results Gallery



- Check the results
- Evaluate and compare spectra (zoom-in, add labels/lines, ...)
- Print/export the data

NEW SOFTWARE FUNCTIONALITY

Standardless Solutions

SMART-QUANT FP and WD

Best standardless analysis with EDXRF and WDXRF

SMART-QUANT is set up to work in full Fundamental Parameter (FP) mode – this means no calibrations necessary!

Excellent for raw material testing and whenever special samples outside the analytical routing need to be measured.

- F to Am (FP) / Na to Am (WD)
- ppm to 100%
- Air, Helium, Vacuum
- 30 and 50 kV



SMART-QUANT: Push-button solution for quick and reliable analysis of unknown samples

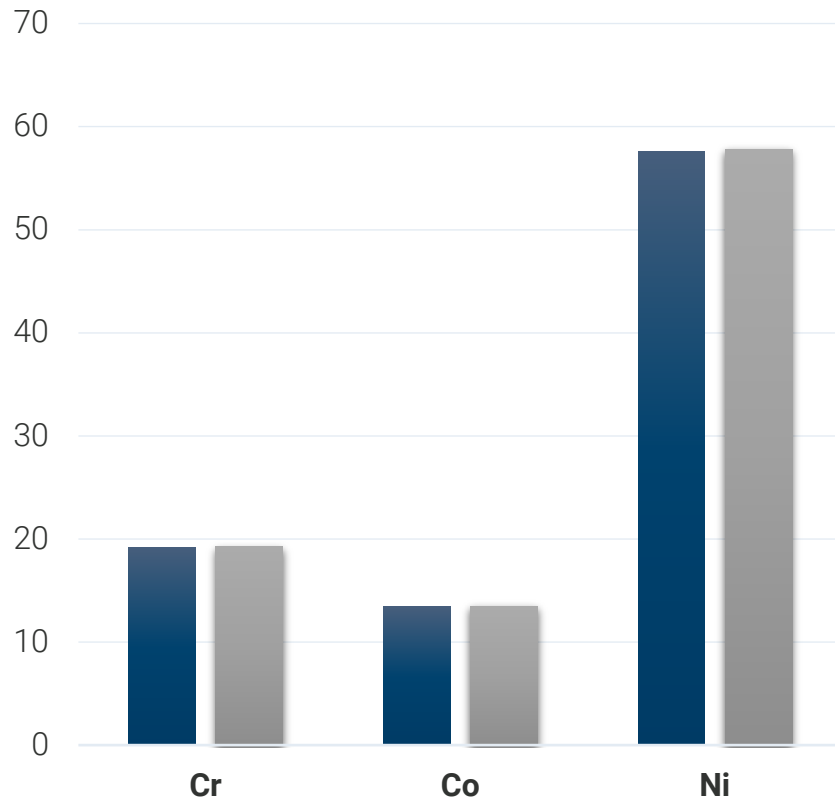


S6 JAGUAR: Full WDXRF performance in a benchtop unit

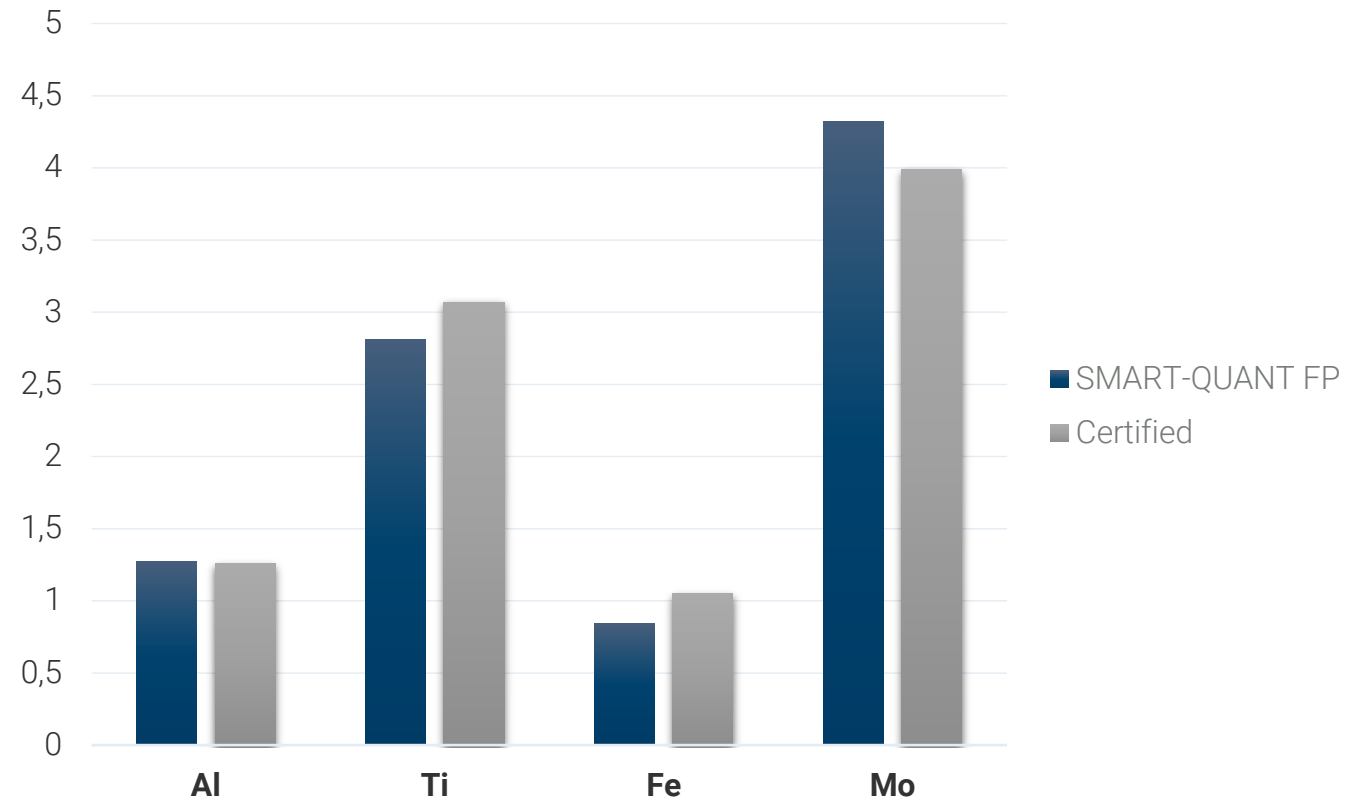
SMART-QUANT FP

Powered by HighSense XP

MAJOR ELEMENTS



MINOR ELEMENTS

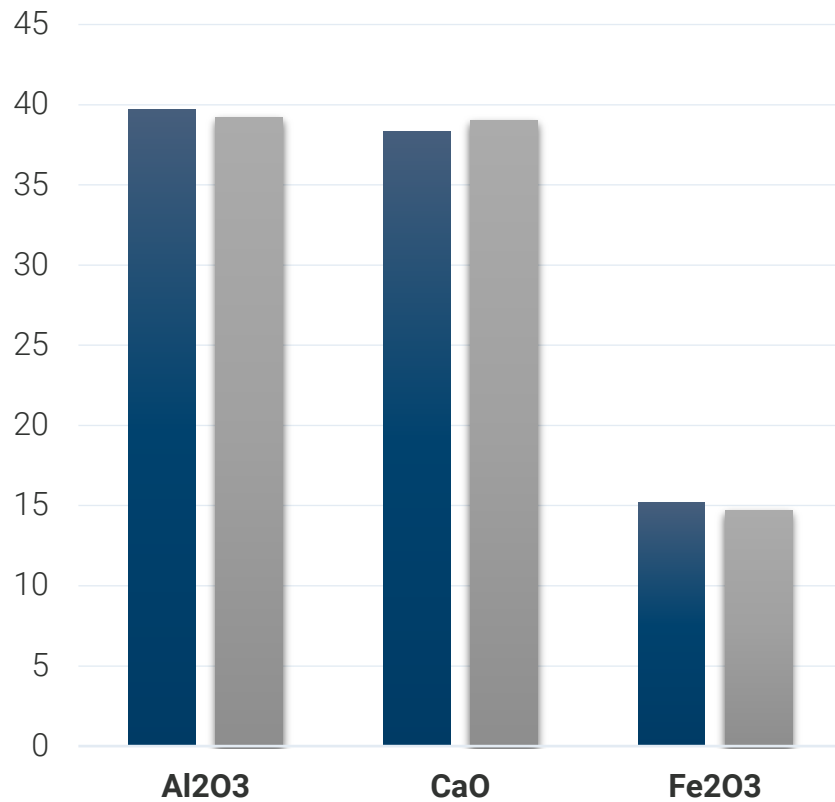


Nickel Alloy – Waspaloy, concentrations in wt%

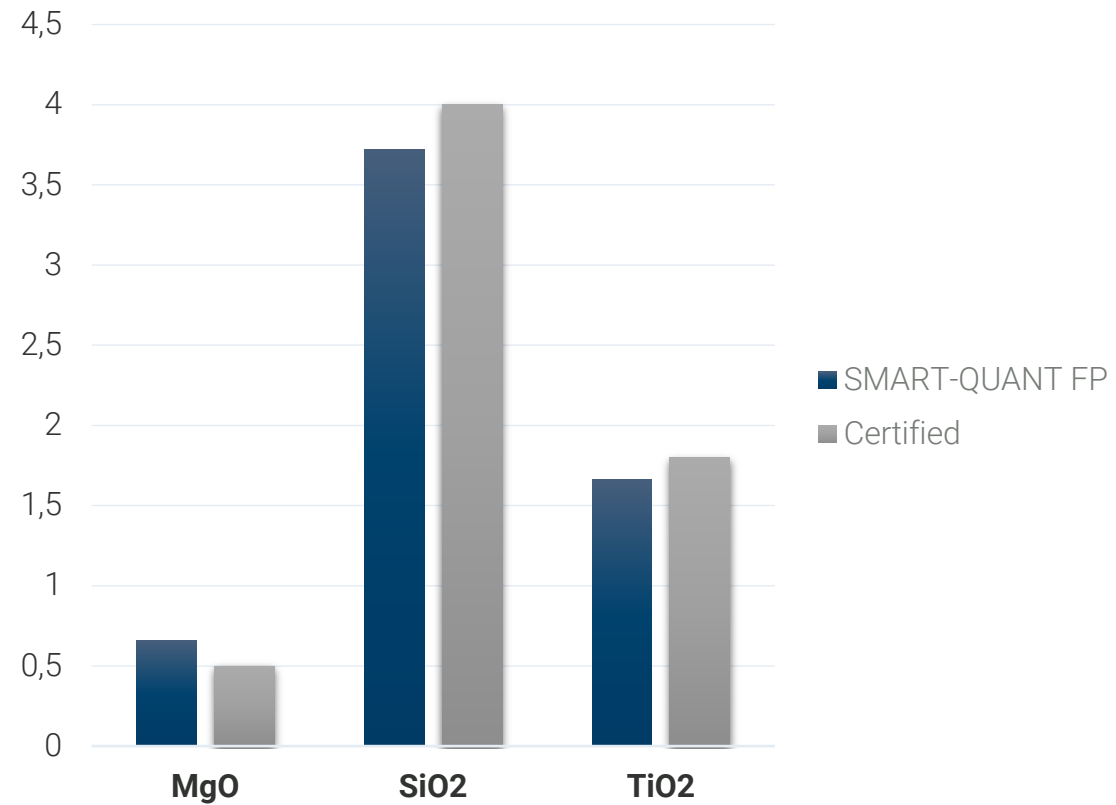
SMART-QUANT FP

Powered by HighSense XP

MAJOR ELEMENTS



MINOR ELEMENTS



High Al Cement, concentrations in wt%

Elemental Analysis: Pharma & Cosmetics

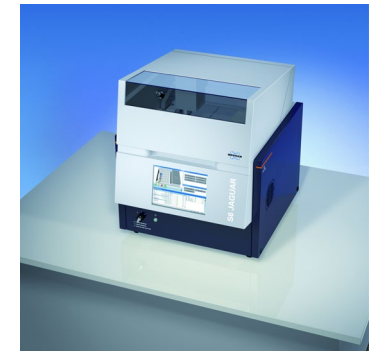
- Strict regulations apply to ensure the quality of resulting medications and other products. This makes reliable and precise analysis inevitable.
- XRF is particularly suitable for
 - quick verification of incoming **raw material**
 - at-line production monitoring (Process Analytical Technology, **PAT**)
 - foreign body identification (**FBI**), and
 - **heavy metal impurity** analysis.
- **Cosmetic** and personal care products must meet high product quality standards due to their applications.



Elemental Analysis: Pharma & Cosmetics

21 CFR Part 11-compliance

- SPECTRA.ELEMENTS is fully compliant
 - The Part 11 features are smoothly integrated to ensure ease-of-use and worry-free operation – being always prepared for the next audit
- *Key features:*
 - Audit trailing
 - Electronic signatures / validation
 - Dedicated user levels
 - Customizable views



Elemental Analysis: Pharma & Cosmetics

IQ/OQ Documentation and Support

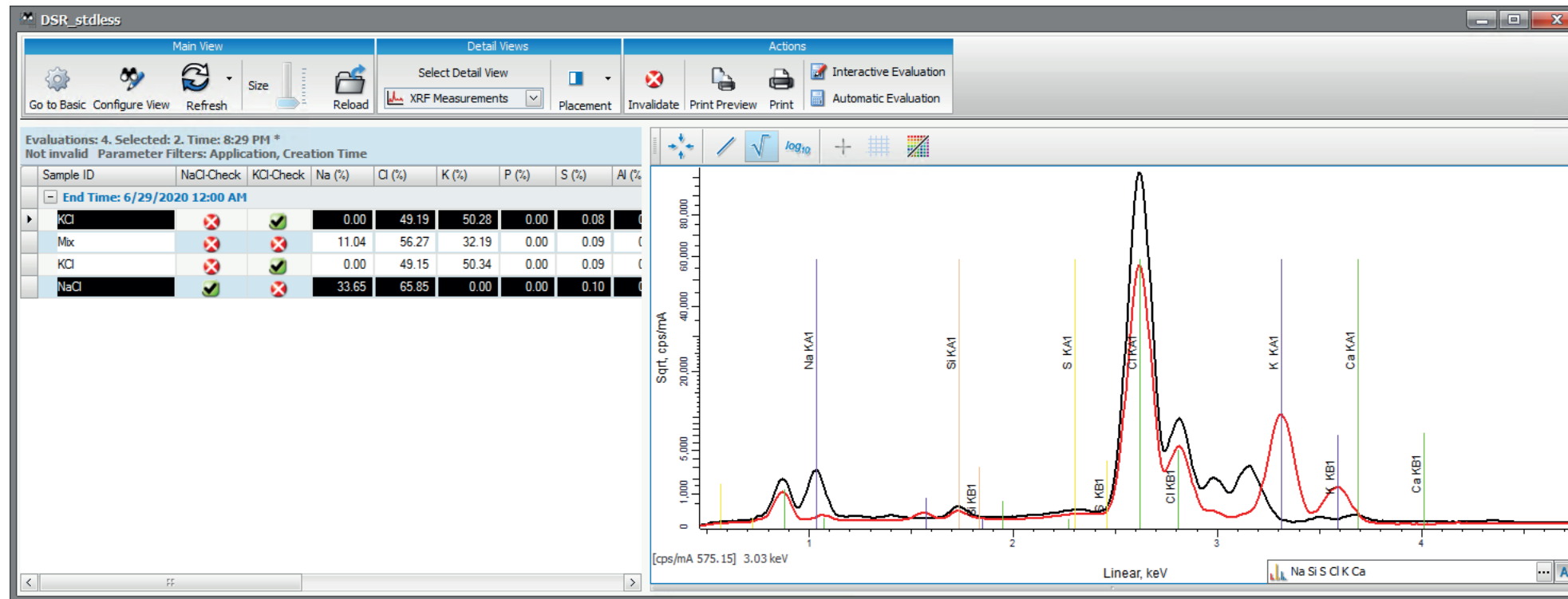
- **Installation Qualification:** Establishes that the instrument is received as designed and specified and that it is properly installed
- **Operation Qualification:** Demonstrates that the instrument will function according to the operational specifications (acceptance testing).
- **IQ/OQ:** Performed together with our Part 11 trained Service Engineer



SMART-QUANT FP

Elemental Analysis: Pharma & Cosmetics

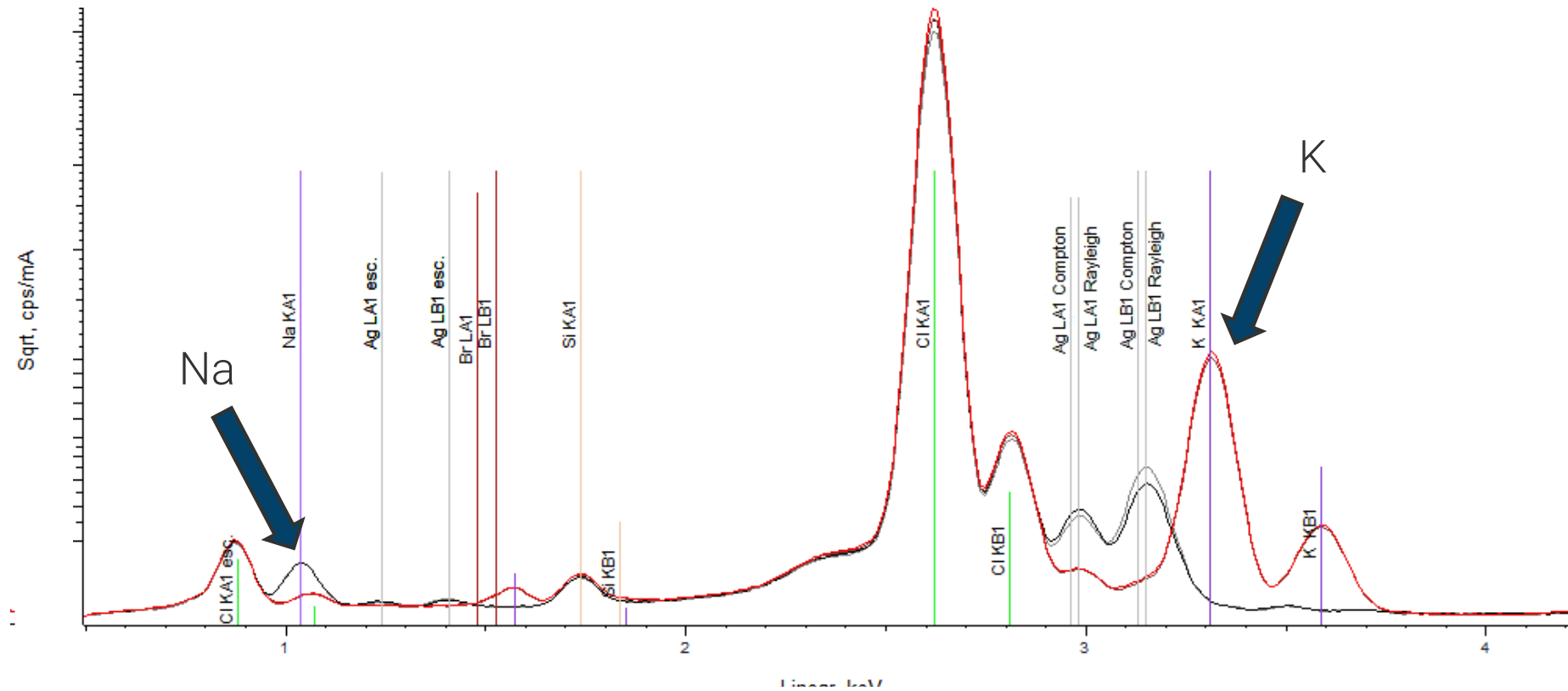
- Customizable concentration thresholds and configurable views allow to make a quick decision (reject or accept)



SMART-QUANT FP

Elemental Analysis: Pharma & Cosmetics

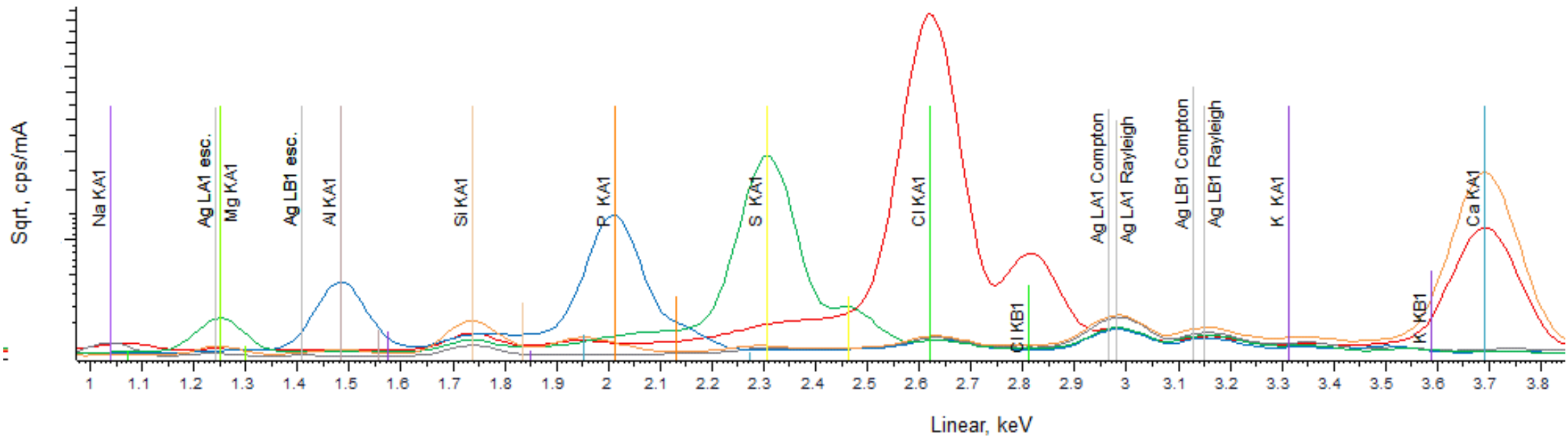
- Differentiate quickly between **KCl** and NaCl



SMART-QUANT FP

Elemental Analysis: Pharma & Cosmetics

- Differentiate quickly between CaCl_2 , MgSO_4 , AlPO_4 , and CaCO_3

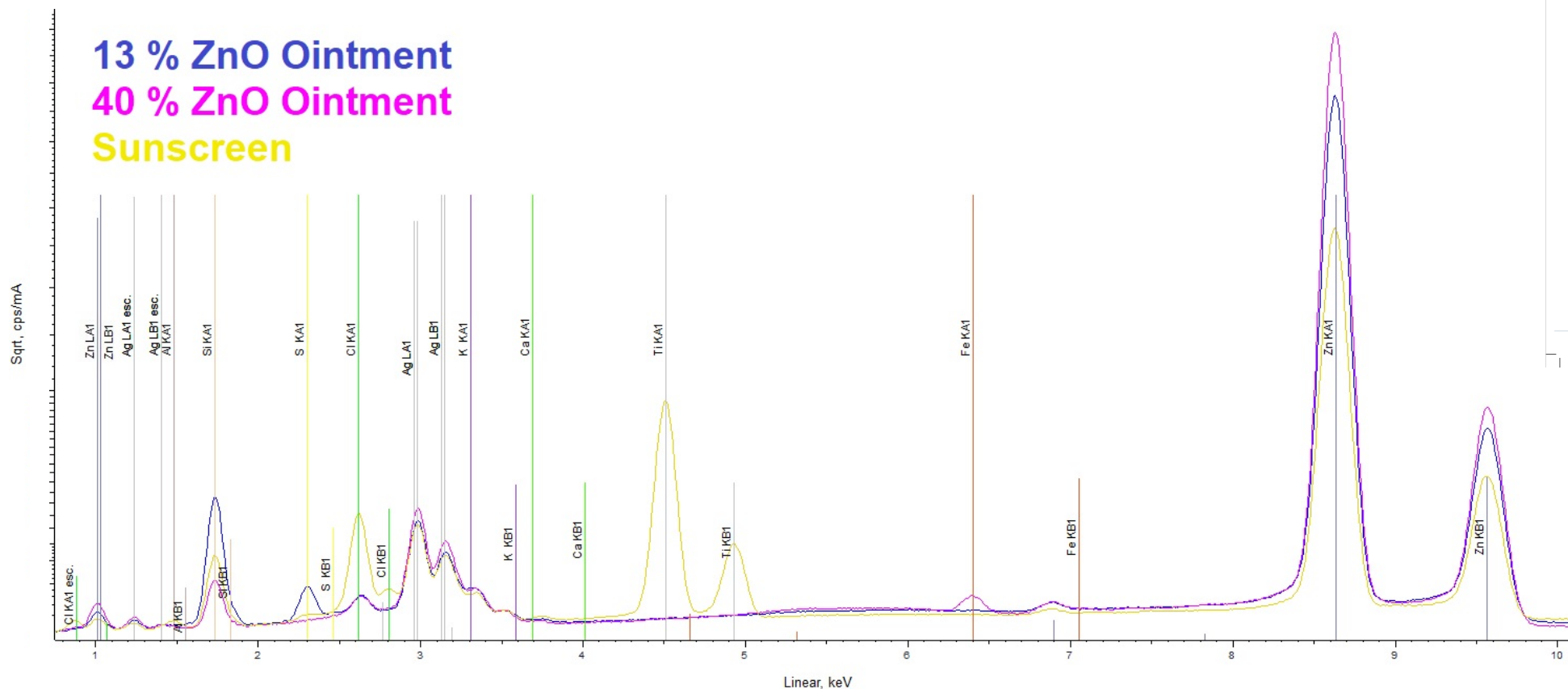


SMART-QUANT FP

Elemental Analysis: Pharma & Cosmetics



- Identify material based on ZnO and/or TiO₂ contents, without providing information about the matrix



Lab Report XRF 174
S2 PUMA Series 2

Material ID and production monitoring made easy and fast

Quick and reliable identification as well as purity verification of raw materials used to formulate pharmaceutical products is critical to meet stringent quality requirements and to produce efficiently. At-line monitoring of the production process to rapidly identify possible impurities is of similar importance. These are two analytical tasks where energy dispersive X-ray fluorescence (EDXRF) excels. Not only is it possible to rapidly identify substances (often in less than 2 minutes), but also the main contaminants can be determined easily. The S2 PUMA Series 2 is the optimal solution for such applications.

- XY Autochanger with 22 positions combining high throughput with flexibility.
- Direct analysis of all sample types (liquids, powders, solids, tablets) without sample preparation, SampleCare™ technology, protecting critical system components for low maintenance.
- Innovative software SPECTRA-ELEMENTS fully compliant with FDA 21 CFR Part 11.
- Sturdy design and robust, high quality components for long lifetime.
- Ergonomic TouchControl™ display for operation without PC peripherals (optional).

Innovation with Integrity

XRF

NEW SOFTWARE FUNCTIONALITY

Summary

SPECTRA.ELEMENTS

Next Generation Spectrometer Software

Faster. Smarter. Easier.

Faster operation

- Optimized hardware-software workflow
- Immediate data processing
- Smooth navigation
- Rapid access to database

Solution				Preparation		
Solution		SMART-Oxides (201)		Values	Preparation = Fused bead (ig...	
Inputs				Basis	Original sample	
	Z	Formula	Concentration	Evaluation ...	Quantified by	Range Name
▶	13	Al ₂ O ₃	1,39 %	Stdless	None	50 kV, Range 1
	14	SiO ₂	35,88 %	Stdless	None	50 kV, Range 1
	16	SO ₃	9,16 %	Stdless	None	50 kV, Range 1
	17	Cl	2,54 %	Stdless	None	50 kV, Range 1
	19	K ₂ O	0,08 %	Stdless	None	50 kV, Range 1
	21	Sc ₂ O ₃	0,03 %	Stdless	None	50 kV, Range 1
	22	TiO ₂	0,11 %	Stdless	None	50 kV, Range 1
	25	MnO	0,06 %	Stdless	None	50 kV, Range 1
	26	Fe ₂ O ₃	0,12 %	Stdless	None	50 kV, Range 1
	27	CoO	0,00 %	Stdless	None	50 kV, Range 1
	38	SrO	0,01 %	Stdless	None	50 kV, Range 1
	39	Y ₂ O ₃	0,00 %	Stdless	None	50 kV, Range 1
	41	Nb ₂ O ₅	0,00 %	Stdless	None	50 kV, Range 1
	45	Rh ₂ O ₃	0,00 %	Stdless	K	50 kV, Range 1
	82	PbO	0,00 %	Stdless	None	50 kV, Range 1
	20	CaO	50,61 %	Stdless	None	
*						

Evaluate your measurements in no time!

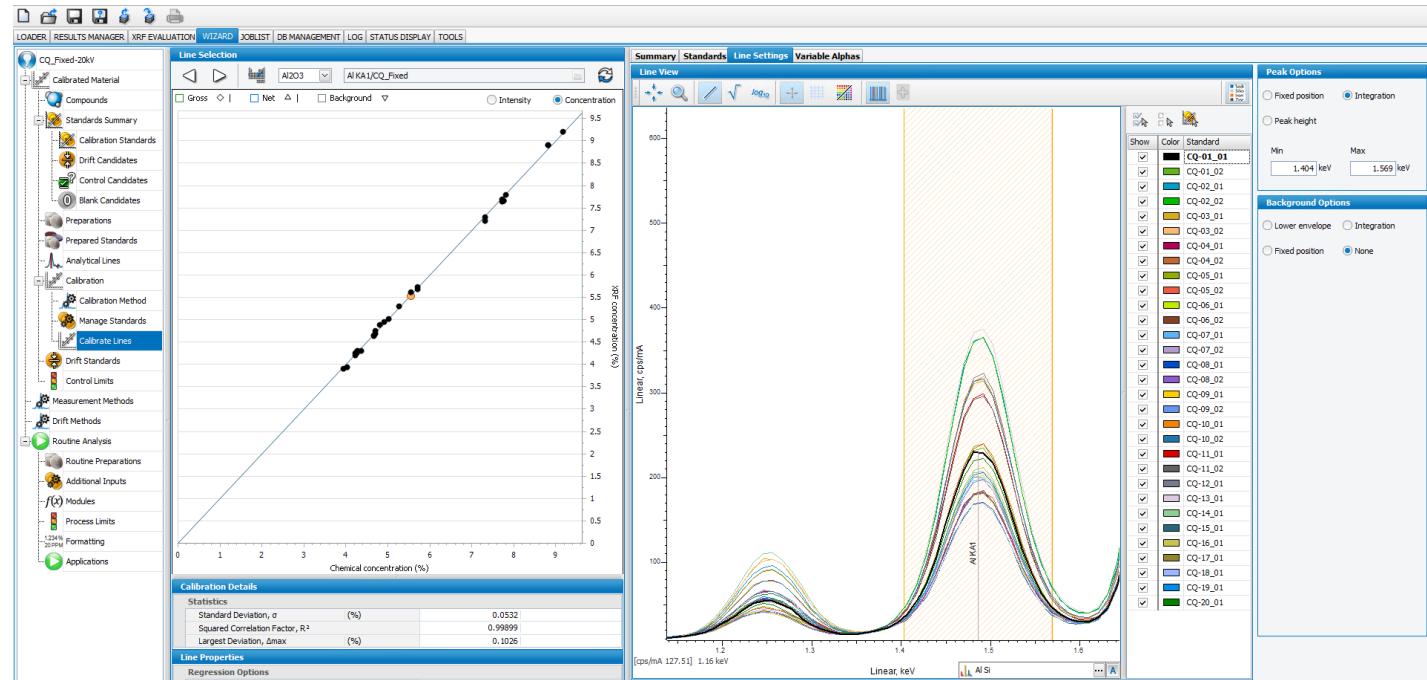
SPECTRA.ELEMENTS

Next Generation Spectrometer Software

Faster. Smarter. Easier.

Smarter features

- Dedicated User Levels
- Basic & Advanced Mode
- Detector Profiling
- Aut-O-Matrix
- Loss-Eliminated Alphas,
- Pressure compensation
- Blanks, duplicates, QC
- Post-Processing
- Automation ready



NAME	VOLTAGE (kV)	FILTER	DETECTOR PROFILE
Range 1	40	Al (500 μ)	Standard
Cu KA1/test	40	Al (500 μ)	Standard
Range 1/40kV	40	Al (500 μ)	High resolution
Zn KA1/test	40	Al (500 μ)	High resolution
Range 1/40kV/Al (5...	40	Al (500 μ)	High count rate
Ni KA1/test	40	Al (500 μ)	High count rate
			High count rate
			High resolution
			Standard

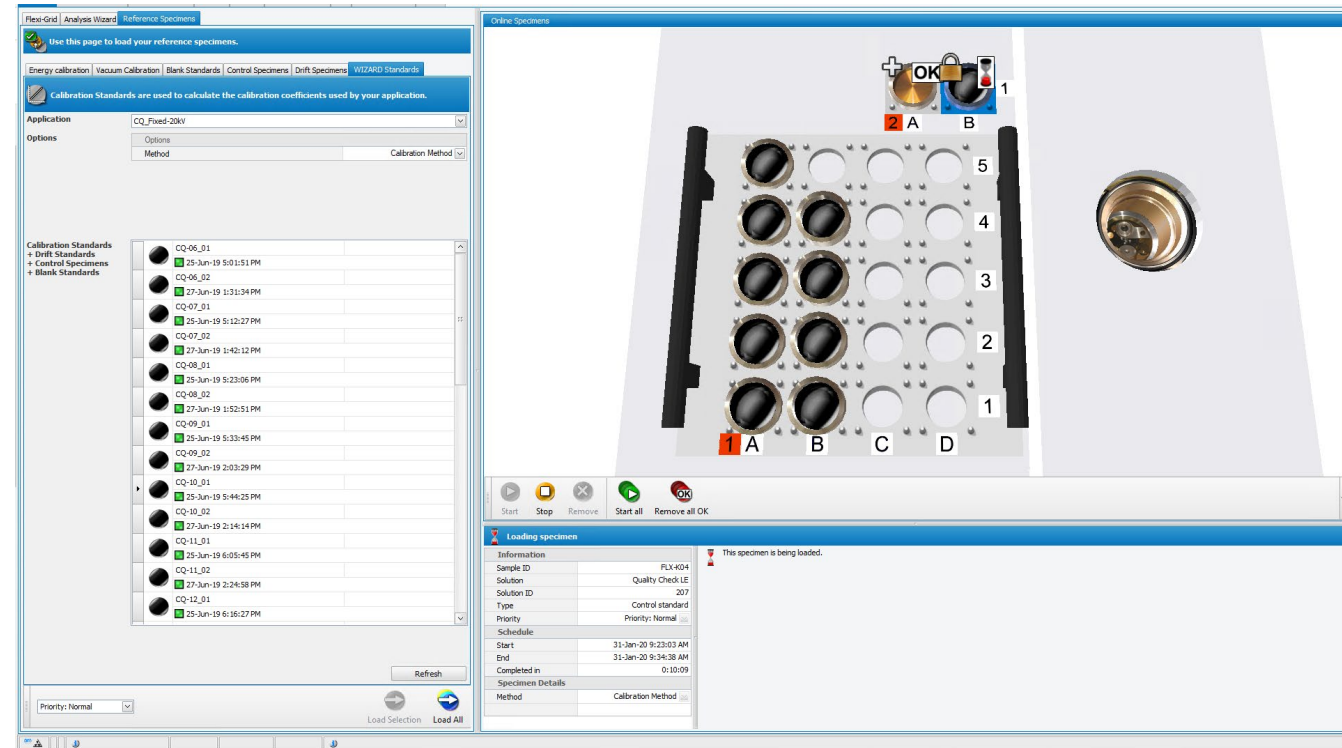
SPECTRA.ELEMENTS

Next Generation Spectrometer Software

Faster. Smarter. Easier.

Easier to use

- Quick learning with new User Interface
- Hints provide help when needed
- WIZARD: the proven tree-structure guide you through the calibration process
- LOADER: Intuitive interface for routine operation
- RESULT MANAGER: Access all your data quickly and get extended reporting



The LOADER: load / unload samples; adjust priorities; start / stop your measurements; view your results.

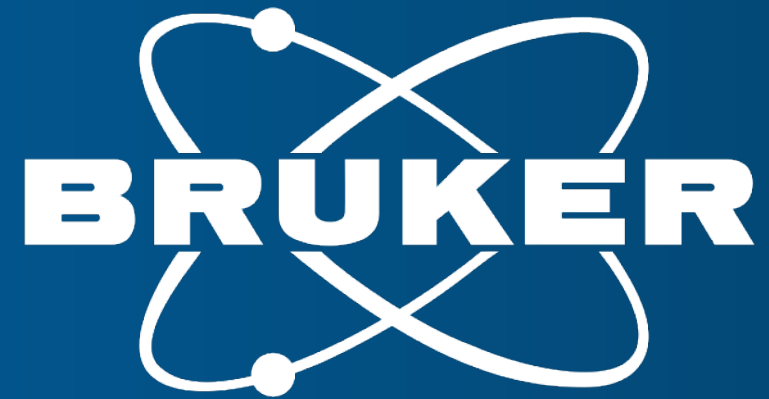
Any Questions?

Learn more about 'Feed and Pet Food Analysis'
In our 15.09.2021 webinar – Sign Up Now!

Thank you!

Kai Behrens, Frank Portala, Adrian Fiege





Innovation with Integrity