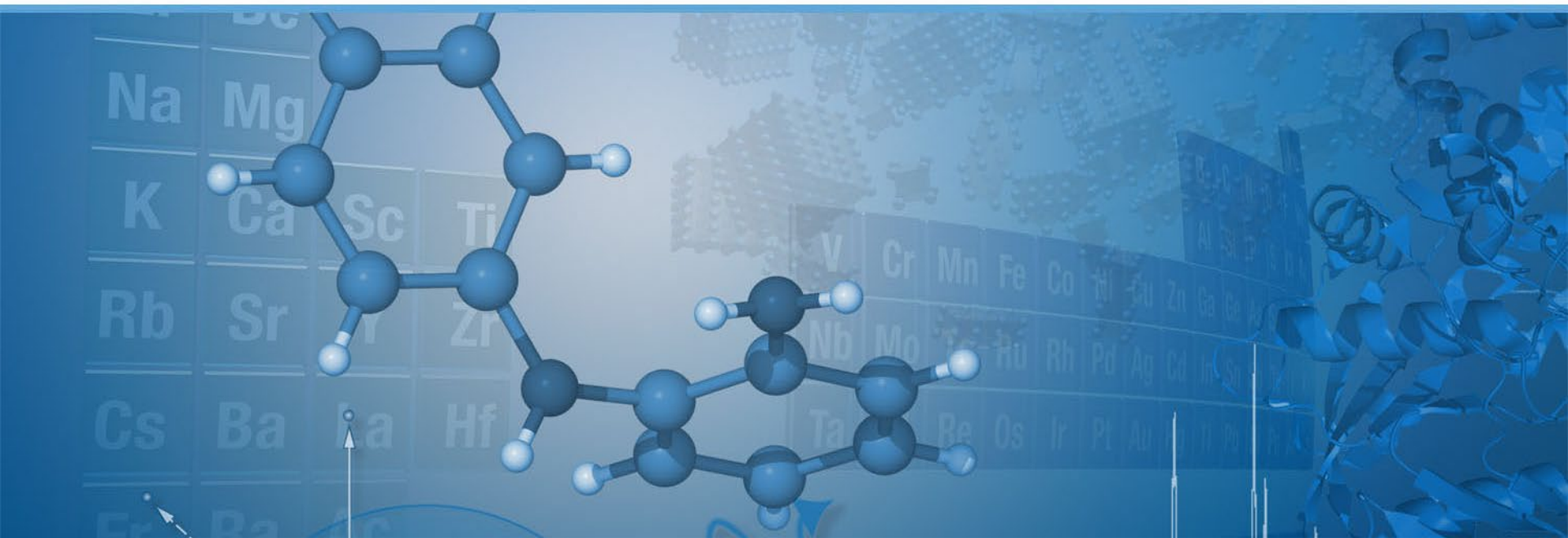


Standardlose Analyse mit SPECTRA.ELEMENTS



SMART-QUANT FP (S2 PUMA) & SMART-QUANT WD (S6 JAGUAR)



Herzlich willkommen!

Standardlose Analytik mit SMART-QUANT



1. SMART-QUANT

- Philosophie & Integration in SPECTRA.ELEMENTS
- Workflow

2. SMART-QUANT FP & WD

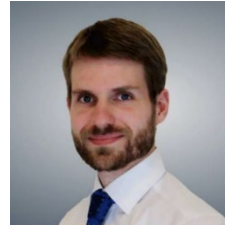
- Unterschiede

3. Beispiele

4. Software & Funktionen



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Elemental Analysis
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Dr. Adrian Fiege
Produktmanager RFA
Karlsruhe, Deutschland

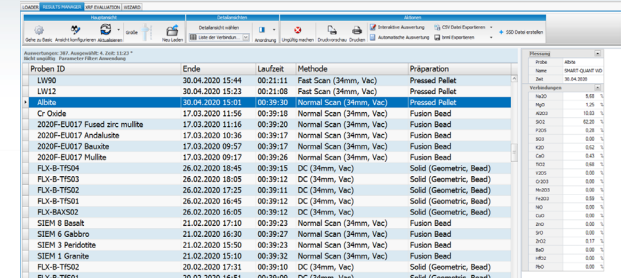


Dr. Kai Behrens
Leiter Produktmanagement RFA
Karlsruhe, Deutschland

SMART-QUANT

Philosophie & Integration in SPECTRA.ELEMENTS

- Warum wird standardlose Analytik benötigt?
 - Referenzmaterial/Standards nicht verfügbar
 - Vollständig unbekannte Proben
 - Black Box oder anpassbare Methode
- Herausforderung
 - Gesamtes Elementspektrum
 - Alle Präparationen
 - Matrix- und Überlagerungskorrekturen
- Einschränkungen
 - Präparationseffekte wie Partikelgrößen können nicht berücksichtigt werden



Problem ID	Ende	Laufzeit	Methode	Präparation
LW90	30.04.2020 15:44	00:21:11	Fast Scan (34mm, Vac)	Pressed Pellet
LW12	30.04.2020 15:23	00:21:08	Fast Scan (34mm, Vac)	Pressed Pellet
Cr Oxide	17.03.2020 11:56	00:39:18	Normal Scan (34mm, Vac)	Fusion Bead
2020F-EU017 Fused zirc mulite	17.03.2020 11:16	00:39:20	Normal Scan (34mm, Vac)	Fusion Bead
2020F-EU017 Andalusite	17.03.2020 10:36	00:39:17	Normal Scan (34mm, Vac)	Fusion Bead
2020F-EU017 Bauxite	17.03.2020 09:57	00:39:17	Normal Scan (34mm, Vac)	Fusion Bead
2020F-EU017 Mullite	17.03.2020 09:17	00:39:26	Normal Scan (34mm, Vac)	Fusion Bead
FLX-B-TS04	26.02.2020 18:45	00:39:15	DC (34mm, Vac)	Solid (Geometric, Bead)
FLX-B-TS03	26.02.2020 18:05	00:39:12	DC (34mm, Vac)	Solid (Geometric, Bead)
FLX-B-TS02	26.02.2020 17:25	00:39:11	DC (34mm, Vac)	Solid (Geometric, Bead)
FLX-B-TS01	26.02.2020 16:45	00:39:12	DC (34mm, Vac)	Solid (Geometric, Bead)
FLX-B-TS00	26.02.2020 16:05	00:39:12	DC (34mm, Vac)	Solid (Geometric, Bead)
SIEM 8 Basalt	21.02.2020 17:10	00:39:23	Normal Scan (34mm, Vac)	Fusion Bead
SIEM 6 Gabbro	21.02.2020 16:30	00:39:27	Normal Scan (34mm, Vac)	Fusion Bead
SIEM 3 Peridotite	21.02.2020 15:50	00:39:23	Normal Scan (34mm, Vac)	Fusion Bead
SIEM 1 Granite	21.02.2020 15:10	00:39:32	Normal Scan (34mm, Vac)	Fusion Bead
FLX-B-TS02	20.02.2020 17:31	00:39:10	DC (34mm, Vac)	Solid (Geometric, Bead)
FLX-B-TS01	19.02.2020 16:41	00:39:10	DC (34mm, Vac)	Solid (Geometric, Bead)



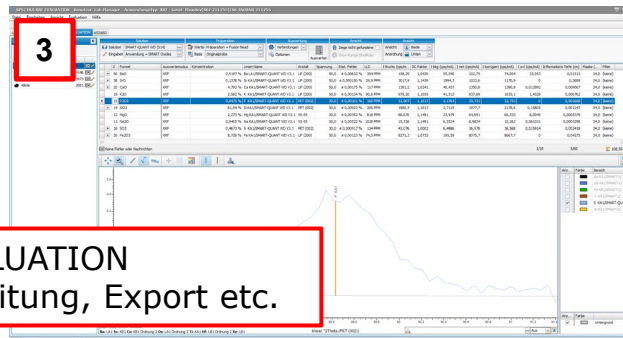
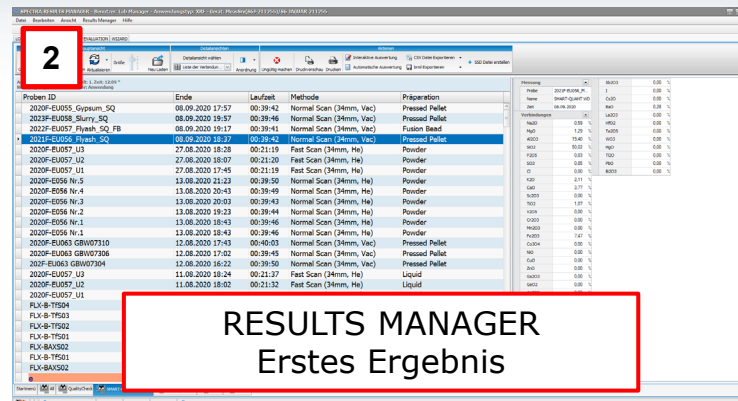
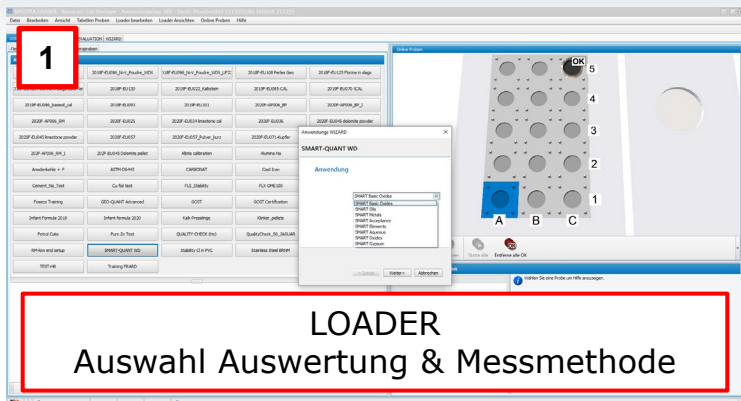
SMART-QUANT

Philosophie – Funktion



- Ansatz in der WDRFA-Analytik
 - Standard-basierte Kalibrierung mit einer Vielzahl von Standards
 - Verwendung theoretischer Korrekturfunktionen (variable Alphas, Überlagerungen)
 - SMART-QUANT WD – S6 JAGUAR
 - QUANT-EXPRESS – S8 TIGER
- Ansatz in der EDRFA-Analytik
 - Berechnung des Probenspektrum und des Fittings anhand der Messung
 - Schließt Berechnung der Konzentrationen mit ein
 - SMART-QUANT FP – S2 PUMA

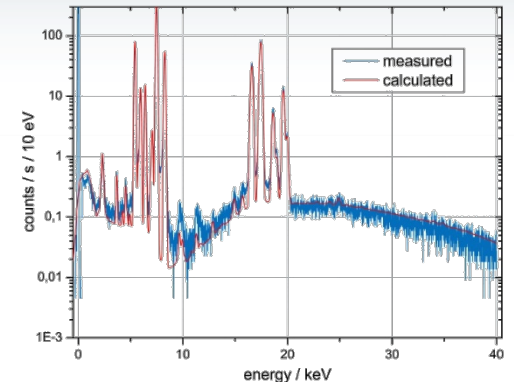
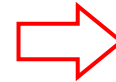
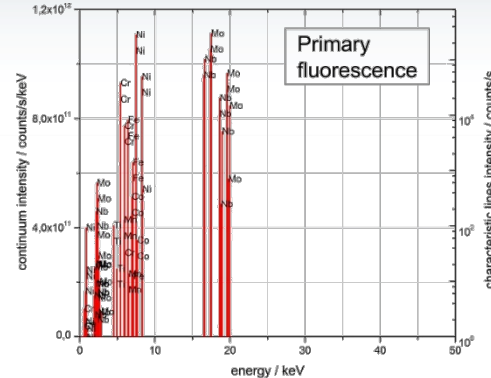
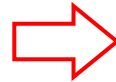
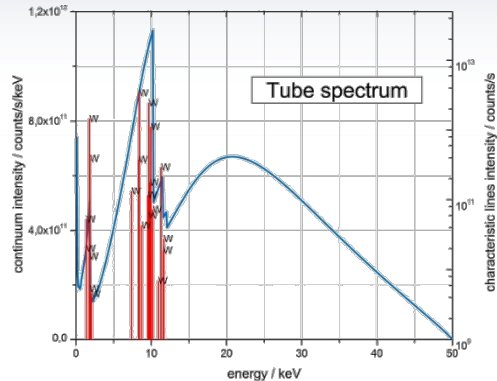
SMART-QUANT Philosophie – Workflow in SPECTRA.ELEMENTS



SMART-QUANT FP & WD

Unterschiede

S2 PUMA SMART-QUANT FP – Fitting & Iteration



Probe

Primärstrahlfilter

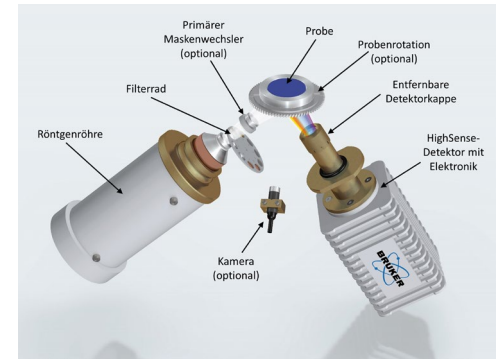
Röhrenfenster

Röntgenröhre

Detektorfenster

Detektor

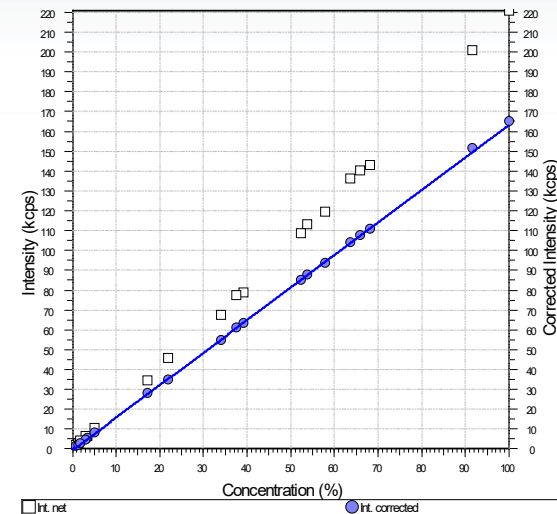
- Eine Probe (MTB2) zur Methodeninstallation



S6 JAGUAR SMART-QUANT WD



- Streng genommen:
Semi-quantitativ, nicht standardlos
- Übertragbare Kalibrierung
 - Methodenspezifische Proben:
 - SMART-QUANT WD (S6 JAGUAR)
FLX-B-TfS04, FLX-B-TfS03, FLX-B-TfS02, FLX-B-TfS01
 - QUANT-EXPRESS (S8 TIGER)
SQ1, SQ2, SQ3, GRA
- Anwendung flexibler Matrixkorrektur
 - Variable Alphas – Neuberechnung für jede Probe
- Theoretische Überlagerungskorrekturen



SMART-QUANT FP & WD

Die Unterschiede



- Semi-quantitative bzw. standardlose Methoden entwickelt, um
 - Weite Element- und Konzentrationsbereiche abzudecken
 - Dem Anwender interaktive Auswertungen zu erlauben und
 - Individuelle Auswertungen und Methoden erstellen zu lassen

Standardlose Methode	System	Element-bereich	Messzeit	Standard-basiert	Modelliert	Kombinierbar mit Kalibrierungen	Individuelle Auswertungen
SMART-QUANT FP	S2 PUMA	(F) Na – Am	• 5 – 10 Minuten • Individuell	✗	✓	✗	✓
SMART-QUANT WD	S6 JAGUAR	(F) Na – Am	• Fast Scan – 21 Minuten • Normal Scan – 40 Minuten	✓	✗	✗	✓
QUANT-EXPRESS	S8 TIGER	(B) F – U	• Fast Screening – 2 Minuten • Full Analysis – 7 Minuten • Best Detection – 17 Minuten	✓	✗	✓	✓

SMART-QUANT FP & WD

Die Unterschiede



- Für die standardlose Pakete wird lediglich die Standardkonfiguration des jeweiligen Systems benötigt
- Für alle Maskengrößen verfügbar

Standardlose Methode	System	Konfiguration
SMART-QUANT FP	S2 PUMA	HighSense (Pd tube) HighSense LE (Ag tube)
SMART-QUANT WD	S6 JAGUAR	Standard • FC, HighSense XE • XS-55, PET, LiF200
QUANT-EXPRESS	S8 TIGER	Standard • FC, SC • 0.23°, 0.46° • XS-55, PET, LiF200

Beispiele

SMART-QUANT FP/WD & QUANT-EXPRESS

SMART-QUANT FP & WD

Leistungsfähigkeit (1)



- BS199A (feste Metallprobe, Ni-Basis, Waspaloy)
- *SMART-QUANT FP/WD & QUANT-EXPRESS*

		S2 PUMA LE	S2 PUMA	S6 JAGUAR	S8 TIGER Series 2 (4 kW)
	CERTIFICATE	SMART-QUANT FP (SPECTRA.ELEMENTS 3.1)	SMART-QUANT FP (SPECTRA.ELEMENTS 3.1)	SMART-QUANT WD (SPECTRA.ELEMENTS 3.1)	QUANT-EXPRESS (SPECTRAplus 4.2.0)
Instrument		250258, External	250061, TouchControl	Proto 2	210207
Al	1,26	1,11	1,37	1,31	1,30
Si	0,05	0,33	0,09	0,13	0,14
Ti	3,07	2,83	2,95	3,07	3,39
V	0,02	n.d.	n.d.	0,00	
Cr	19,25	18,88	18,92	20,13	20,2
Mn	0,014	0,11	0,17	0,02	
Fe	1,05	0,78	0,94	1,07	1,12
Co	13,47	13,57	13,58	13,71	12,8
Ni	57,8	58,08	57,61	59,50	60,5
Nb	0,04	0,01	0,04	0,01	0,04
Mo	3,99	4,00	3,78	3,90	4,30
False Positives > 0,05		Ca, W	S, Ca, W	Na, Cl, Sc, Cd, Sn, I	Yb = 2,61 Er = 1,70 (not conv.) Na = 0,10 S = 0,05

SMART-QUANT FP & WD

Leistungsfähigkeit (2)



- FLX-RAW24 (Schmelztablette, Zement)
- *SMART-QUANT FP/WD & QUANT-EXPRESS*

		S2 PUMA LE	S2 PUMA	S6 JAGUAR	S8 TIGER Series 2 (4 kW)
	CERTIFICATE	SMART-QUANT FP (SPECTRA.ELEMENTS 3.1)	SMART-QUANT FP (SPECTRA.ELEMENTS 3.1)	SMART-QUANT WD (SPECTRA.ELEMENTS 3.1)	QUANT-EXPRESS (SPECTRAplus 4.2.0)
Instrument		250258, External	250061, TouchControl	Proto 2	210207
Na2O	0,02	n.d.		0,42	0,75
MgO	0,5	0,63		0,00	0,58
Al2O3	39,2	39,09	39,11	40,72	41,2
SiO2	4,0	4,57	3,56	4,32	4,46
P2O5	0,07	n.d.	n.d.	0,08	0,10
K2O	0,05	n.d.	n.d.	0,06	0,10
CaO	39	39,12	39,08	40,59	39,5
TiO2	1,8	1,69	1,71	1,25	1,85
Cr2O3	0,11	0,06	0,08	0,15	0,11
Mn2O3	0,06	n.d.	n.d.	0,05	0,04
Fe2O3	14,7	14,66	15,74	16,72	15,07
ZnO	0,004	n.d.	n.d.	0,01	0,01
SrO	0,02	0,02	0,02	0,02	0,02
False Positives > 0,05		Cl	SO3, Cl, Sc2O3	Cl, SO3, BaO	F, SO3, Cl, ZrO2, Ru

Bruker Training Office Hours Elemental Analysis



- Thanks for joining!
 - We'll leave the session open for a few more minutes so you can read answers to questions
- To ask a question:
 - Use the Q&A panel
 - We'll be answering questions on this week's topic throughout the hour
 - Note that many topics will be addressed in upcoming sessions
- Contact:
 - www.bruker.com
 - application.baxs.emea@bruker.com

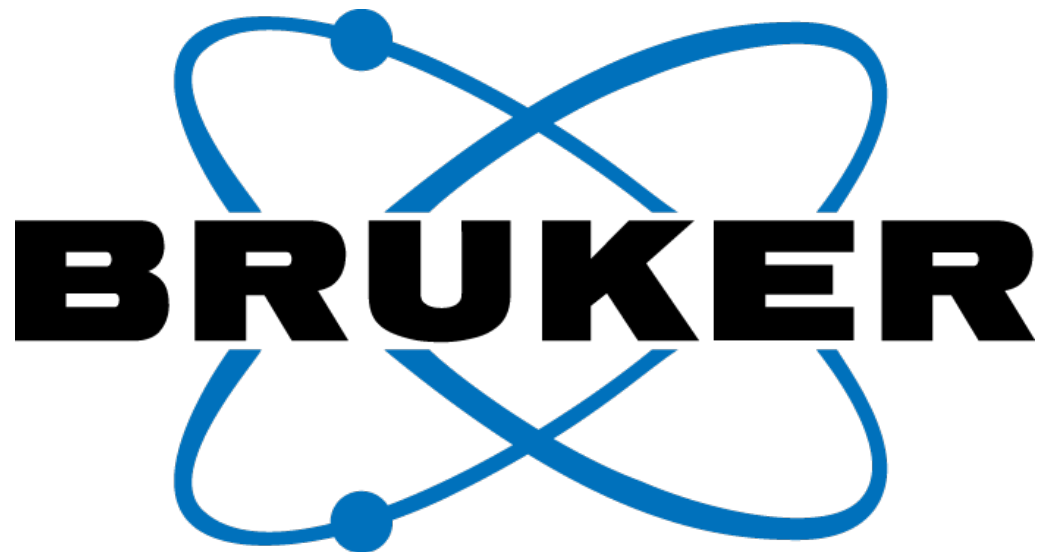


Bruker Training Office Hours

Open to existing users of Bruker [X-ray Diffraction \(XRD\)](#), [X-ray Microscopy \(XRM or Micro-CT\)](#), [X-ray Fluorescence \(XRF\)](#), [Optical Emission Spectrometry \(OES\)](#), [CS/ONH Analysis](#), and [Single Crystal X-ray Diffraction \(SC-XRD\)](#) instruments, Bruker Training Office Hours are free, 1-hour, online, live, interactive, weekly Applications Training sessions, offered in three different time zones and multiple languages. These sessions will not be recorded or offered on-demand. Each series will be extended with new topics approximately every 4 weeks, based on your feedback and suggestions. Sign up once for a series and attend as many of its live weekly sessions as you like. We'll send you an attendance reminder before each session starts. Drop in for a few minutes or stay the hour, learn new methods during the brief training presentation, chat with your fellow attendees, bring your questions, and discuss your applications with our experts.

Check out the upcoming schedule:

<https://my.bruker.com/acton/media/2655/bruker-training-office-hours-series>



Innovation with Integrity