Thermo Scientific iCAP 7000 Series ICP-OES

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Topics to be covered

- Configurations and Specifications
- Hardware
  - Technology and features
- Challenging matrices
  - Hydrocarbon samples
  - High saline samples
- Software
  - Principles of software
  - Work flows
  - Key features
- Element Finder
  - Fully automated method development

Thermo Scientific™ iCAP™ 7000 Series ICP-OES

- Lowest cost ICP-OES analysis, the highest quality data
  - *iCAP 7200 ICP-OES* - Entry level, cost-effective analysis for low sample thru-put requirements.
  - *iCAP 7400 ICP-OES* - For routine analysis requirements and mid-range sample thru-put.
  - *iCAP 7600 ICP-OES* - Highest productivity and maximum sample thru-put with advanced, flexible accessory support, such as laser ablation.

iCAP 7200 ICP-OES

- Entry level, cost-effective analysis for low sample thru-put requirements.
- *Perfect analytical solution for restricted budgets*

- Powerful analyte detection & resolution
- Analysis-ready sample introduction for consistent performance & ease of use
- User selectable method templates for minimized method development
- Field upgradeable technology to iCAP 7400 ICP-OES

Who's it for:

- Routine labs with a low budget
- Less demanding liquids applications
- Low sample numbers

iCAP 7200 ICP-OES – Specification

SIMPLE PRE-OPTIMIZED SAMPLE INTRODUCTION

- Duo plasma viewing
- Pre-set 1150W plasma power
- Manual (pressure regulated) gas flow controls

POWERFUL PERFORMANCE & PRODUCITIVTY

- Powerful resolution and DLs from iCAP 7000 Series ICP-OES
- Optimized productivity for small sample batches (≤ 100 samples per day)
  - Approximately 4 minutes per sample for a 15 element method
- Simple, intuitive software tools for reduced method development
  - Pre-loaded methods for Enviro, Food/Toy Safety and WEEE/RoHS applications
  - Downloadable methods from the on-line library
- ***Wavelength range 175-847 nm***
  - Access to most sensitive As, P, Hg, Tl, Sn and I wavelengths

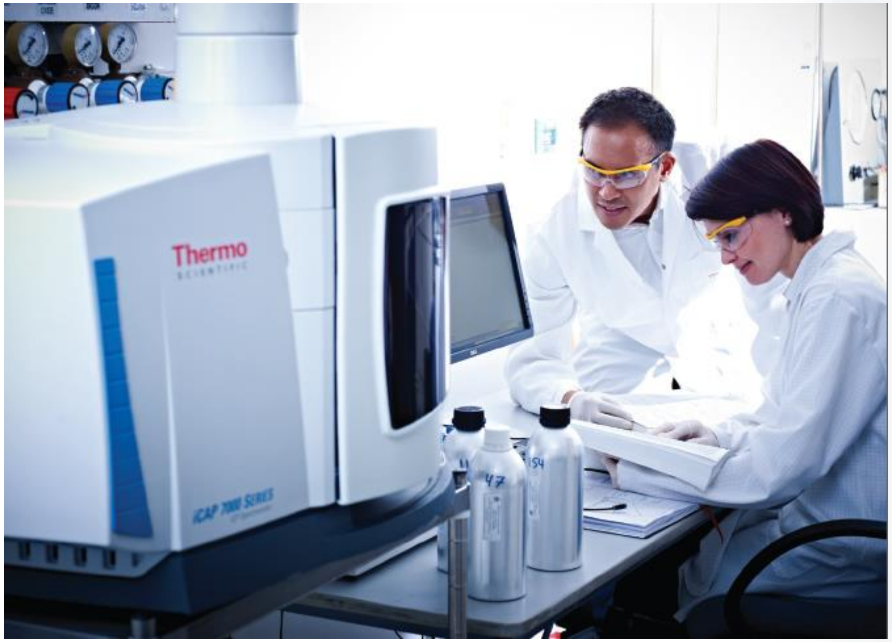
Future Proof Field Upgradeable iCAP 7200 ICP-OES

The iCAP 7200 ICP-OES can evolve with the customer’s analytical requirements and be **field upgraded** to iCAP 7400 ICP-OES **Duo** specification

- iCAP 7200 ICP-OES Upgrade Kit
  - Provides full wavelength range of 166-847nm
  - Provides MFC controlled nebuliser for enhanced long term stability
  - Provides enhanced flexibility for Peristaltic Pump control to enhance productivity
  - Provides enhanced flexibility for Plasma RF power (e.g. for volatile organics analysis)
  - Enhanced productivity (precision mode enables analysis of 15 elements in <2 mins)
  - Fullframe for advanced method development and data acquisition

iCAP 7400 ICP-OES

- For routine analysis requirements and mid-range sample thru-put.
- *Ideal for QA/QC laboratories that require highest sensitivity from full wavelength coverage*



- Powerful analyte detection & resolution
- Choice of plasma orientation to enable enhanced application suitability
- Intuitive software tools for optimized liquid sample introduction
- Advanced gas flow control for optimized liquid sample introduction
- Flexible data acquisition modes for routine method development operations

Who's it for

- Routine analytical laboratories
- Moderate-high throughput liquid applications

iCAP 7600 ICP-OES

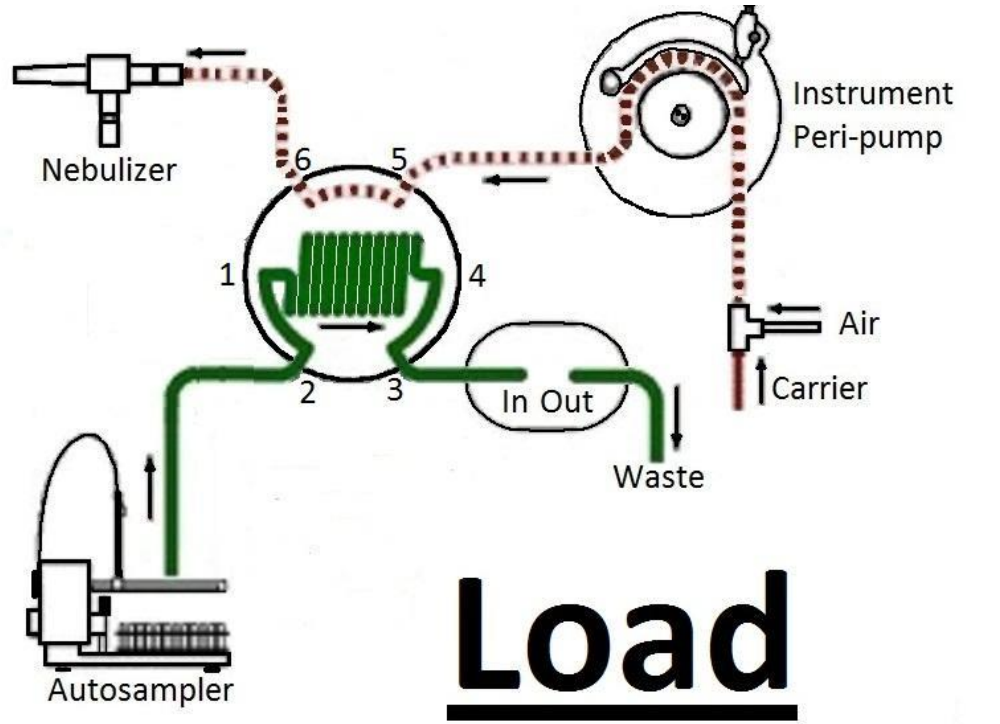
- Highest productivity and maximum sample thru-put with advanced sprint valve sample introduction , flexible accessory support
- *Best solution for laboratories experiencing the most challenging analytical demands, such as large contract, or R&D facilities*

- Powerful analytical detection & resolution
- Choice of plasma orientation to enable enhanced application suitability
- Intelligent software for powerful auto-optimization of the sample intro system
- Advanced data acquisition including ‘Sprint’ modes for ultimate productivity & versatility
- Comprehensive accessory compatibility for liquid & solid sampling

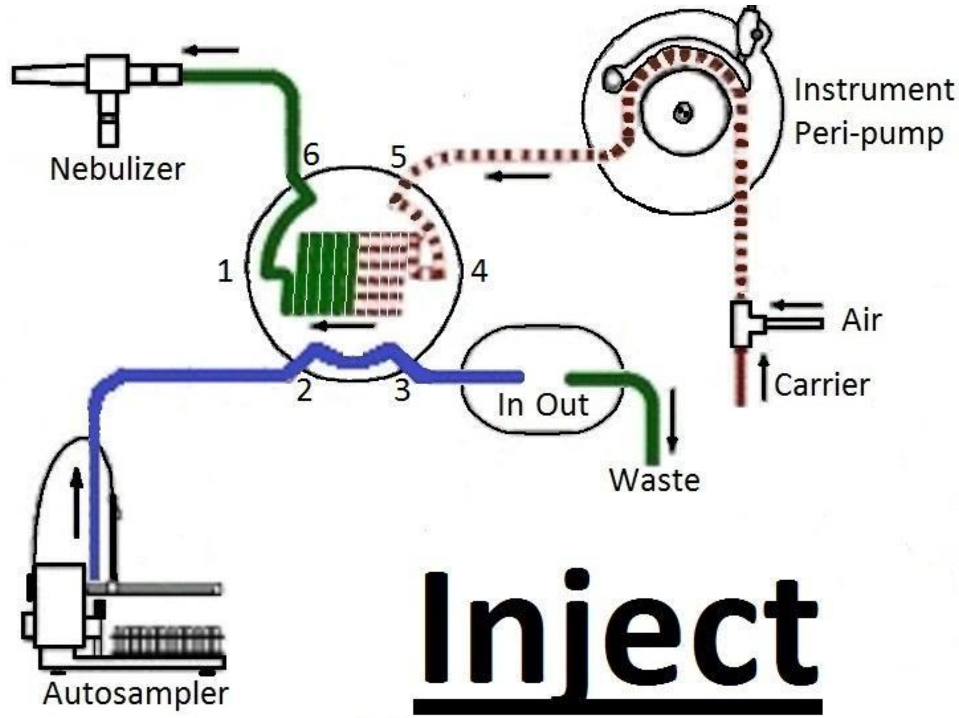
Who’s it for

- Labs requiring the extreme productivity
- Labs who perform highly variable & demanding research-based applications
- Labs who require solid sampling capability

Sprint valve system – How does it work?



Sprint valve system – How does it work?



iCAP 7000 Series ICP-OES – Plasma View Configurations

Duo

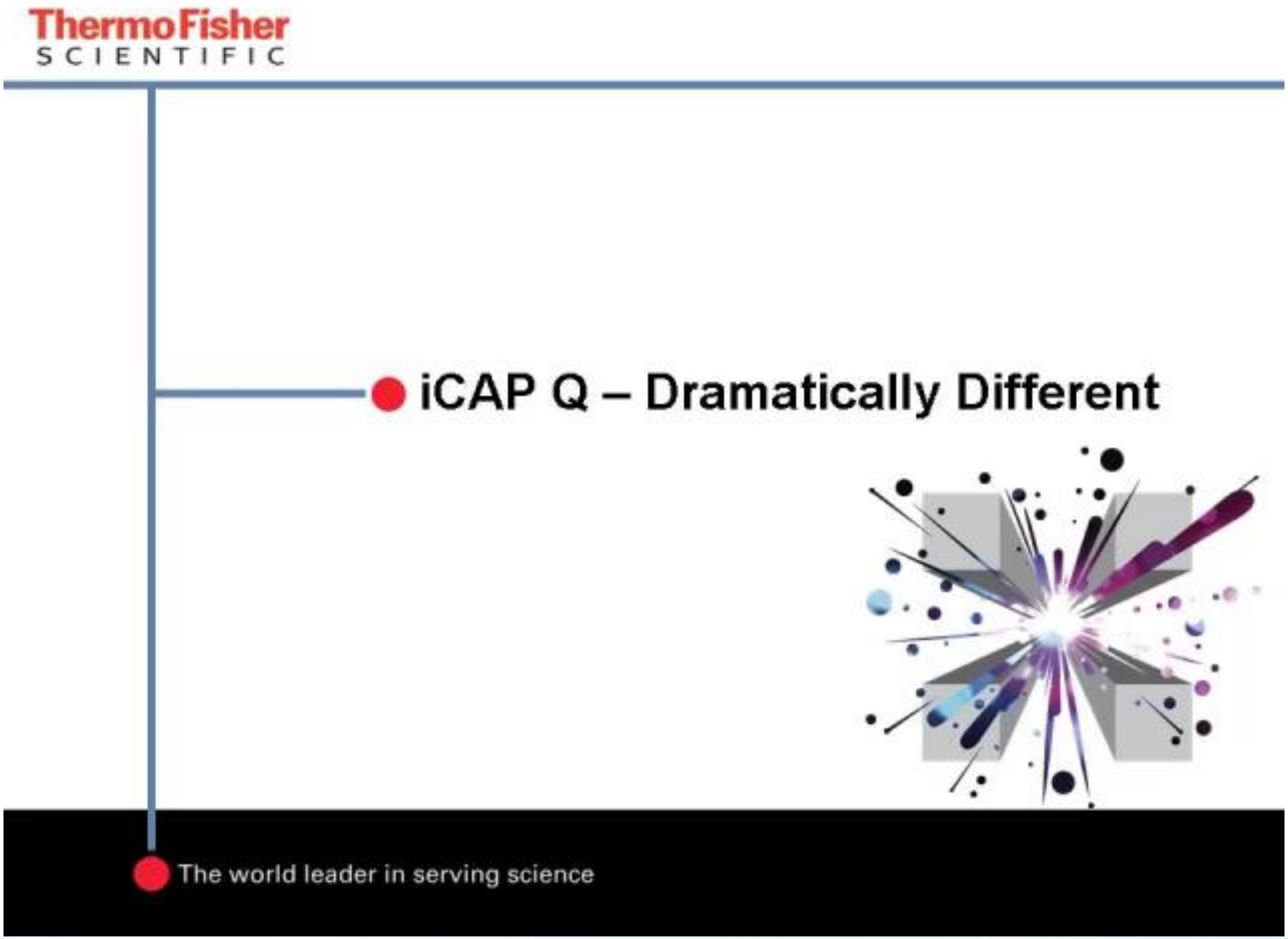
iCAP 7200 ICP-OES

iCAP 7400 ICP-OES

iCAP 7600 ICP-OES

Radial

iCAP 7000 RF Generator MK III performance prove



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Thermo Scientific iCAP 7000 Series ICP-OES

	iCAP 7200 ICP-OES	iCAP 7400 ICP-OES	iCAP 7600 ICP-OES
Plasma View	Duo	Radial or Duo	Radial or Duo
λ Range	175 – 847 nm	166 – 847 nm	166 – 847 nm
Gas Flow Controls	Pressure/Solenoid	~~Neb~~/MFC	**Full MFC**
Additional Gas	No	No	**Yes as stand**
Full Spectrum Capture	No	Fullframe	Fullframe
Spray Chamber/Neb	Aqueous (as std) Others Available	Aqueous (as std) Others Available	Aqueous (as std) Others Available
Detector	CID86	CID86	CID86
Sample Pump	3-channel std peri pump	**4-channel mini pump**	**4-channel mini pump & Integrated Loop**
RF Source	Pre-optimized 1150 W	1500W	1600W
Operating Gas Cons. (L/min)	14	16	16
Detection Capability	Standard iCAP – 1ppb	Standard iCAP – 1ppb	Standard iCAP – 1ppb
Software	**Qtegra Basic**	**Qtegra Standard**	**Qtegra Enhanced**
Method Templates (MT)	**Enhanced set of MT**	**Enhanced set of MT**	**Enhanced set of MT**

iCAP 7000 Series ICP-OES – IDLs with Axial Plasma Viewing

Element	Wavelength (nm)	DL (15s integrations) ug/L
Ag	328.068	0.32
Al	167.079	0.12*
Al	308.215	4.1
As	189.042	1.43
As	193.759	2.14
Ba	455.403	0.03
Be	311.107	0.017
Ca	393.366	0.003
Cd	214.438	0.07
Co	228.616	0.51
Cr	205.560	0.21
Cu	324.754	0.39
Fe	259.940	0.25
Hg	184.950	0.14
Hg	194.227	0.66
K	766.490	0.60
Li	670.784	0.03
Mg	279.553	0.010

Element	Wavelength (nm)	DL (15s integrations) ug/L
Mn	257.610	0.07
Mo	202.030	0.38
Na	589.592	0.37
Ni	231.604	0.36
P	177.495	1.55
P	213.618	2.12
Pb	220.353	1.06
S	180.731	1.05
Sb	206.833	3.25
Se	196.090	3.05
Sn	189.989	1.10
Sn	283.999	4.14
Sr	407.771	0.010
Ti	336.121	0.30
Tl	190.856	1.16
Tl	276.787	4.40
V	309.311	0.23
Zn	213.856	0.19

***Not applicable for iCAP 7200 ICP-OES**

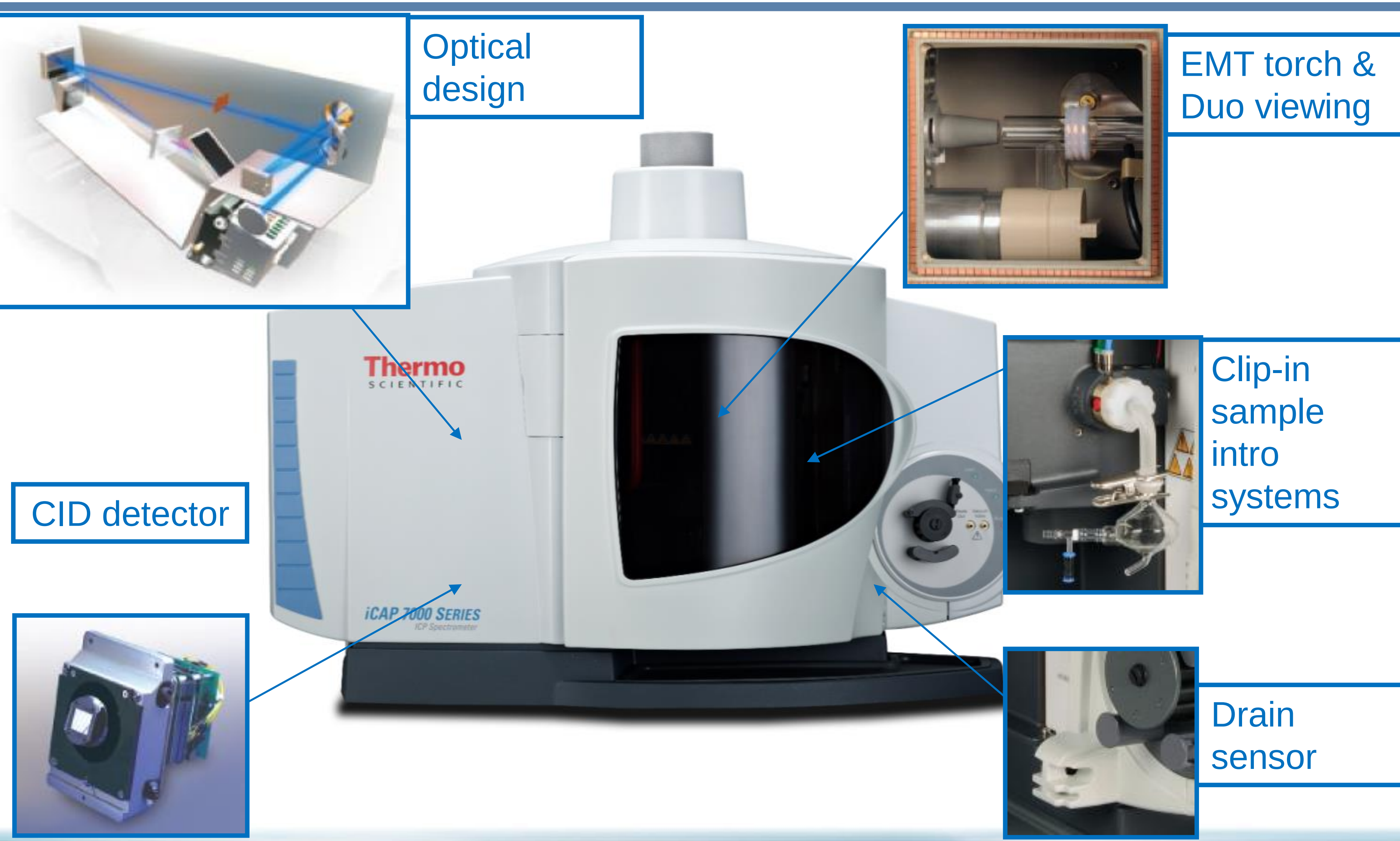
(All instrument detection limits calculated using the 3σ model)

iCAP 7000 Series ICP-OES – IDLs with Radial Plasma Viewing

Element	Wavelength (nm)	DL (15s integrations) ug/L
Ag	328.068	2.46
Al	167.079	1.51
As	189.042	4.74
Ba	455.403	0.17
Be	311.107	0.07
Ca	393.366	0.02
Cd	214.438	0.19
Co	228.616	1.16
Cr	205.560	0.85
Cu	324.754	2.36
Fe	259.940	0.80
Hg	184.950	1.10
K	766.490	5.10
Li	670.784	0.83
Mg	279.553	0.04
Mn	257.610	0.21
Mo	202.030	1.11
Na	589.592	1.80
Ni	231.604	2.29
P	177.495	5.66
Pb	220.353	4.50
S	180.731	2.22
Sb	206.833	9.36
Se	196.090	7.36
Sn	189.989	1.57
Sr	407.771	0.04
Ti	336.121	0.58
Tl	190.856	7.33
V	309.311	0.80
Zn	213.856	0.6

(All instrument detection limits calculated using the 3σ model)

The iCAP 7000 Series ICP-OES Core Technologies



Sample Introduction Kits for iCAP 7000 Series ICP-OES

- Liquid handling kits for Duo & Radial ICP-OES
  - Aqueous Kits
  - Organics Kits
  - Volatile Organics Kits
  - High Solids Kits
  - HF Resistant Kits
- All kits include EMT torches
- User selectable injectors tubes
  - 1.0, 1.5, 2.0 mm quartz tube
  - 2.0 mm ceramic tubes
- **Pump tubing is not included**

Open Access Sample Introduction Compartment

- Large fully opening outer door
  - Improved user access
- Clear view of plasma source
  - Simplifies optimization
- Easy access to sample introduction
  - Simple change of components
- Peri-pump
  - 12 roller for smooth flow, micro tension control
- Drain Sensor
  - Monitors drain, detects leaks or blockages
- Accessories
  - Easy connection of Argon Humidifier, Hydride Generation and Laser Ablation accessories

“Better user access, compatible with all accessories”

EMT Torch for Ease of Use for Routine Maintenance

TORCH ORIENTATION LOCK

- Auto alignment of the torch in the torch box
- Automatically establishes robust plasma gas connections

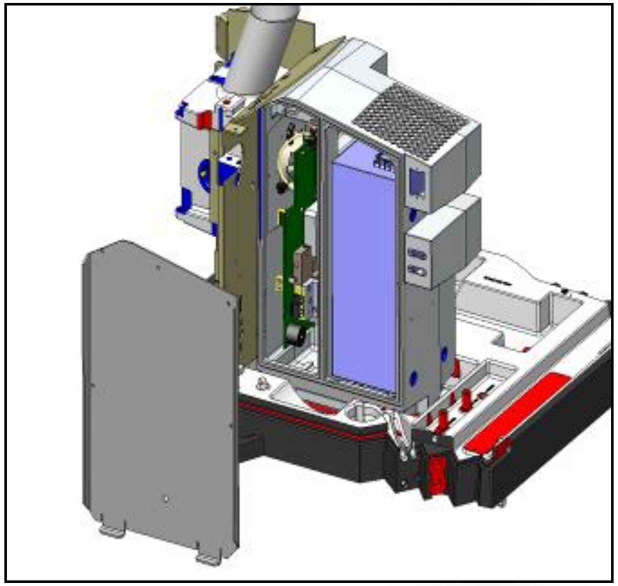
SCREW-THREADED CENTRE TUBE HOLDER

- Simple routine maintenance operations with the plasma on!

Still the best torch design and common ICP-OES/ICP-MS

High Efficiency RF Generator Design

- 27 MHz Swing Frequency design for enhanced stability
- High efficiency (>78%) enables operation at lower power
- Conformal coated PCBs for corrosion resistance
- Reduced thermal stresses on key components
  - Re-optimized air circulation
  - Re-optimized water flow thresholds
  - In-line water filters
- Ease of serviceability and fault diagnosis
  - Modular control board and software diagnostic tools
  - Modular Power Supply Unit and software diagnostic tools



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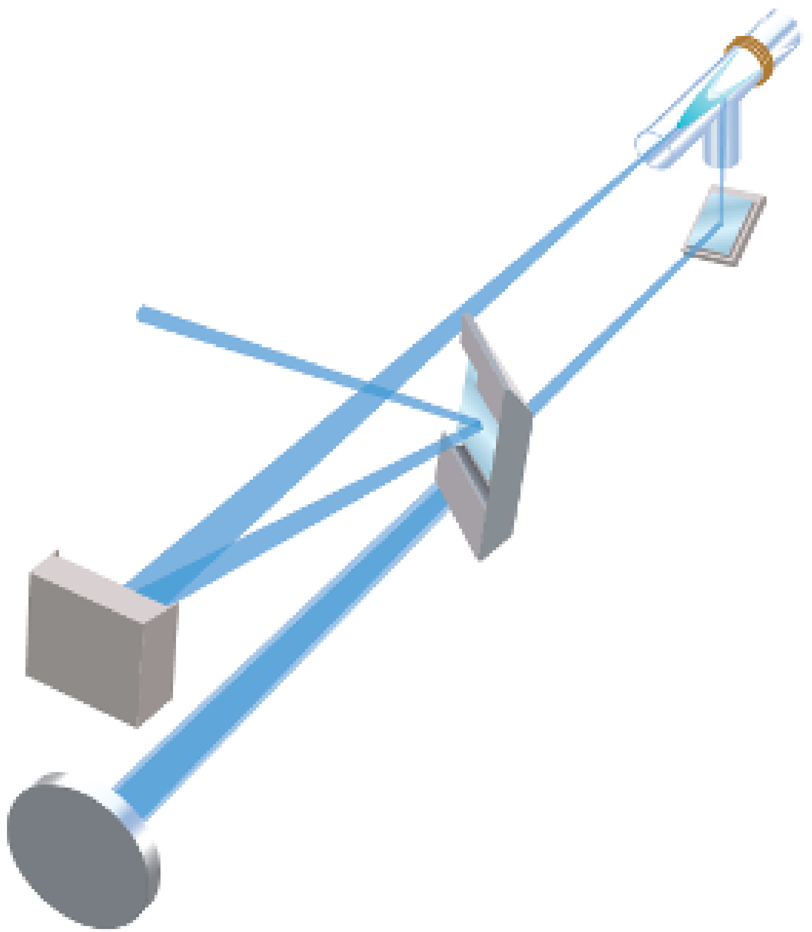
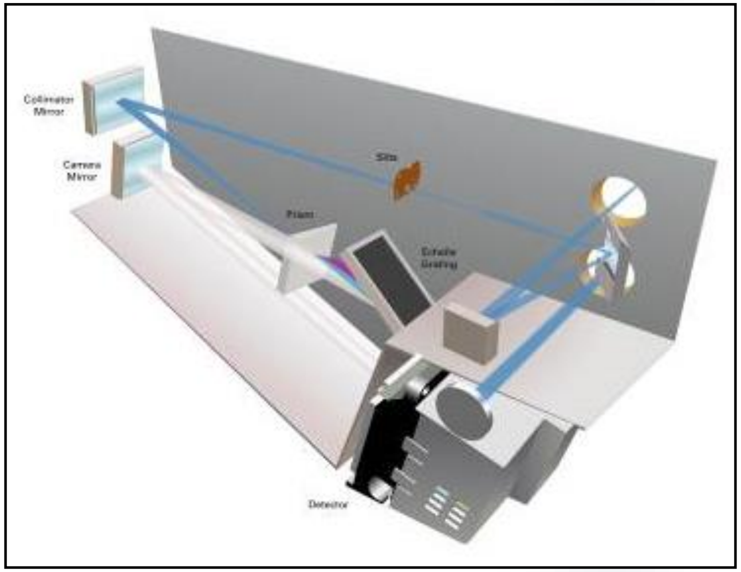
iCAP 7000 Series ICP-OES Optics – Fore Optics



- Duo View & Radial View Options
- Telephoto system (concave & convex mirror)
  - *Low aberrations (efficient collection of light)*
- Convex mirror (before slit) steerable in 2 directions
  - *selects view (in Duo)*
  - *allows peaking of plasma view (in Radial)*

iCAP 7000 Series ICP-OES Optical Design – Echelle Polychromator

- High optical stability & accuracy
  - *Compact optical design (thermally insulated with heater control to 0.1 ^{0}C)*
  - *Automated optical correction on GetReady*
  - *New wavelength calibration – accurate to <1 pixel*
- High resolution and image quality
  - *7 pm @ 200nm*
  - *Aberration compensation over whole chip*
  - *Reduced stray light effects*
  - *Anamorphic magnification focuses all lines on the chip*
- High sensitivity
  - *Compact design with reduced optical surfaces*
  - *Shorter integration times for faster analysis*
  - *UV & Vis slits for optimized light transmission*
- Low running costs
  - *Compact design allows fast purge & reduced gas consumption*



Improving robustness for ICP-OES analysis

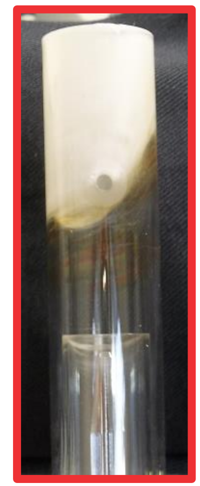
Overview

- What samples cause problems for ICP-OES?
  - Types of sample
  - Challenges they cause
- How can these problems be solved?
  - Nebuliser, spray chamber, torch and purged radial view window
  - Sheath gas (for radial ICP-OES) and humidifier
- Example applications
- Improving productivity with ICP-OES
  - High speed analysis options
  - Automated sample preparation and intelligent dilution
  - Automated method development using enhanced software (Element Finder)

What samples cause problems for ICP-OES?

- Types of sample
  - Saline matrices (e.g. sea water, brine)
  - Metal / metal alloy digests
  - Organic materials (e.g. engine lubrication oils)

- Challenges
  - Nebuliser blockage
  - Torch devitrification and cracking
  - Injector degradation and blocking
  - For dual view systems, coating of radial view window



How can these problems be solved? - 1

- Nebulisers
  - Parallel path – Burgener
  - Large capillary concentric devices (e.g. SeaSpray)
  - V-groove
  - Resistant to blocking
- Spray chamber
  - Baffled cyclonic type
  - Reduced sample loading on plasma
  - Improved long term stability

How can these problems be solved? - 2

- Torch
  - Ceramic torch: very high tolerance to aggressive sample matrices, radial and Duo options
  - Fully demountable for simplified maintenance
  - Duo design incorporates fibre optic connection to allow plasma on status to be detected
  - Ideal for saline materials, fusions, metal digests
- Purged radial view window (iCAP 7000 Duo)
  - Holes in base allow Ar purge gas flow through the window and out through tapered nozzle
  - Prevents sample deposition on base of window so eliminates related signal drift
  - Improves sensitivity, especially in the UV range and enhances long term stability
  - Reduces user maintenance

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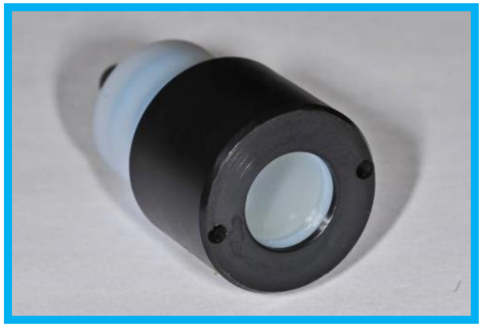
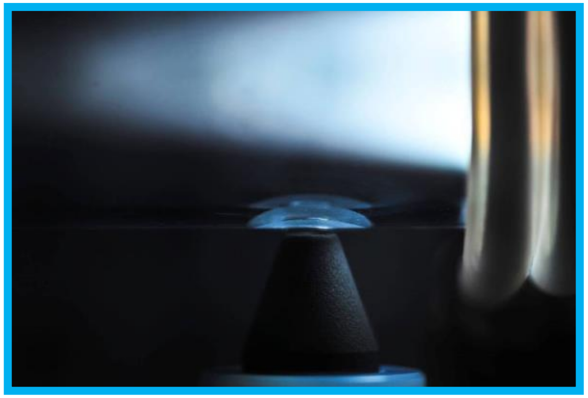
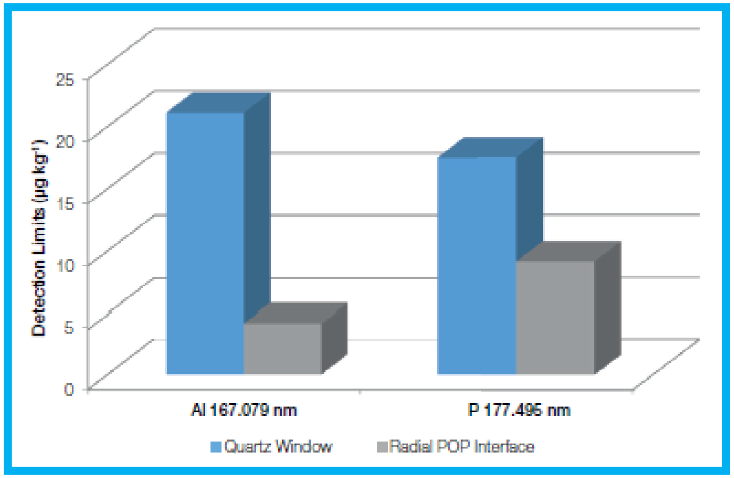
How can these problems be solved? - 3

Purged radial view window







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How can these problems be solved? - 4

- Sheath gas adaptor
  - Creates barrier between aerosol and injector surface
  - Prevents sample build up on the injector tip
  - Enhances the long term stability of high solid samples
  - Improves detection limits and avoids contamination by eliminating the need for sample dilution
  - Connects directly to the Thermo Scientific™ iCAP™ 7400/7600 ICP-OES additional gas accessory
- Argon humidifier, if sheath gas option not available
  - Nebuliser gas line fed through chamber containing water
  - Water permeates through gas line and wets the argon
  - Prevents salting up on nebuliser tip caused by drying effect of nebuliser gas flow
  - Example shown here - ESI *pergo* system

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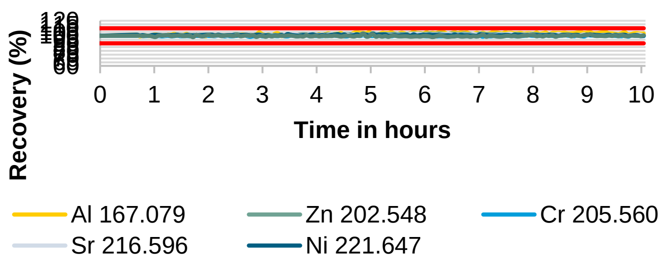
Example application 1: Analysis of 25% NaCl samples

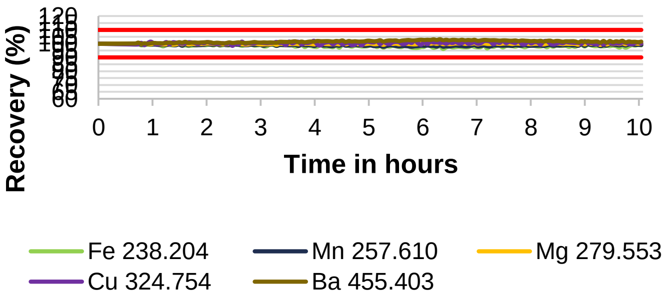
- iCAP 7400 ICP-OES Radial
  - Burgener MiraMist nebuliser
  - Ceramic torch (aka the D-Torch)

- Long term stability: Recovery ±5% during 10 h analysis
- Detection limits: Mostly single digit ppb (see later slide)
- Reduced wash time of 30 sec.

10 h stability in 25% NaCl, λ <230nm (without internal standard correction)

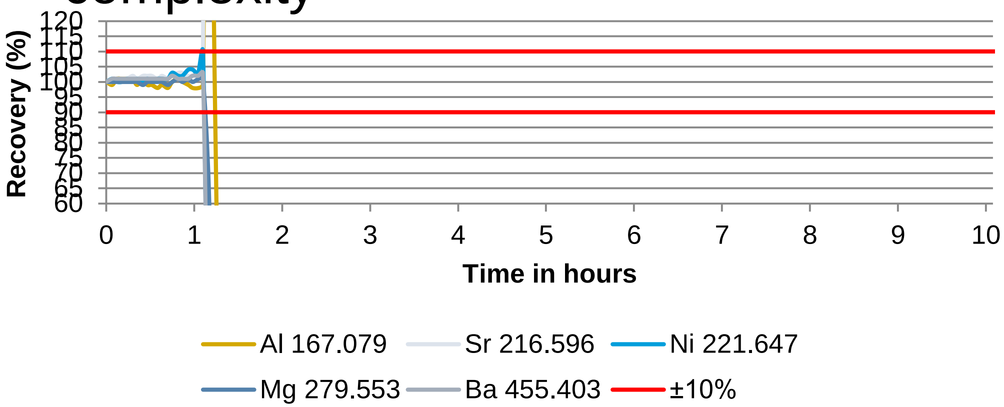


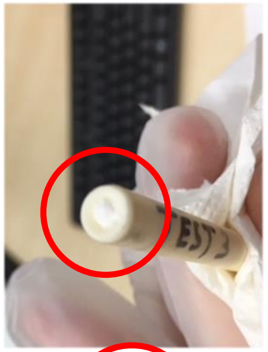
10 h stability in 25% NaCl, λ >230nm (without internal standard correction)



Measurement without sheath gas adaptor

- Without sheath gas
  - Completely blocked injector tube after < 2h, signal lost
  - If sheath gas option not available, argon humidifier would be required – additional cost, complexity





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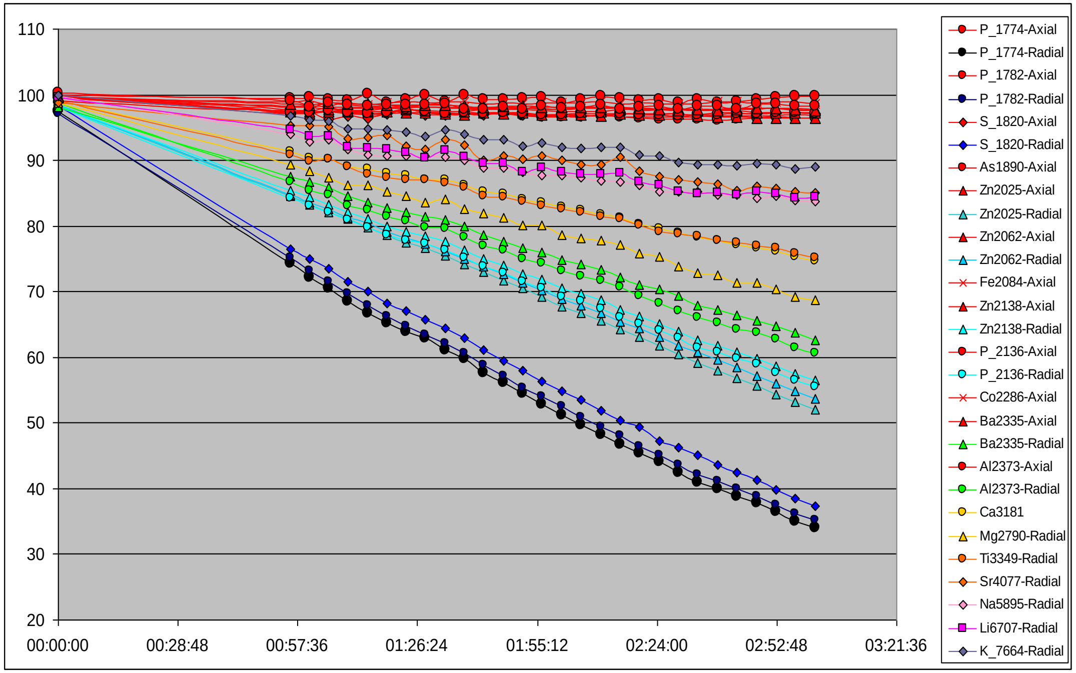
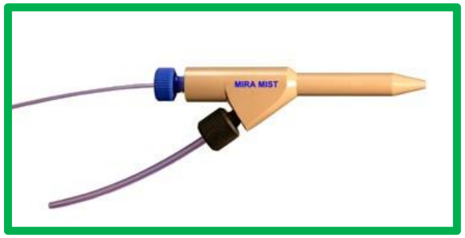
25% NaCl analysis results summary

Element and wavelength (nm)	R^2	Internal standard wavelength (nm)	Known spike concentration (µg·L^{-1})	Measured spike concentration (µg·L^{-1})	Recovery (%)	MDL (µg·L^{-1})
Al 167.079	0.9997	Y 224.306	500	497.2	97.2	4.1
Ba 455.403	1.0000	Y 317.030	500	499.9	99.9	0.9
Co 228.616	0.9999	Y 224.306	500	500.6	100.6	10.6
Cr 205.560	0.9999	Y 224.307	500	500.5	100.5	4.5
Cu 324.754	0.9999	Y 324.228	500	501.7	101.7	13.0
Fe 238.204	0.9995	Y 320.332	500	503.2	103.6	8.8
Mg 279.553	0.9999	Y 320.332	500	501.0	101.0	0.5
Mn 257.610	0.9999	Y 320.332	500	501.1	101.1	1.7
Ni 221.647	0.9999	Y 224.306	500	500.8	100.8	8.0
Sr 216.596	0.9999	Y 224.306	500	501.3	101.3	10.2
Zn 202.548	1.0000	Y 224.306	500	499.9	99.9	2.0

Example application 2: Concentrated metal digests

Aqua regia 10g/L vanadium concentrate analysis using iCAP 7400 Duo, without internal standard correction

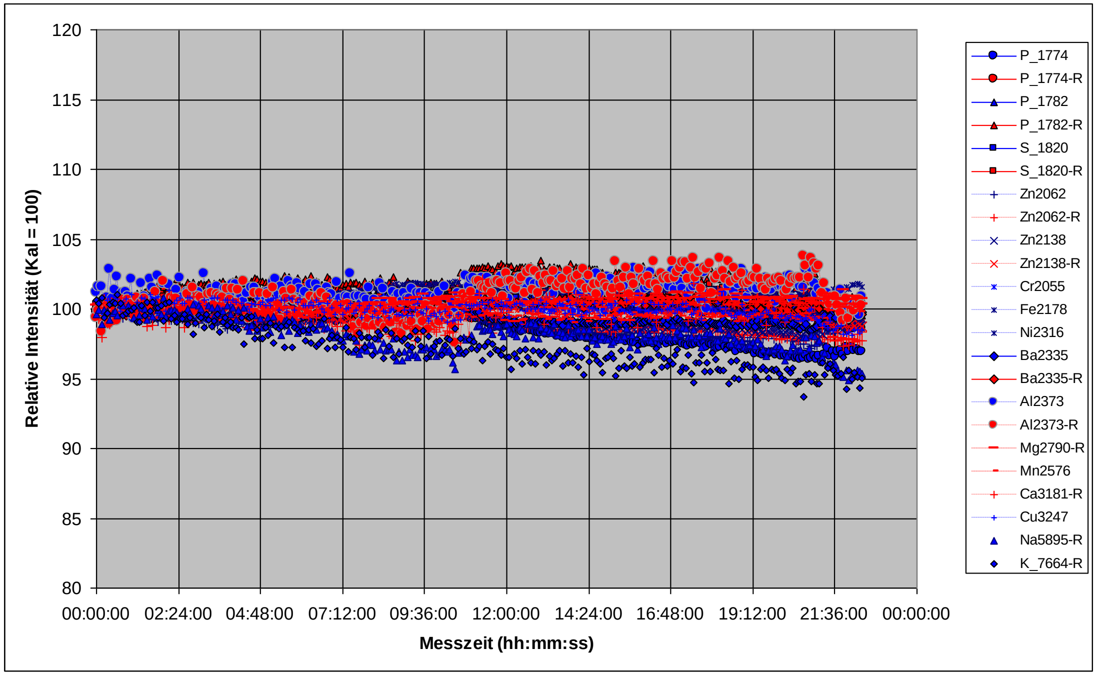


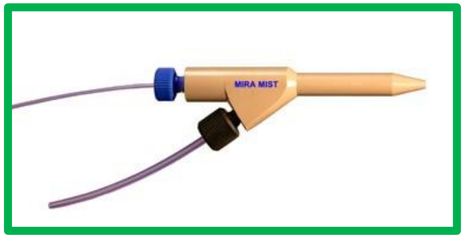


Repeat analysis over 3 hours using the standard quartz radial view window: Axial (red) signals stable, but radial signals drift

Example application 2: Concentrated metal digests

Aqua regia 10g/L vanadium concentrate analysis using iCAP 7400 Duo, without internal standard correction





Repeat analysis over > 21 hours using the purged radial window:

Axial (red) and radial (blue) signals both stable

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Results summary for concentrate metal digests analysis

300 samples monitored over > 21 hours, results normalised to 100%

Data obtained with purged radial view window, with Y internal standard correction

Line	Observation	Avg	*RSD*	min	max	*Δ*
	ax/rad	%	%	%	%	%
P_1774	axial	98,6	*1,2*	96,1	100,0	*3,9*
P_1774-2	radial	100,5	*0,6*	98,4	101,5	*3,1*
P_1782	axial	100,5	*0,6*	98,7	101,4	*2,7*
P_1782-2	radial	102,0	*0,7*	100,0	103,5	*3,5*
S_1820	axial	100,6	*0,4*	99,3	101,4	*2,2*
S_1820-2	radial	100,8	*0,5*	99,2	102,0	*2,8*
As1890	axial	99,6	*0,6*	97,7	101,2	*3,5*
Zn2025	axial	96,5	*1,9*	93,1	100,1	*7,0*
Zn2025-2	radial	96,8	*1,7*	93,9	99,9	*6,0*
Cr2055	axial	100,1	*0,4*	99,0	101,0	*2,0*
Zn2062	axial	99,0	*0,9*	97,2	100,9	*3,7*
Zn2062-2	radial	99,0	*0,6*	97,4	100,1	*2,7*
Fe2084	axial	98,9	*1,0*	97,1	100,2	*3,1*
P_2136	axial	100,1	*0,4*	99,3	101,1	*1,8*
P_2136-2	radial	100,2	*0,3*	99,3	100,9	*1,6*
Zn2138	axial	99,2	*0,5*	98,1	100,2	*2,1*
Zn2138-2	radial	99,9	*0,3*	98,5	100,5	*2,1*
Fe2178	axial	100,1	*0,3*	98,9	100,7	*1,8*
Pb2203	axial	100,9	*0,6*	99,8	102,2	*2,4*
Ni2216	axial	101,2	*0,8*	99,7	102,6	*2,9*
Co2286	axial	99,9	*0,5*	99,2	101,2	*2,0*
Ni2316	axial	101,0	*0,5*	99,9	102,0	*2,1*
Ba2335	axial	99,5	*0,5*	98,5	100,9	*2,4*
Ba2335-2	radial	100,2	*0,3*	99,3	101,1	*1,8*

Example application 3: Analysis of engine lubrication oils

- iCAP 7400 ICP-OES Radial
  - V-groove nebuliser
  - Ceramic D-Torch
  - Baffled cyclonic spray chamber
- Wear metals in oil materials analysed
  - Quartz 7000 oil (unused – New)
  - Quartz 7000 oil (200 hours use – Intermediate)
  - Quartz 7000 oil (400 hours use - Old)
- Samples diluted 10x with xylene and measured 8 consecutive times
- Y used as internal standard

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Engine lubrication oils analysis results

Element and wavelength	New oil	Intermediate oil	Old oil
Ag 338.389 nm	0.76	0.87	0.94
Al 308.215 nm	0.09	0.05	0.05
B 208.959 nm	2.14	1.63	2.46
Ba 223.527 nm	ND	0.46	0.82
Ca 184.006 nm	1103	2293	3014
Cd 214.438 nm	0.15	0.17	0.27
Cr 267.716 nm	0.12	1.15	2.54
Cu 324.754 nm	0.58	2.03	3.49
Fe 238.204 nm	2.76	23.2	30.8
Mg 279.553 nm	870.8	631.2	323.4
Mn 293.930 nm	0.21	0.63	0.89

Element and wavelength	New oil	Intermediate oil	Old oil
Mo 281.615 nm	ND	0.16	0.38
Na 589.592 nm	5.71	5.2	3.71
Ni 231.604 nm	0.73	0.59	0.48
P 178.284 nm	972.4	1045	984.1
Pb 220.353 nm	16	12.1	8
S 180.731 nm	5731	5776	5134
Si 212.412 nm	7.15	10.3	10.8
Sn 283.999 nm	7.7	4.58	2.53
Ti 334.941 nm	0.4	0.48	0.51
V 309.311 nm	2.2	1.46	0.7
Zn 213.856 nm	1038	1143	1106

- Results in mg/kg in the undiluted oil
- Increased concentration of key elements indicative of engine wear
  - Ca, Cr, Cu, Mn, Fe
- Certain elements (e.g. Mg) decrease with oil use; Mg sulfonates used as detergents to help keep engines clean so possibly lost by precipitation as oil ages with engine use

Improving productivity with ICP-OES

Achieving higher sample throughput with less manual labour

Ultrafast Sample Introduction

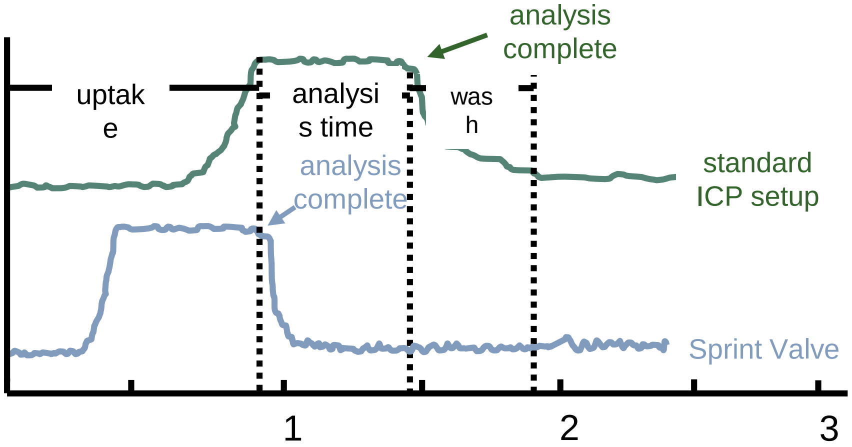
Automated Sample Preparation and Intelligent Dilution

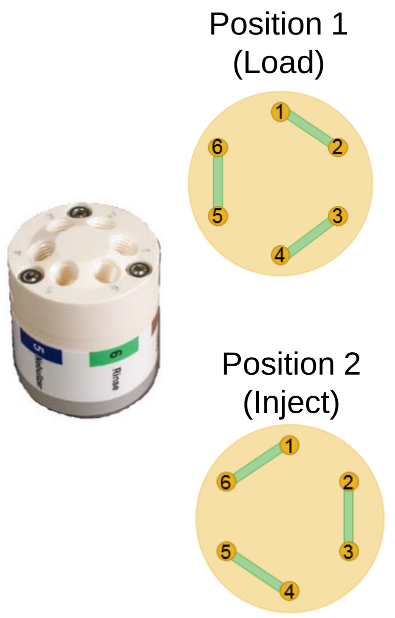
Automated and simplified method set up:

Element Finder^{TM}

Ultrafast sample introduction (standard with iCAP 7600)

- Rapid sample introduction with automated Sprint Valve
  - 6 ports, 2 positions (load, inject)
  - Fast sample loading into injection loop using integrated vacuum pump
  - Short connection from valve to nebulizer – rapid uptake time when valve switches to inject position
  - Fast washout when loop switches back to load position



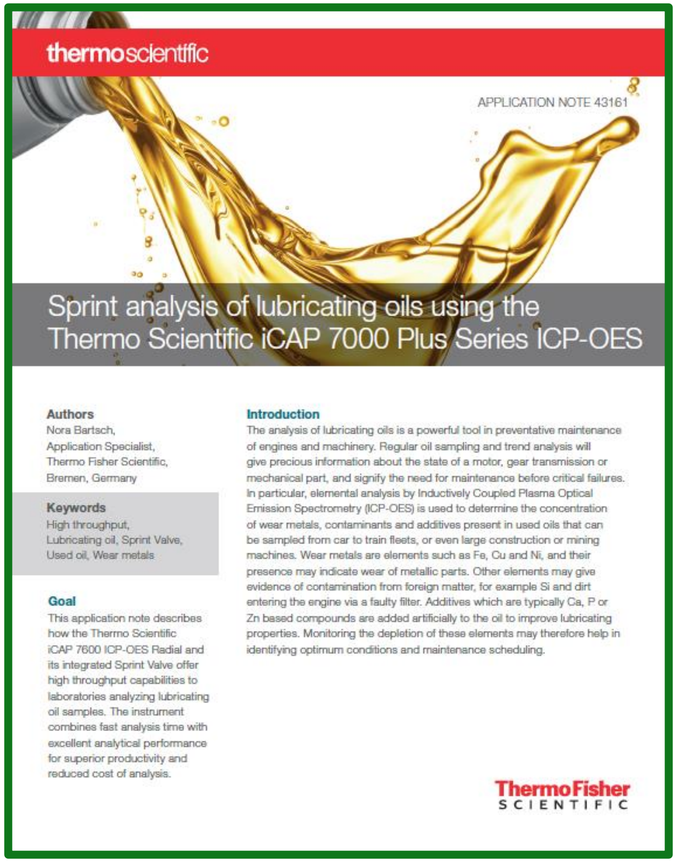


Standard ICP setup: 2 min

Sprint Valve: 1 min

Sprint valve operation applied to lubricating oils analysis - summary

- Samples diluted 10x with white spirit solvent
- Yttrium internal standard used
- Sprint valve method
    - Total analysis time per sample - sample load, inject, uptake and acquisition time = 1 minute
    - Acquisition parameters = 2 repeats, 5 seconds integration time per repeat
    - Number of analytes = 22
    - Detection limits (3 x standard deviation of 10 consecutive blanks) in the range 0.5 to 50 mg/kg in undiluted samples
- For more details see application note AN 43161



thermoscientific

APPLICATION NOTE 43161

Sprint analysis of lubricating oils using the Thermo Scientific iCAP 7000 Plus Series ICP-OES

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Keywords
High throughput,
Lubricating oil, Sprint Valve,
Used oil, Wear metals

Goal
This application note describes how the Thermo Scientific iCAP 7600 ICP-OES Radial and its integrated Sprint Valve offer high throughput capabilities to laboratories analyzing lubricating oil samples. The instrument combines fast analysis time with excellent analytical performance for superior productivity and reduced cost of analysis.

Introduction
The analysis of lubricating oils is a powerful tool in preventative maintenance of engines and machinery. Regular oil sampling and trend analysis will give precious information about the state of a motor, gear transmission or mechanical part, and signify the need for maintenance before critical failures. In particular, elemental analysis by Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES) is used to determine the concentration of wear metals, contaminants and additives present in used oils that can be sampled from car to train fleets, or even large construction or mining machines. Wear metals are elements such as Fe, Cu and Ni, and their presence may indicate wear of metallic parts. Other elements may give evidence of contamination from foreign matter, for example Si and dirt entering the engine via a faulty filter. Additives which are typically Ca, P or Zn based compounds are added artificially to the oil to improve lubricating properties. Monitoring the depletion of these elements may therefore help in identifying optimum conditions and maintenance scheduling.

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Automated sample preparation and intelligent dilution

Teledyne CETAC SDX$_{HPLD}$

- Serial dilution
- Vortex mixing
- Max. 50

ESI prep*FAST*

- Online dilution
- Syringe system
- I ut

Both systems are capable of **Prescriptive Dilution** and **Intelligent Dilution**

Qtegra software used to define dilution parameters

Fully integrated with iCAP 7000 Plus Series ICP-OES and iCAP Qnova Series ICP-MS with the Qtegra ISDS Software

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Auto-dilution systems – Prescriptive dilution

Running Samples

- Autodilution

- Prescriptive dilution allows sample specific dilution in a single analytical run
- Advantage over fixed dilution approaches such as:
  - Liquid dilution via ratios of peristaltic pump tubing internal diameters
  - Manual off-line dilution with fixed sample and solvent volumes

TELEDYNE CETAC
SDX_{HPLD}

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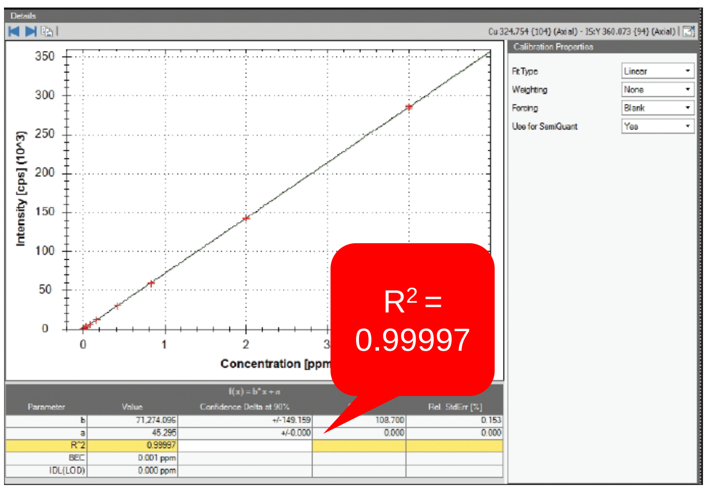
Prescriptive dilution – building a calibration curve

Running Samples

- Autodilution

- Automatic generation of 0.01 to 4 ppm calibration line from single stock standard



Dilution of one stock standard

	Label	Sample Type	Standard	Rack	Vial	prepFAST DF
1	BLK	AVERAGE BLK		1	2	1
2	BLK	AVERAGE BLK		1	2	1
3	BLK	AVERAGE BLK		1	2	1
4	0.010 ppm	STD	4 ppm stock	1	3	400
5	0.013 ppm	STD	4 ppm stock	1	3	300
6	0.020 ppm	STD	4 ppm stock	1	3	200
7	0.040 ppm	STD	4 ppm stock	1	3	100
8	0.080 ppm	STD	4 ppm stock	1	3	50
9	0.160 ppm	STD	4 ppm stock	1	3	25
10	0.4 ppm	STD	4 ppm stock	1	3	10
11	0.8 ppm	STD	4 ppm stock	1	3	5
12	2 ppm	STD	4 ppm stock	1	3	2
13	4 ppm	STD	4 ppm stock	1	3	1

- Dual stocks can be used to further extend automated calibration ranges

Auto-dilution systems – Intelligent Dilution

Running Samples

- Autodilution

- Advanced, intelligent auto-dilution of analyses based on specific criteria, e.g.:
  - Out-of-range analyte concentration with respect to calibration curve
  - Internal standard suppression indicating that matrix concentrations are too high
- Auto-dilution setting is automatically calculated and applied on a sample by sample basis

ESI prep*FAST*

Qtegra™

Intelligent Scientific Data Solution™

The world leader in serving science

iCAP 7000 Series ICP-OES – Qtegra driven!

What is Qtegra?

Qtegra is a workflow driven software platform for analytical instruments which allows a complete intuitive and state of the art user experience.

It is for sample measurement and data processing in consideration of traceability and transparency to meet formal guidelines such as electronic records and signatures as described in FDA regulation 21 CFR Part 11.

The four pillars of Qtegra ISDS

Workflow

- **PRODUCTIVE**
- **Simple workflow**
  - Dashboard
  - Protocol
  - LabBooks
- **Time saving**
  - One click ‘Get Ready’
  - 5 clicks to LabBook
- **Relevant Results**
- **Relevant Reporting**
- Feel / Ease of use
- Start-up
- Commonality

Scalability

- **Large and growing number of instruments on Qtegra**
- **Large number of peripherals supported**
- Tree of techniques
- Interfaces
- Inputs
- Plug-ins
- Training
- Commonality

Compliance

- Regulations
- Security
- Data integrity
- Simplified validation
- Commonality

Data Management

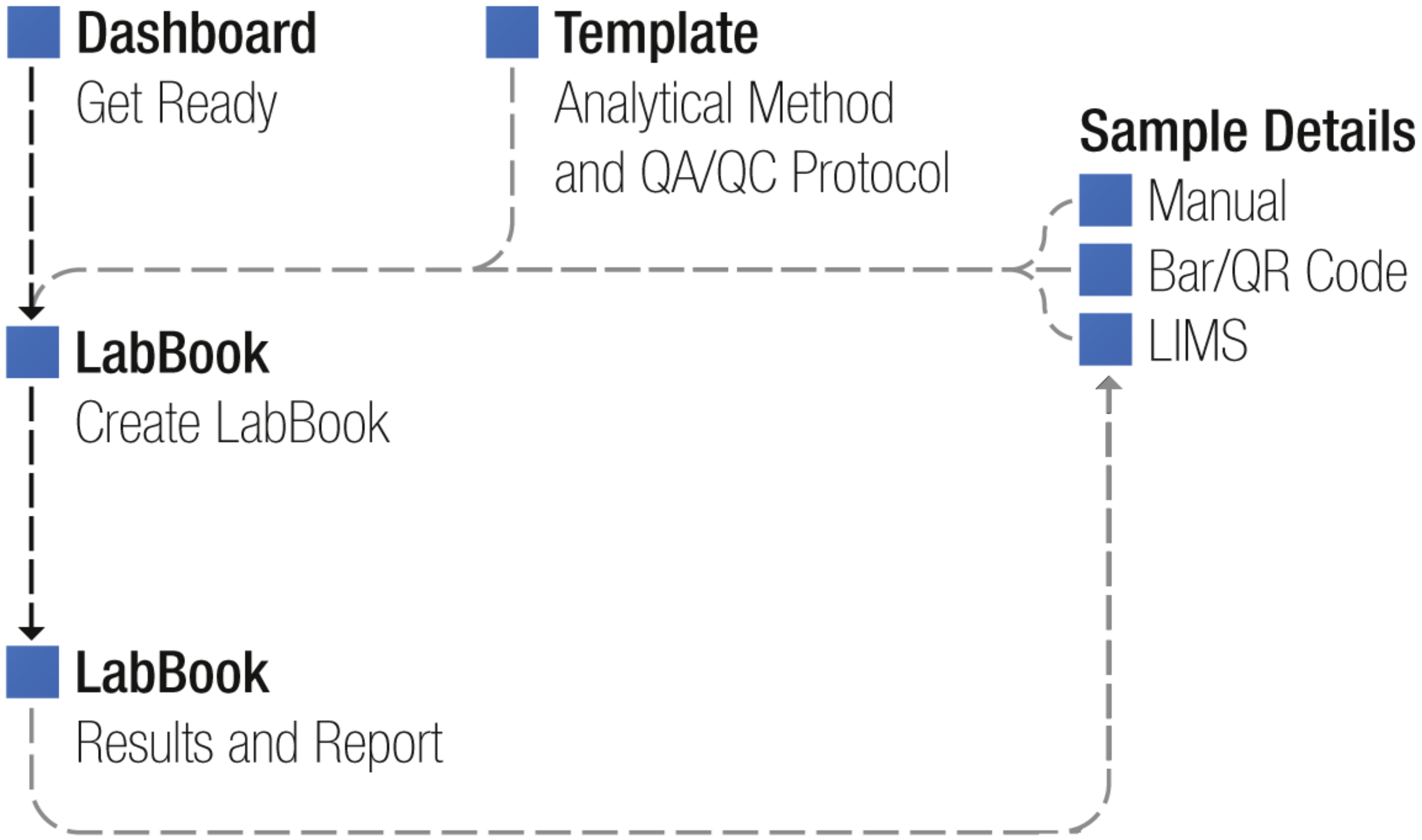
- Data connectivity
- LIMS connectivity
- Data search and amalgamation
- Report outputs
- Relevant reporting
- Commonality

Workflow – How to get from sample to results

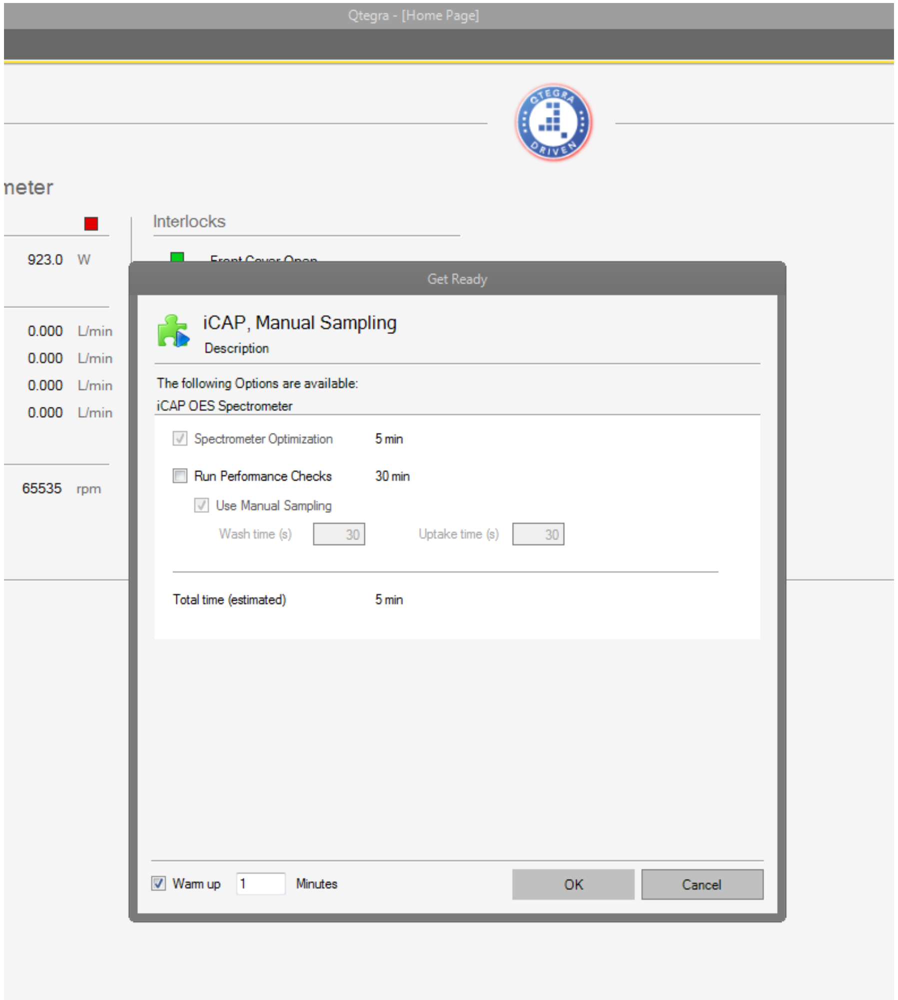
Qtegra intelligent workflows drive to results:

- Simplified pathways
- Reduced number of steps
- Save time with automation
- Reduce training
- Increase productivity

Workflow from a template to a LabBook



Workflow - Dashboard - *'Get Ready'*



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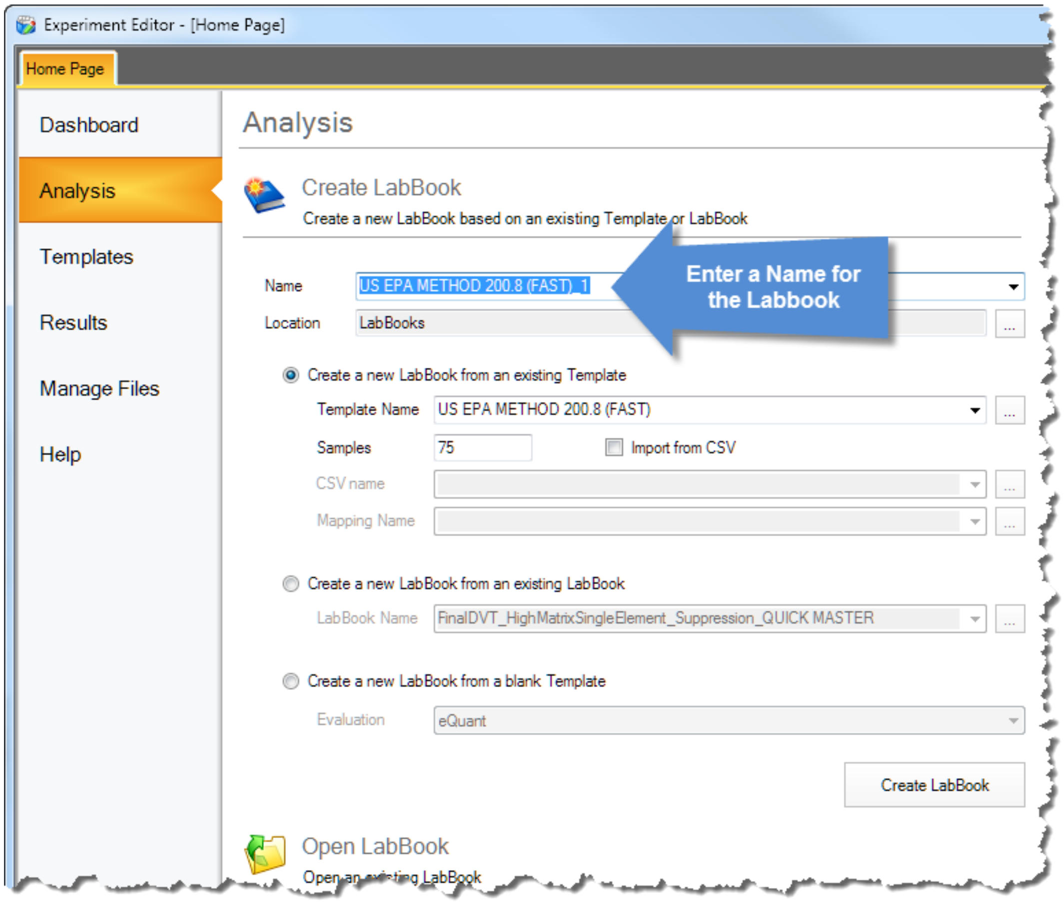
Workflow - Dashboard – *'Get Ready'*

- Prepares system for analysis
  - Confirms performance

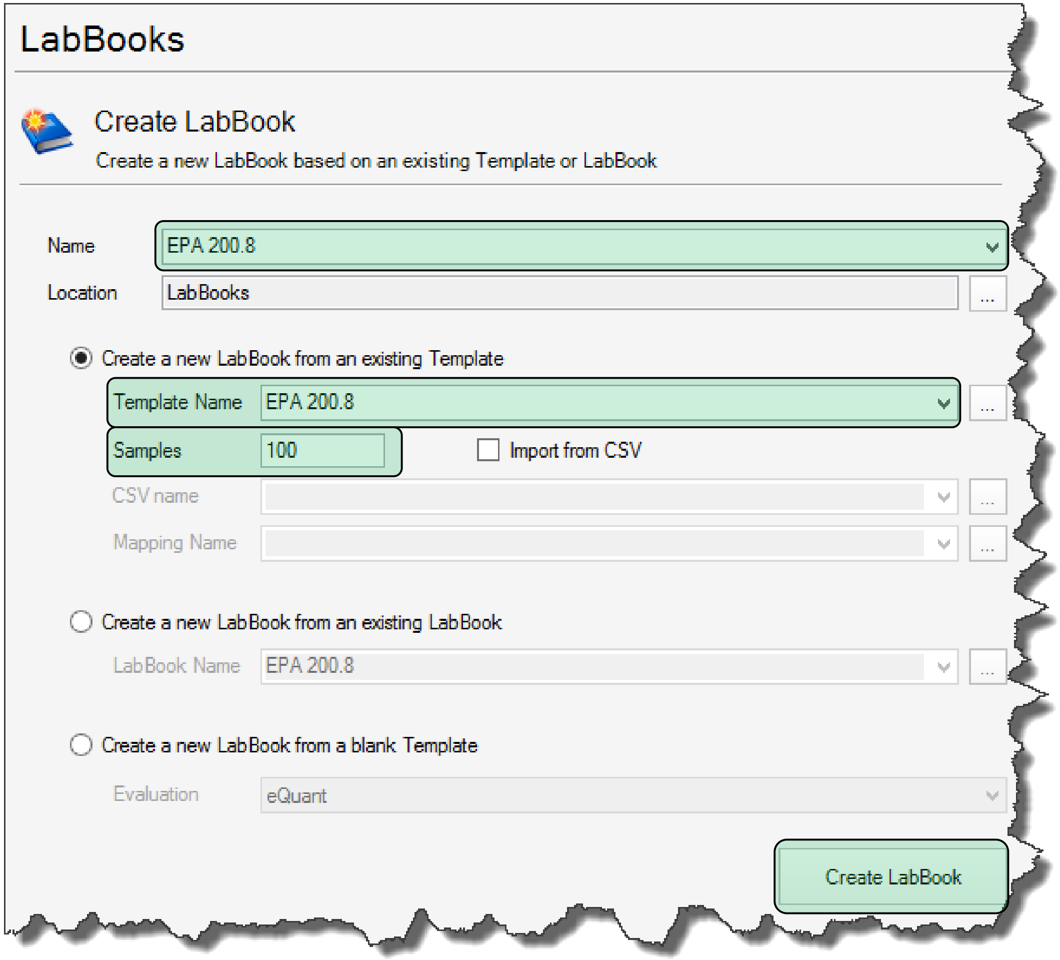
- Improves quality of results
- Saves time
- Reduces requirement for training
- Improves productivity

Workflow - Qtegra LabBook



- Prepared in 4 clicks
- LabBook contains:
  - Method
  - Analytical protocol
  - Intelligent sequence checks
  - Data
  - Results
  - Report
  - Audit logs

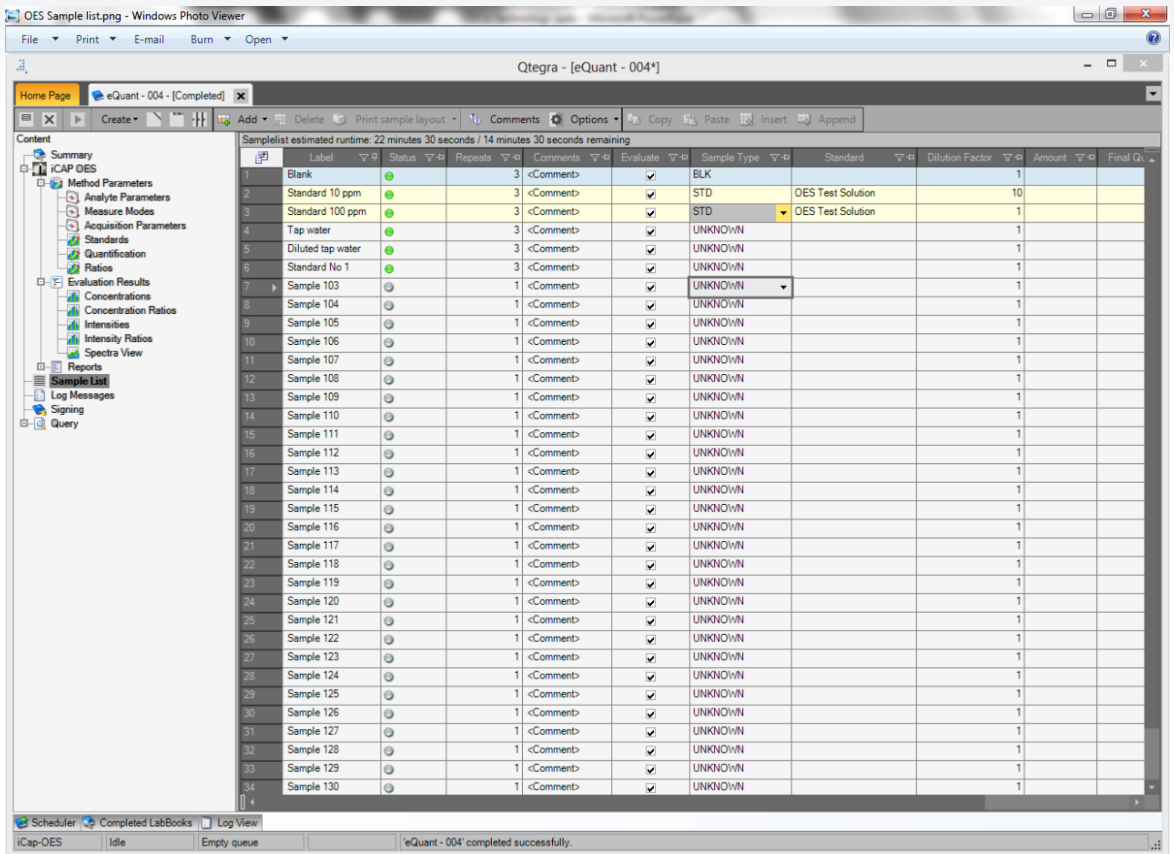
Four steps to an EPA compliant analysis



1. Insert a name
2. Select a template
3. Enter the number of samples or import from LIMS
4. Click create

LabBook Sample List

- List of samples for analysis: Standards, Unknowns & QC
- Can be modified whilst the sample list is running



Comprehensive quality control tests

Blank Verification	Continuous Calibration Blank (CCB) Initial Calibration Blank (ICB) Memory Blank Test (MTB) Preparation Blank (PRB)
Calibration Verification	Continuous Calibration Verification (CCV) Initial Calibration Verification (ICV) Laboratory Control Standard (LCS) Quality Control Standard (QCS)
Paired Sample Tests	Duplicate (DUP) Serial Dilution (SER)
Matrix Tests	Laboratory fortified Blank (LFB) Matrix Spike (MXS) Post Digestion Spike (PDS)
Continuous Tests	Regression Coefficient Verification (RCV) Relative Stability Verification (RSV)
Internal Standard Test	Internal Standard Test (IST)

Data presentation

Guiding principle:

Present only data which are valuable to a certain time

- Hide data set complexity
- Guide user in an intelligent way to the required data set
- Bring attention to suspicious data
- Offer tools to simplify laboratory workflows

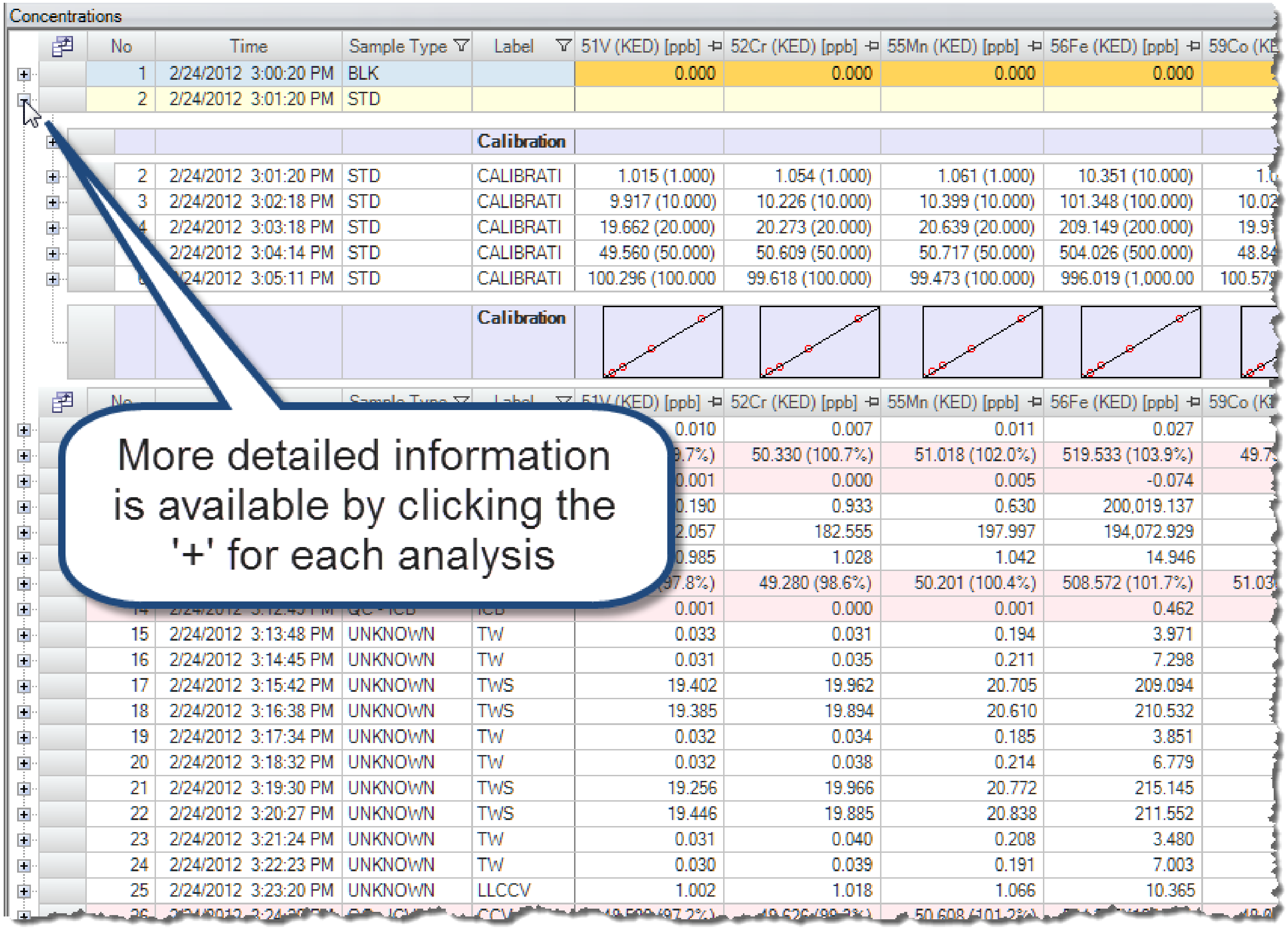
Workflow – LabBook Data presentation

Concentrations

No	Time	Sample Type	Label	51V (KED) [ppb]	52Cr (KED) [ppb]	55Mn (KED) [ppb]	56Fe (KED) [ppb]
1	2/24/2012 3:00:20 PM	BLK		0.000	0.000	0.000	0.000
2	2/24/2012 3:01:20 PM	STD					
7	2/24/2012 3:06:07 PM	UNKNOWN	RINSE	0.010	0.007	0.011	0.027
8	2/24/2012 3:07:04 PM	QC - ICV	ICV	49.839 (99.7%)	50.330 (100.7%)	51.018 (102.0%)	519.533 (103.9%)
9	2/24/2012 3:08:03 PM	QC - ICB	ICB	0.001	0.000	0.005	-0.074
10	2/24/2012 3:09:02 PM	UNKNOWN	ICSA	0.190	0.933	0.630	200,019.137
11	2/24/2012 3:10:00 PM	UNKNOWN	ICSAB	192.057	182.555	197.997	194,072.929
12	2/24/2012 3:10:57 PM	UNKNOWN	LLCCV	0.985	1.028	1.042	14.946
13	2/24/2012 3:11:53 PM	QC - ICV	CCV	[illegible]	49.280 (98.6%)	50.201 (100.4%)	508.572 (101.7%)
14	2/24/2012 3:12:49 PM	QC - ICB	ICB	[illegible]	[illegible]	[illegible]	0.462
15	2/24/2012 3:13:48 PM	UNKNOWN	TW	[illegible]	[illegible]	[illegible]	3.971
16	2/24/2012 3:14:45 PM	UNKNOWN	TW	[illegible]	[illegible]	[illegible]	7.298
17	2/24/2012 3:15:42 PM	UNKNOWN	TWS	[illegible]	[illegible]	[illegible]	209.094
18	2/24/2012 3:16:38 PM	UNKNOWN	TWS	[illegible]	[illegible]	[illegible]	210.532
19	2/24/2012 3:17:34 PM	UNKNOWN	TW	[illegible]	[illegible]	[illegible]	3.851
20	2/24/2012 3:18:32 PM	UNKNOWN	TW	[illegible]	[illegible]	[illegible]	6.779
21	2/24/2012 3:19:30 PM	UNKNOWN	TWS	[illegible]	[illegible]	[illegible]	215.145
22	2/24/2012 3:20:27 PM	UNKNOWN	TWS	[illegible]	[illegible]	[illegible]	211.552
23	2/24/2012 3:21:24 PM	UNKNOWN	TW	[illegible]	[illegible]	[illegible]	3.480
24	2/24/2012 3:22:23 PM	UNKNOWN	TW	0.030	0.039	0.191	7.003
25	2/24/2012 3:23:20 PM	UNKNOWN	LLCCV	1.002	1.018	1.066	10.365
26	2/24/2012 3:24:20 PM	QC - ICV	CCV	48.588 (97.2%)	49.626 (99.3%)	50.608 (101.2%)	514.245 (102.8%)
27	2/24/2012 3:25:18 PM	QC - CCB	CCB	0.005	0.000	0.000	0.084
28	2/24/2012 3:28:41 PM	UNKNOWN	TW	0.031	0.033	0.198	3.422
29	2/24/2012 3:29:38 PM	UNKNOWN	TW	0.028	0.038	0.205	7.096
30	2/24/2012 3:30:35 PM	UNKNOWN	TWS	19.565	19.954	21.044	209.265
31	2/24/2012 3:31:31 PM	UNKNOWN	TWS	19.634	19.865	20.810	212.177
32	2/24/2012 3:32:28 PM	UNKNOWN	TW	0.030	0.037	0.194	3.367
33	2/24/2012 3:33:25 PM	UNKNOWN	TW	0.026	0.039	0.225	7.157
34	2/24/2012 3:34:21 PM	UNKNOWN	TWS	19.576	20.160	21.230	214.227
35	2/24/2012 3:35:19 PM	UNKNOWN	TWS	19.446	19.962	20.854	211.176
36	2/24/2012 3:36:16 PM	UNKNOWN	TW	0.028	0.037	0.203	3.349
37	2/24/2012 3:37:16 PM	UNKNOWN	TW	0.030	0.037	0.212	7.025

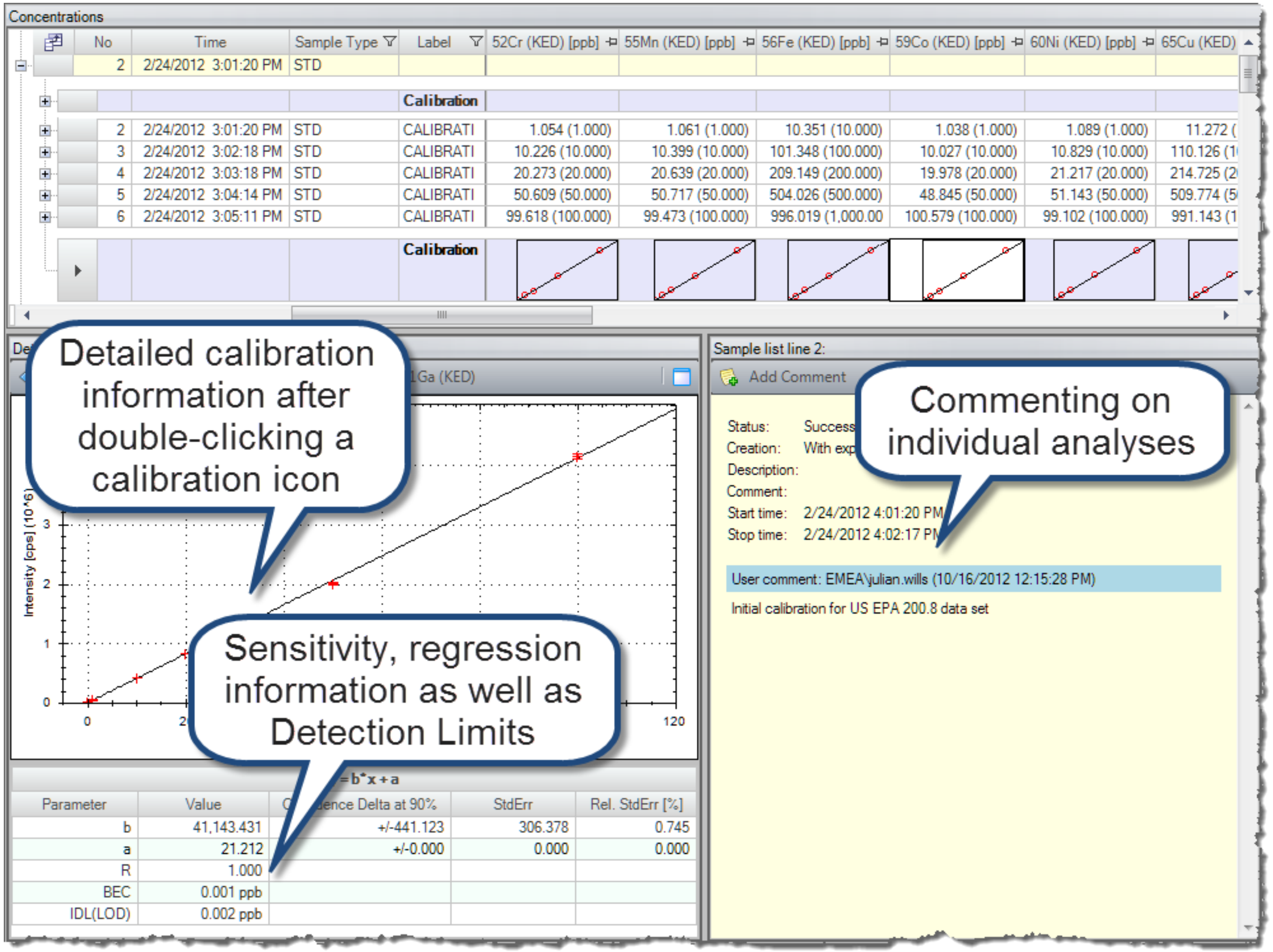
The initial display focus on the most important values - the final concentrations

Workflow – LabBook Data presentation



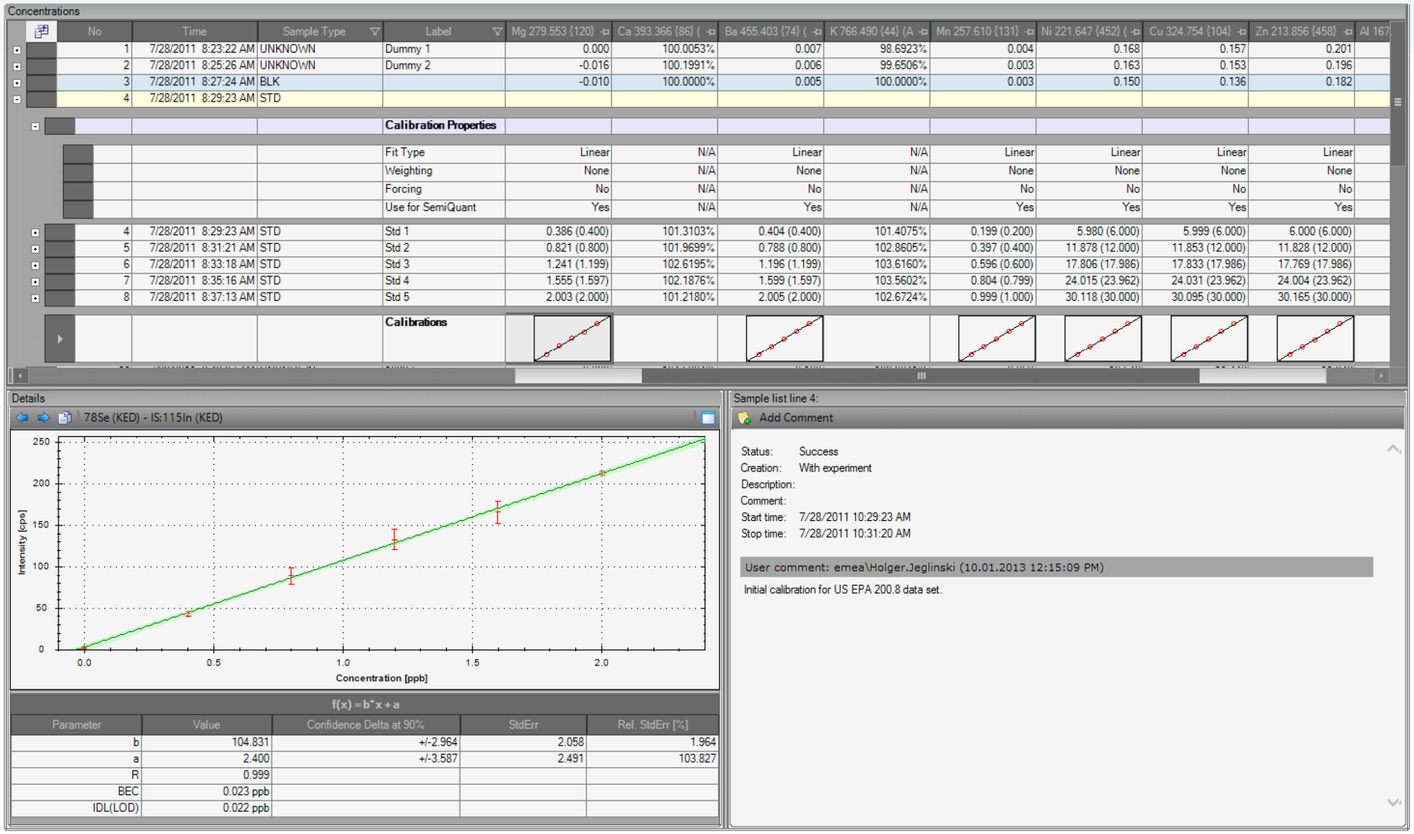
No	Time	Sample Type	Label	51V (KED) [ppb]	52Cr (KED) [ppb]	55Mn (KED) [ppb]	56Fe (KED) [ppb]	59Co (KE
1	2/24/2012 3:00:20 PM	BLK		0.000	0.000	0.000	0.000	
2	2/24/2012 3:01:20 PM	STD						
			Calibration					
2	2/24/2012 3:01:20 PM	STD	CALIBRATI	1.015 (1.000)	1.054 (1.000)	1.061 (1.000)	10.351 (10.000)	1.(
3	2/24/2012 3:02:18 PM	STD	CALIBRATI	9.917 (10.000)	10.226 (10.000)	10.399 (10.000)	101.348 (100.000)	10.02
4	2/24/2012 3:03:18 PM	STD	CALIBRATI	19.662 (20.000)	20.273 (20.000)	20.639 (20.000)	209.149 (200.000)	19.9
	2/24/2012 3:04:14 PM	STD	CALIBRATI	49.560 (50.000)	50.609 (50.000)	50.717 (50.000)	504.026 (500.000)	48.84
	/24/2012 3:05:11 PM	STD	CALIBRATI	100.296 (100.000	99.618 (100.000)	99.473 (100.000)	996.019 (1,000.00	100.57
			Calibration					
				0.010	0.007	0.011	0.027	
				9.7%)	50.330 (100.7%)	51.018 (102.0%)	519.533 (103.9%)	49.7
				0.001	0.000	0.005	-0.074	
				0.190	0.933	0.630	200,019.137	
				2.057	182.555	197.997	194,072.929	
				0.985	1.028	1.042	14.946	
				97.8%)	49.280 (98.6%)	50.201 (100.4%)	508.572 (101.7%)	51.03
14				0.001	0.000	0.001	0.462	
15	2/24/2012 3:13:48 PM	UNKNOWN	TW	0.033	0.031	0.194	3.971	
16	2/24/2012 3:14:45 PM	UNKNOWN	TW	0.031	0.035	0.211	7.298	
17	2/24/2012 3:15:42 PM	UNKNOWN	TWS	19.402	19.962	20.705	209.094	
18	2/24/2012 3:16:38 PM	UNKNOWN	TWS	19.385	19.894	20.610	210.532	
19	2/24/2012 3:17:34 PM	UNKNOWN	TW	0.032	0.034	0.185	3.851	
20	2/24/2012 3:18:32 PM	UNKNOWN	TW	0.032	0.038	0.214	6.779	
21	2/24/2012 3:19:30 PM	UNKNOWN	TWS	19.256	19.966	20.772	215.145	
22	2/24/2012 3:20:27 PM	UNKNOWN	TWS	19.446	19.885	20.838	211.552	
23	2/24/2012 3:21:24 PM	UNKNOWN	TW	0.031	0.040	0.208	3.480	
24	2/24/2012 3:22:23 PM	UNKNOWN	TW	0.030	0.039	0.191	7.003	
25	2/24/2012 3:23:20 PM	UNKNOWN	LLCCV	1.002	1.018	1.066	10.365	

Workflow – LabBook Data presentation



LabBook Results

- Results can be displayed in concentration, intensity etc
- Top level display plus the ability to drill down to individual replicates



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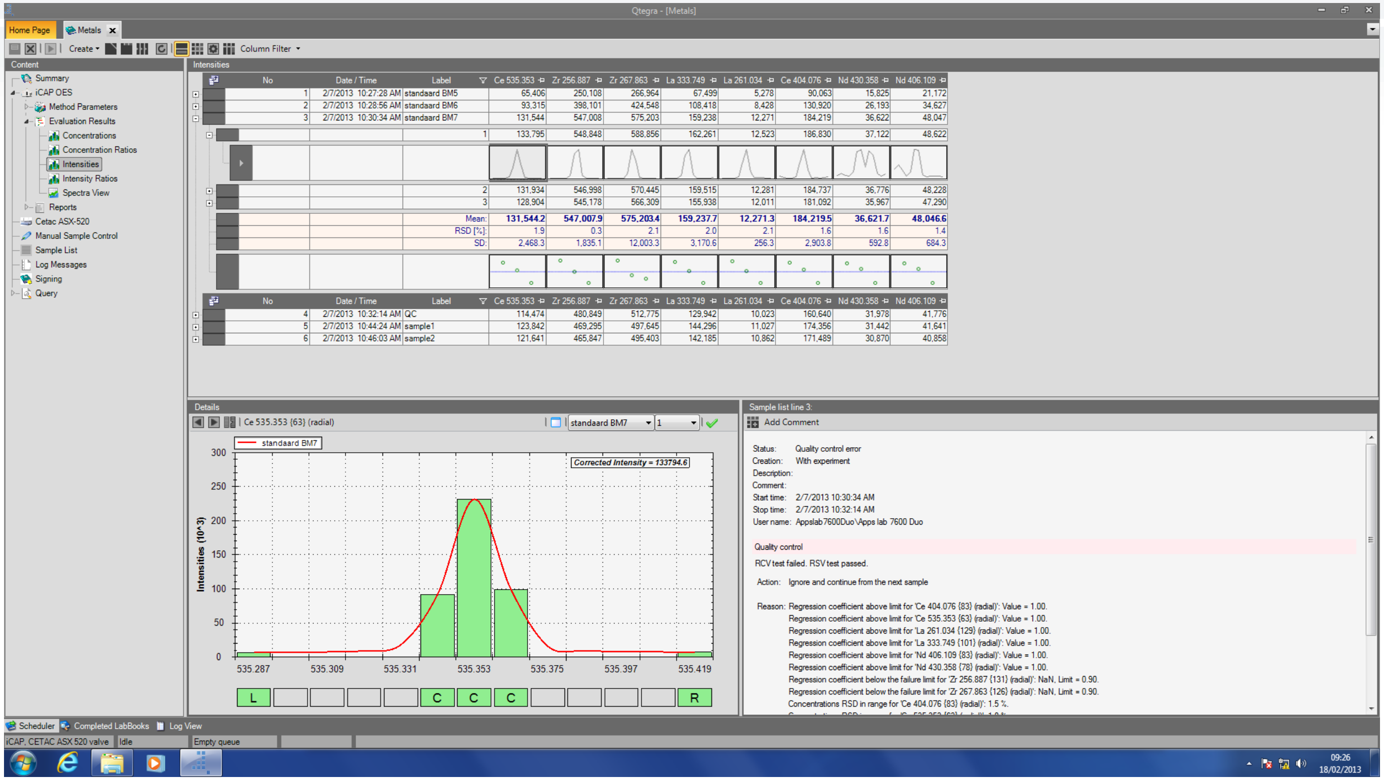
LabBook Results

- Check for interference
- Optimize background points
- Overlay data from previous runs



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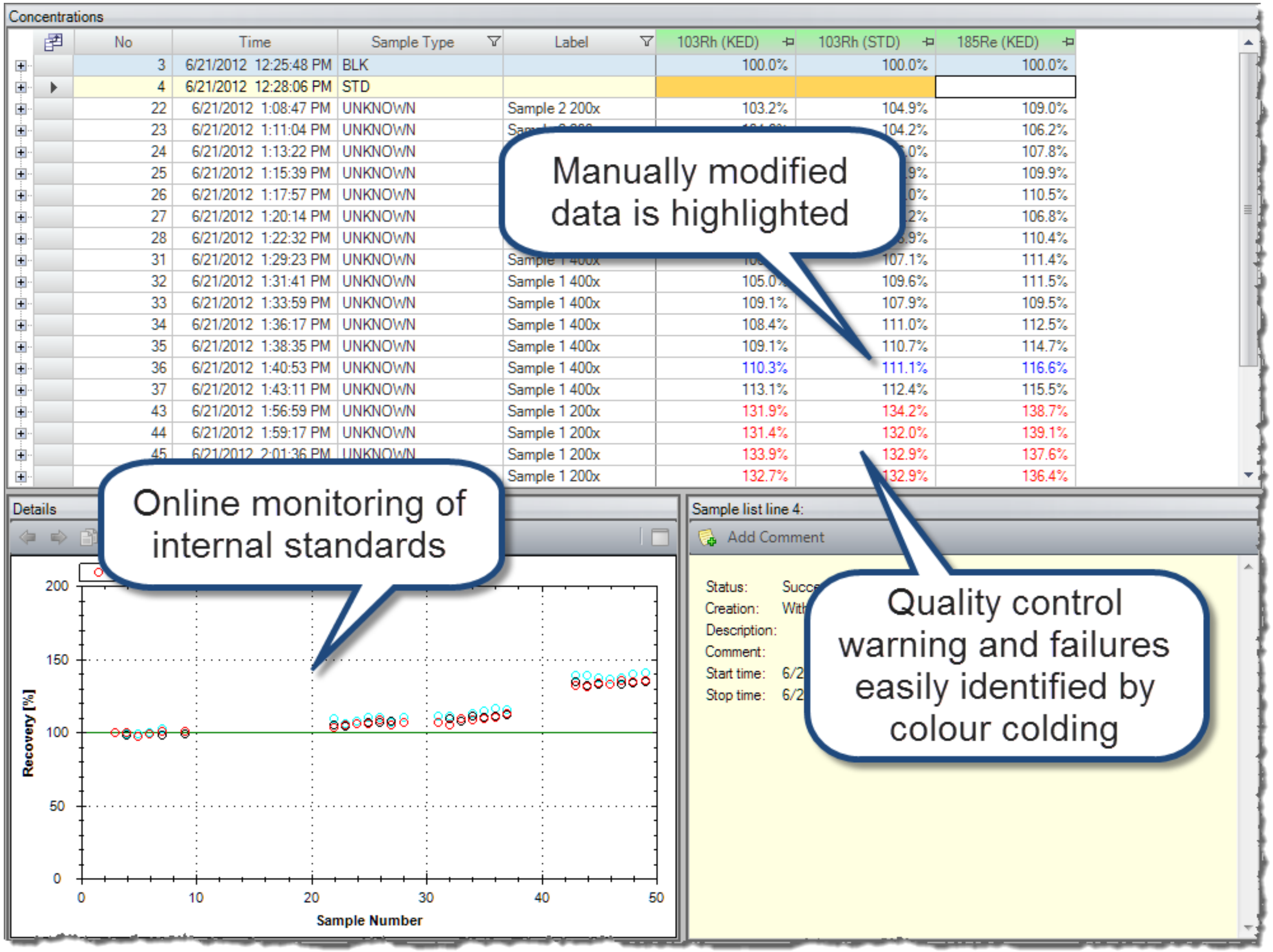
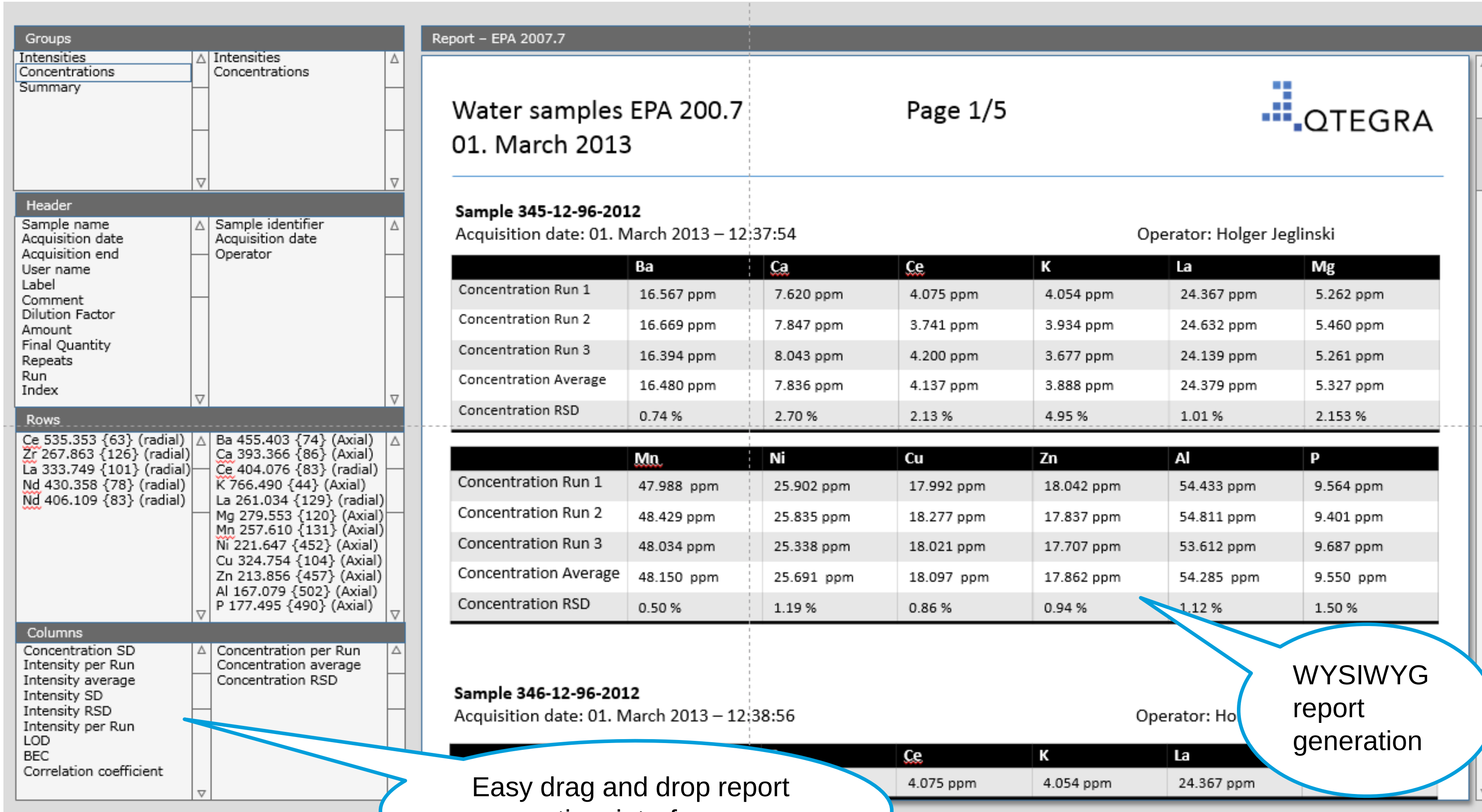
Qtegra: Data presentation



Customizable reports for tailored data presentation



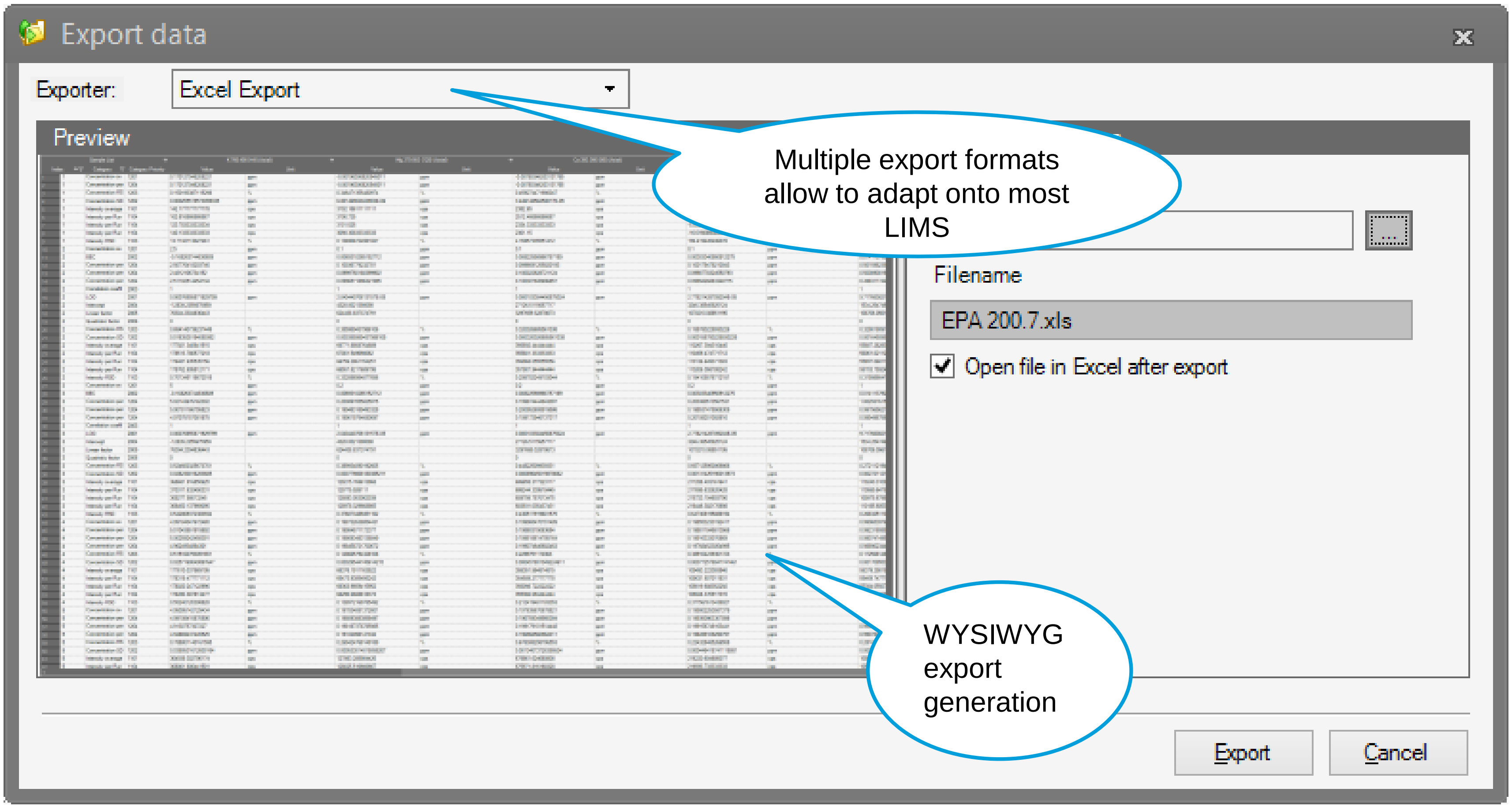
	Ba	Ca	Ce	K	La	Mg
Concentration Run 1	16.567 ppm	7.620 ppm	4.075 ppm	4.054 ppm	24.367 ppm	5.262 ppm
Concentration Run 2	16.669 ppm	7.847 ppm	3.741 ppm	3.934 ppm	24.632 ppm	5.460 ppm
Concentration Run 3	16.394 ppm	8.043 ppm	4.200 ppm	3.677 ppm	24.139 ppm	5.261 ppm
Concentration Average	16.480 ppm	7.836 ppm	4.137 ppm	3.888 ppm	24.379 ppm	5.327 ppm
Concentration RSD	0.74 %	2.70 %	2.13 %	4.95 %	1.01 %	2.153 %

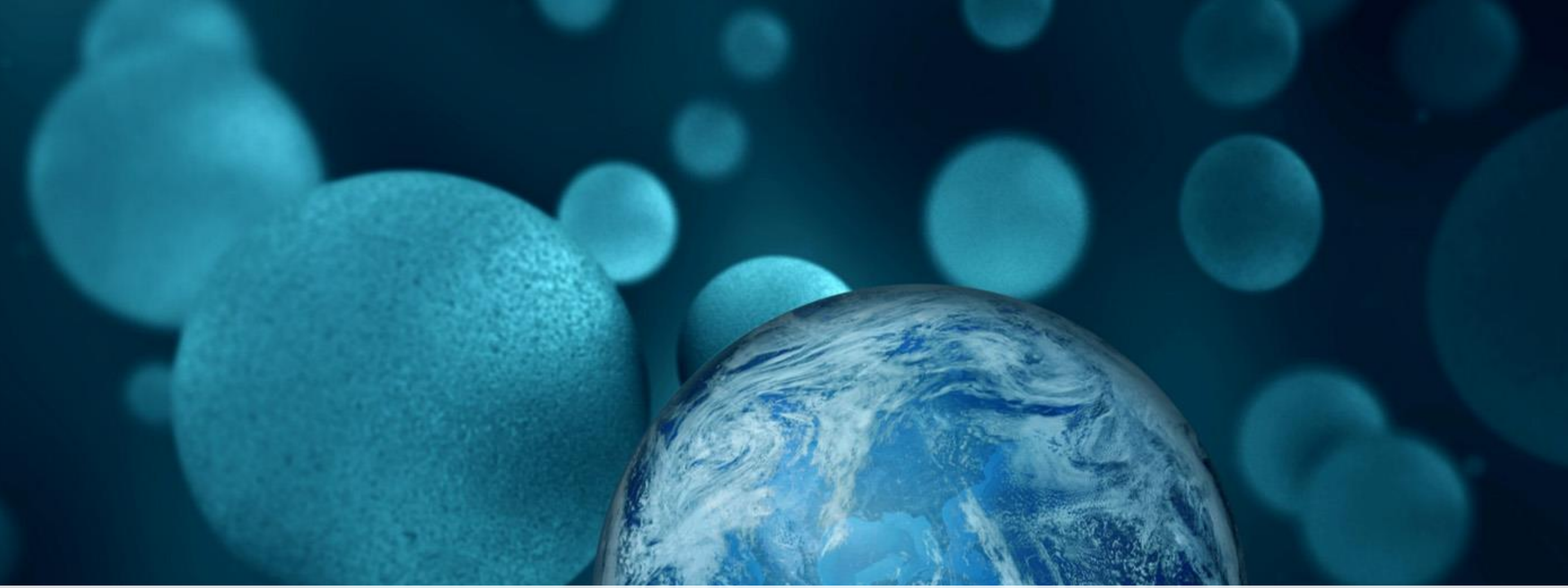
	Mn	Ni	Cu	Zn	Al	P
Concentration Run 1	47.988 ppm	25.902 ppm	17.992 ppm	18.042 ppm	54.433 ppm	9.564 ppm
Concentration Run 2	48.429 ppm	25.835 ppm	18.277 ppm	17.837 ppm	54.811 ppm	9.401 ppm
Concentration Run 3	48.034 ppm	25.338 ppm	18.021 ppm	17.707 ppm	53.612 ppm	9.687 ppm
Concentration Average	48.150 ppm	25.691 ppm	18.097 ppm	17.862 ppm	54.285 ppm	9.550 ppm
Concentration RSD	0.50 %	1.19 %	0.86 %	0.94 %	1.12 %	1.50 %

WYSIWYG report generation

Easy drag and drop report generation interface

Free customizable data exports





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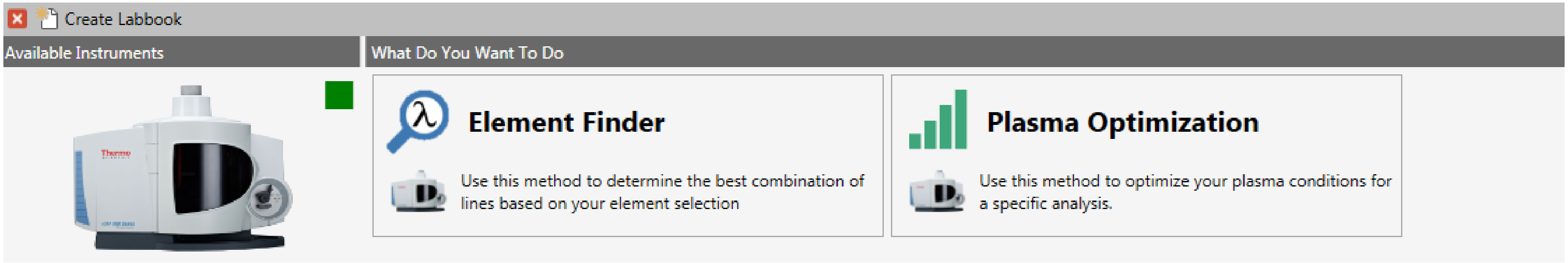
Element Finder plug-in Applications and Competition

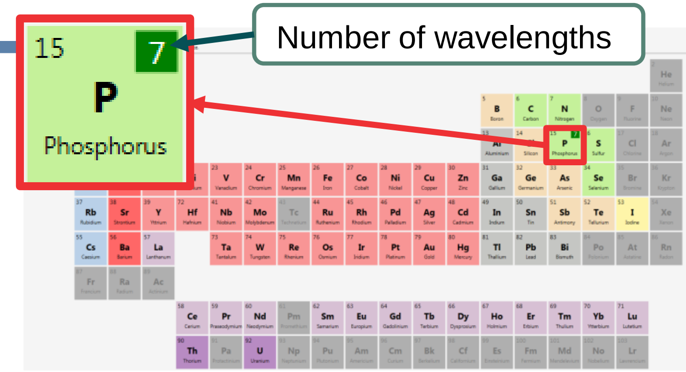
What is the Element Finder plug-in?

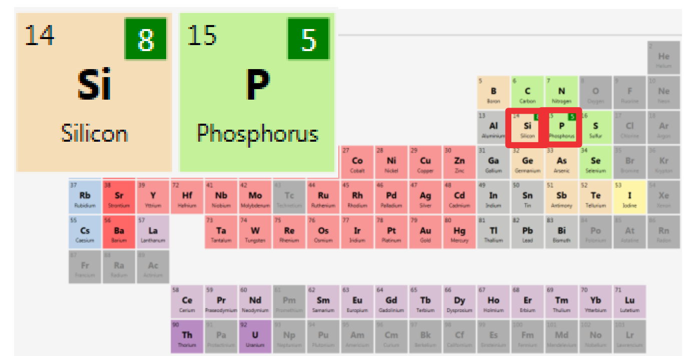
- An intuitive user-friendly method development tool
- Automated selection of analytical wavelengths, free from potential interferences
- Automated plasma optimization, based on the elements of interest and the elements present in the sample matrix
- The software intelligently selects wavelengths and plasma conditions

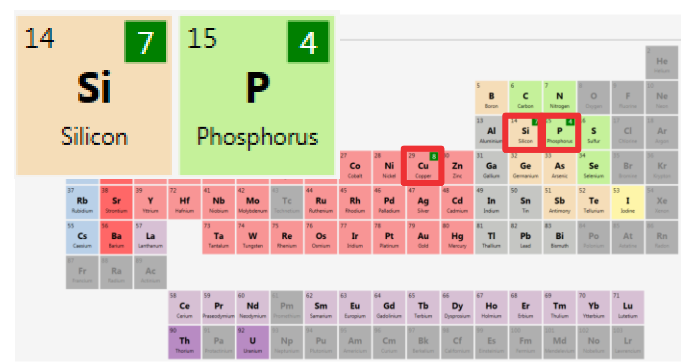


How does the Element Finder plug-in work?

- User input of analyte elements
  - Each element has the number of wavelengths for analysis
  - As more analytes are added the wavelengths are refined and reduced
  - Selection based on know interferences
  - The same happens when adding matrix elements
  - No wavelength selection by the user is taking place
- **The user is just selecting elements!**

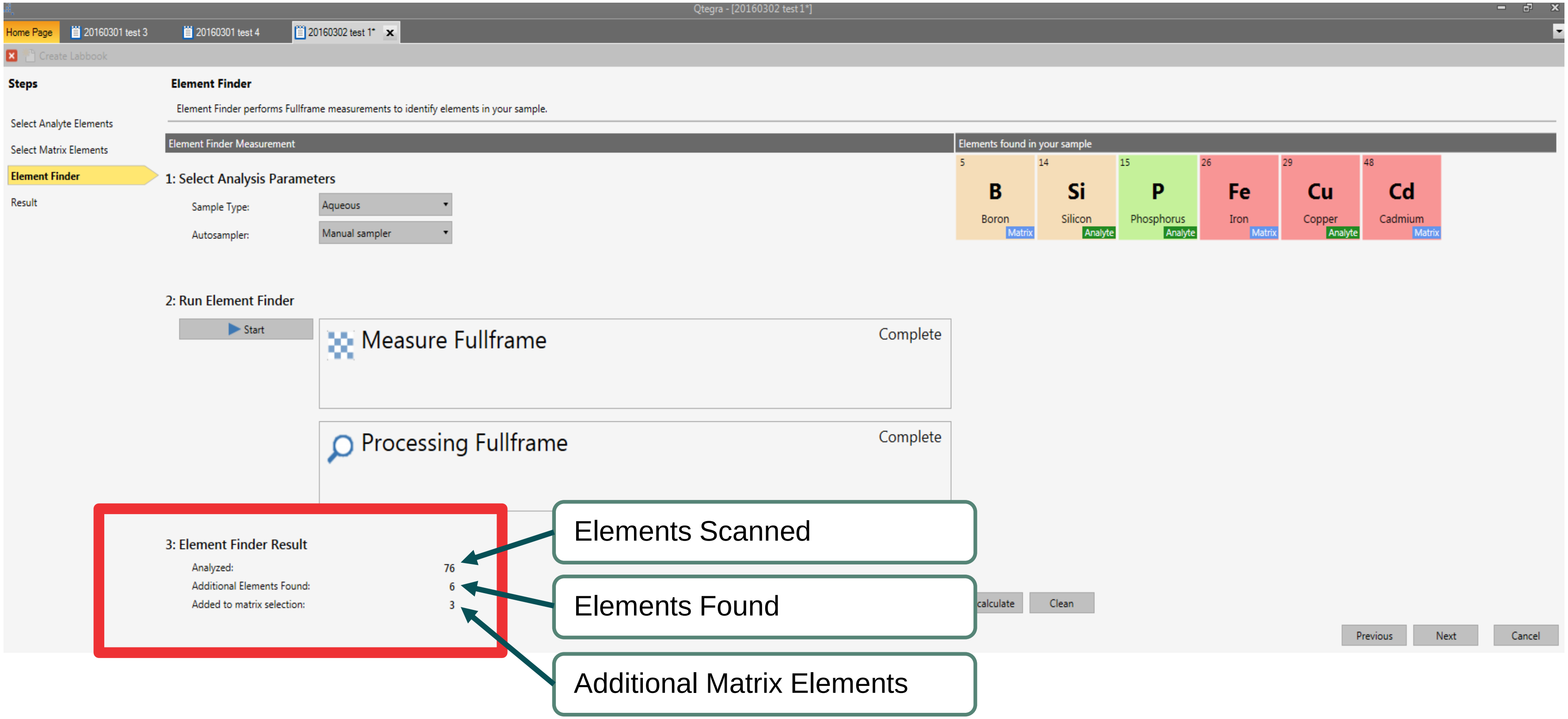






Element Finder – Analysis of an unknown sample

- <u>**Takes less than 5 minutes and uses just 8mL of sample!**</u>



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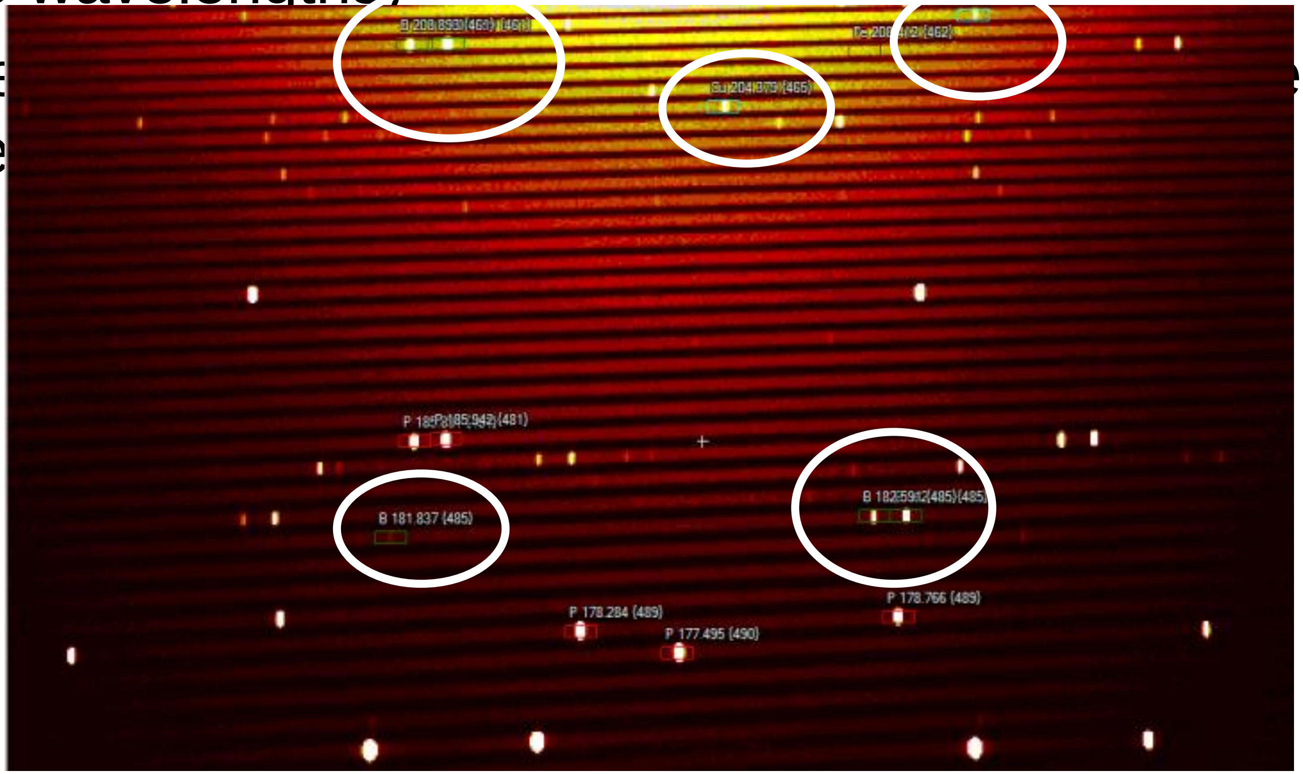
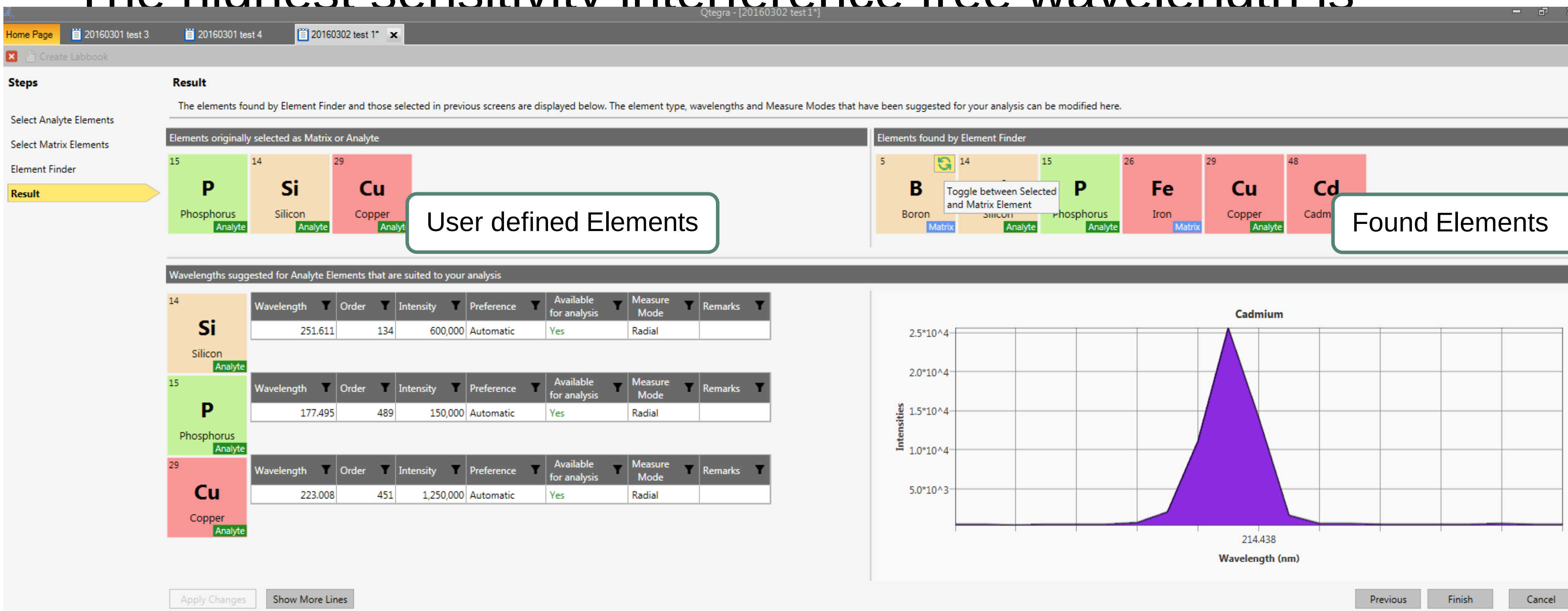
Element Finder – Analysis of an unknown sample

- Fullframes are used to collect the spectrum of the sample
- The Element Finder plug-in analyses the Fullframes and confirms the present of a element (when it is present at multiple wavelengths)
- The use ented with the

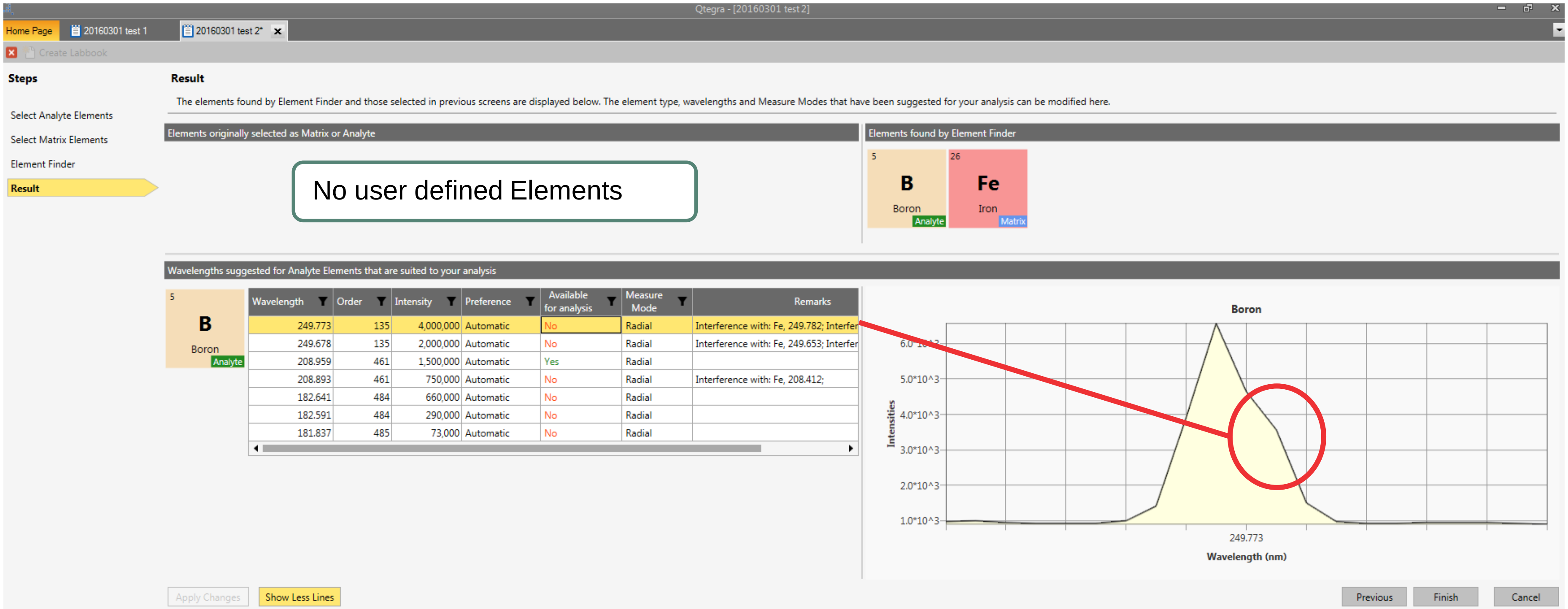


Element Finder plug-in results of Fullframe

- Elements selected by the displayed (analyte and Matrix)
- Elements found by Element Finder are displayed
  - Found elements are assumed to be matrix elements (unless already defined
  - User can convert to analyte elements
- The highest sensitivity interference free wavelength is

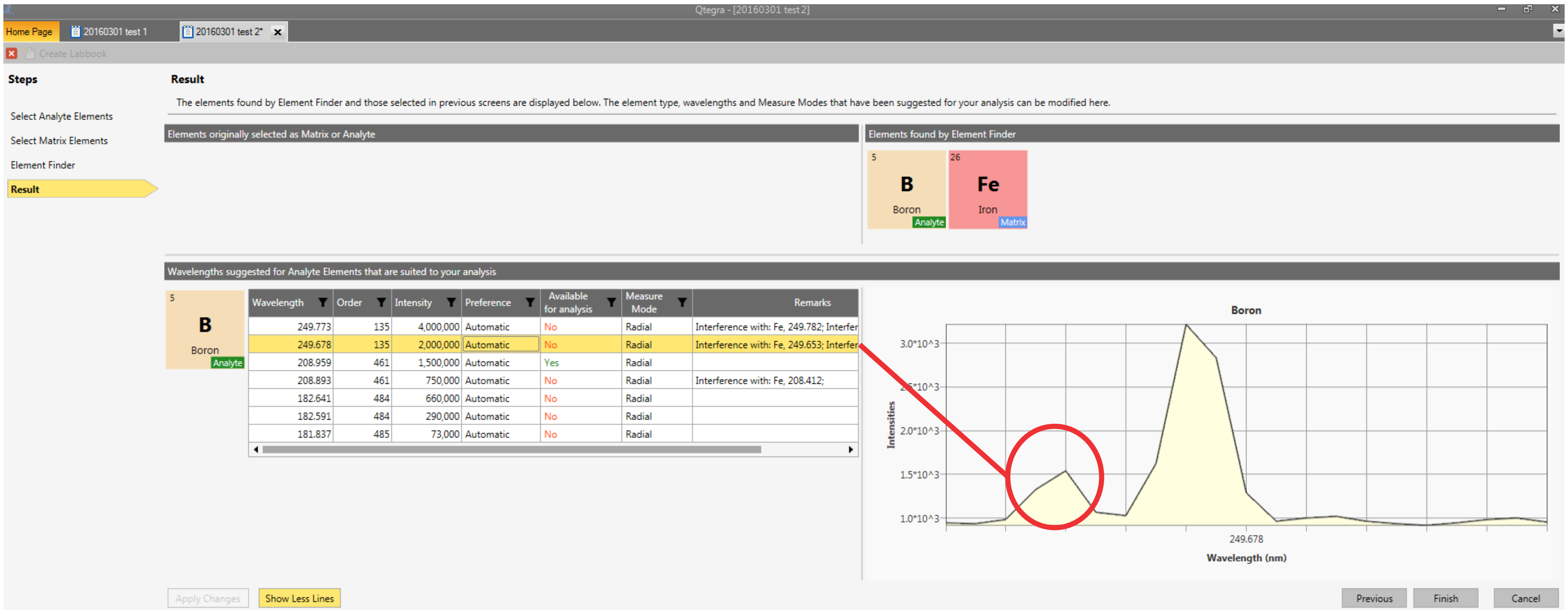


Element Finder – Analysis of an unknown sample



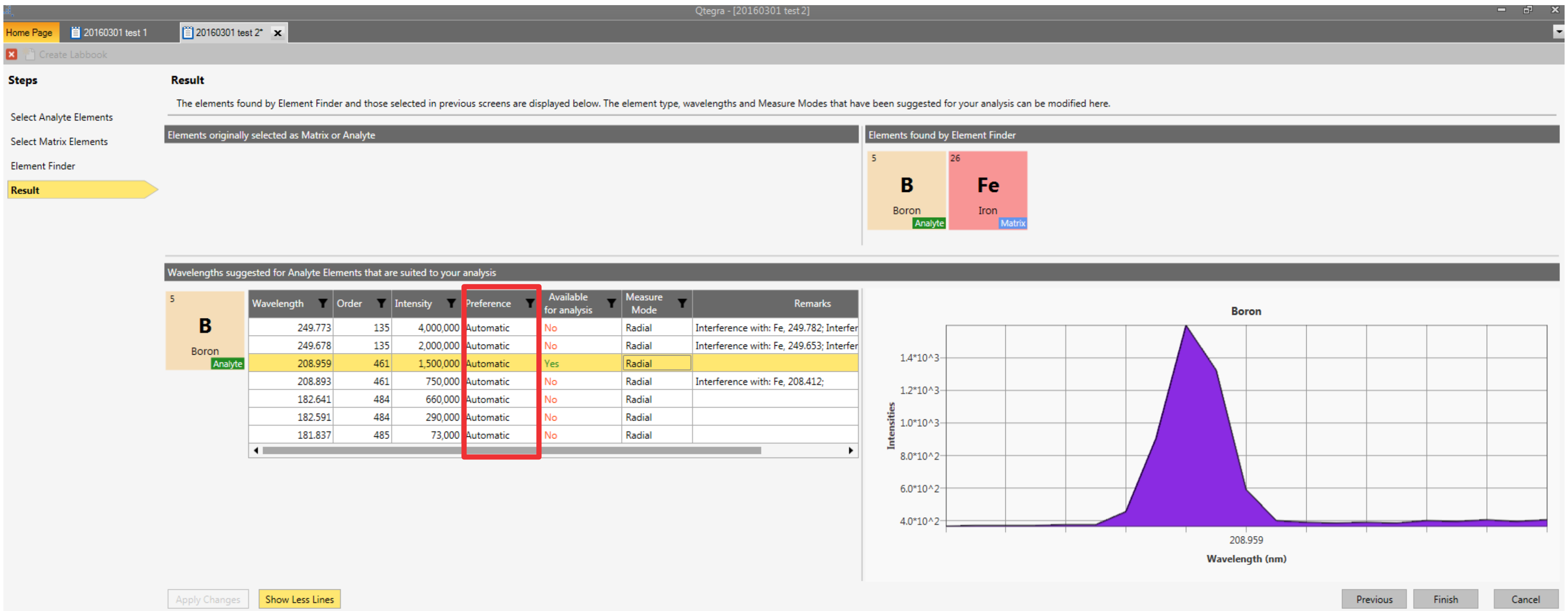
Wavelength	Order	Intensity	Preference	Available for analysis	Measure Mode	Remarks
249.773	135	4,000,000	Automatic	No	Radial	Interference with: Fe, 249.782; Interfer
249.678	135	2,000,000	Automatic	No	Radial	Interference with: Fe, 249.653; Interfer
208.959	461	1,500,000	Automatic	Yes	Radial	
208.893	461	750,000	Automatic	No	Radial	Interference with: Fe, 208.412;
182.641	484	660,000	Automatic	No	Radial	
182.591	484	290,000	Automatic	No	Radial	
181.837	485	73,000	Automatic	No	Radial	

Element Finder – Analysis of an unknown sample

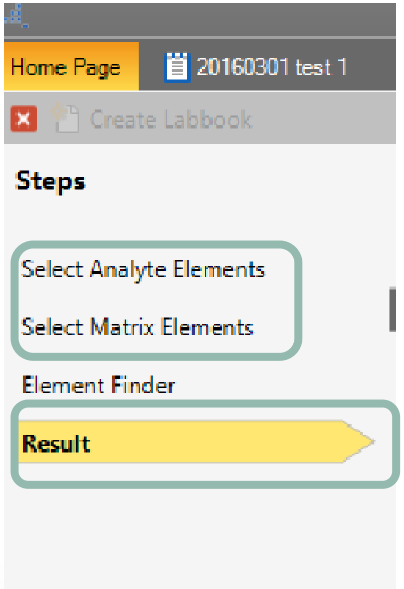


Element Finder – Analysis of an unknown sample

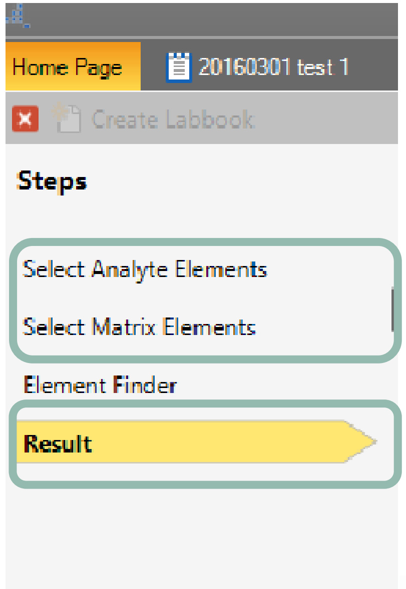
- The wavelength with the highest sensitivity that is free from interferences will be selected for analysis
- Additional wavelengths can be selected



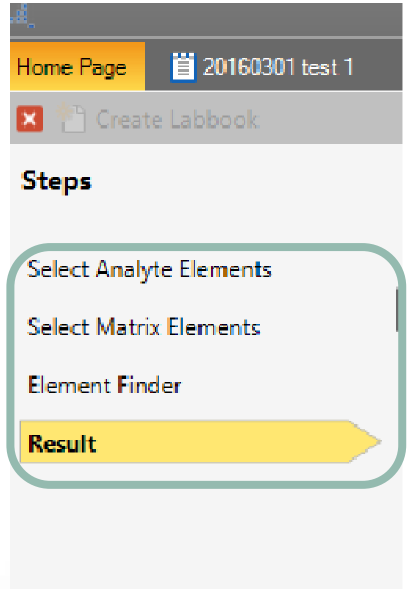
Methods of element input and selection



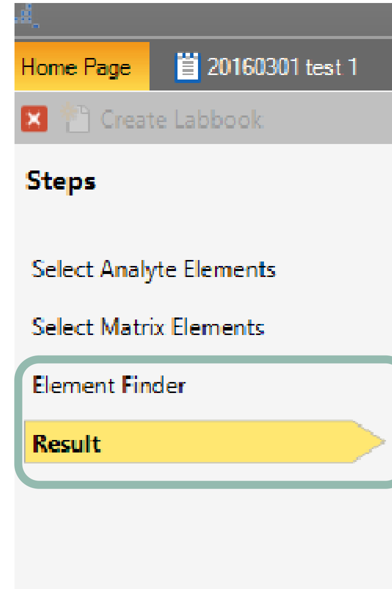
- **iCAP 7200 ICP-OES**
- **Manual element selection (from periodic tables, Analyte or Matrix)**



- iCAP 7400/7600 ICP-OES
- Manual element selection



- **iCAP 7400/7600 ICP-OES**
- **Manual element selection**
- **Element Finder with Fullframe**



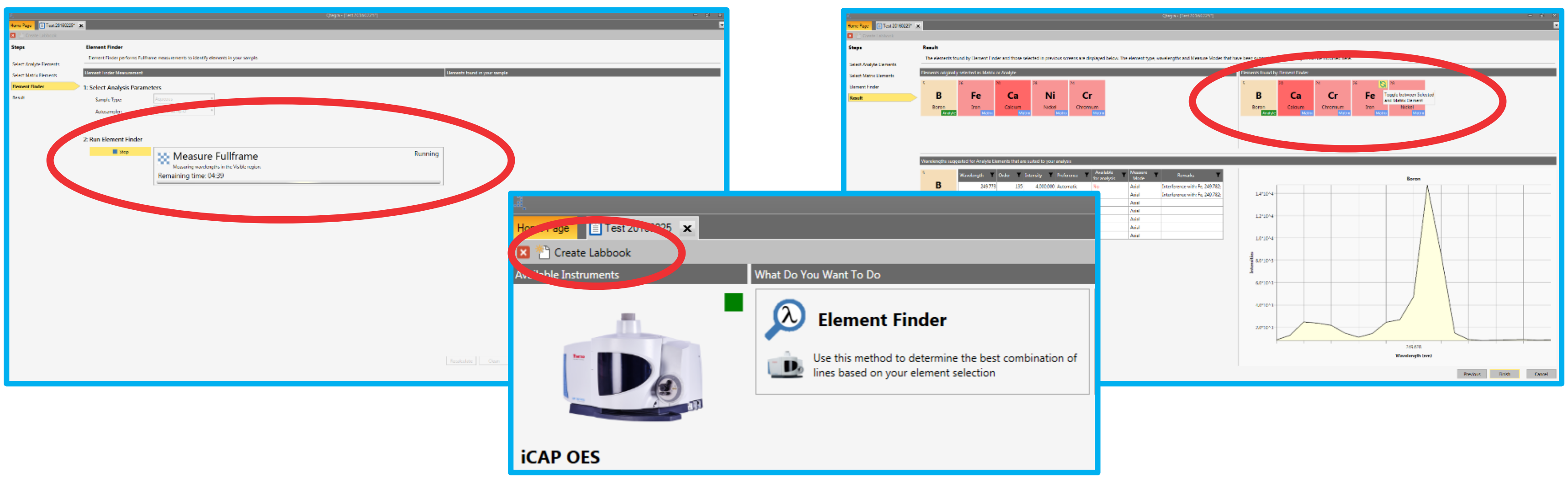
- iCAP 7400/7600 ICP-OES
- Element Finder with Fullframe

Wavelength Selection in Just Three Steps!!

Analyze
- Measure sample using a Fullframe within the Element Finder plug-in

Select
- Select the elements you would like to analyze

Import
- Import the results in to plasma optimization or directly into a LabBook



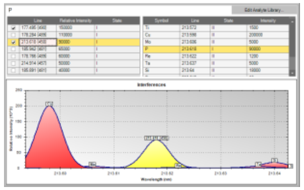
Manual Wavelength Selection (without Element Finder)

Method

- Create a basic method to measure within the software

Select

- Select the wavelengths
- Based on knowledge of the sample
- Based on knowledge of wavelength tables

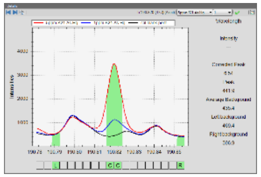


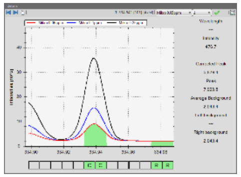
Analyze

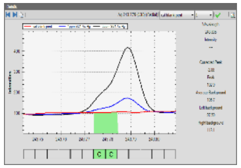
- Analyze a sample

Examine

- Look at the results/peaks
- Is there an interference?
- Repeat for every wavelength



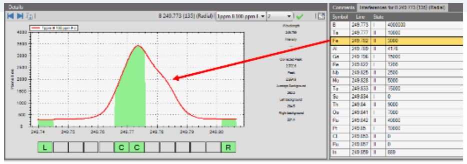




Manual Wavelength Selection (without Element Finder)

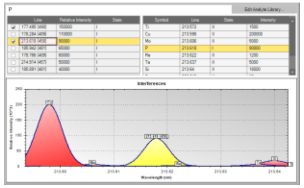
Identify

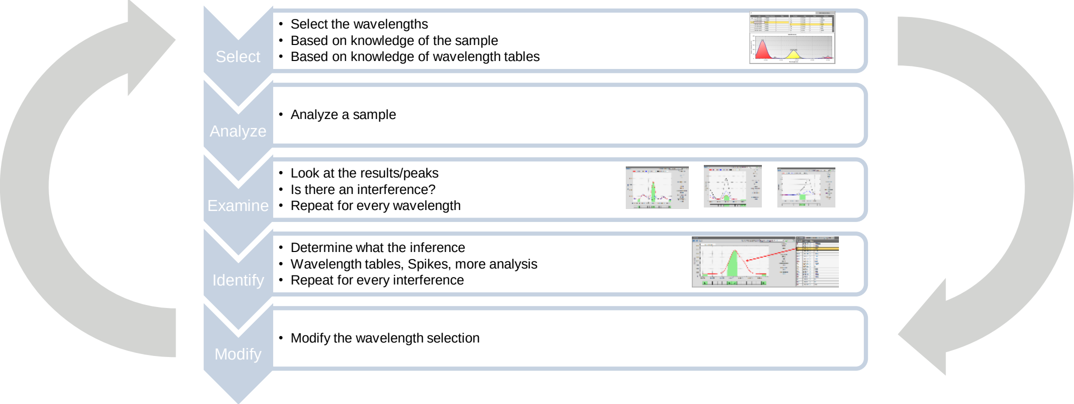
- Determine what the inference
- Wavelength tables, Spikes, more analysis
- Repeat for every interference



Modify

- Modify the wavelength selection





Use

- Use the wavelengths in a method and move on to manual plasma optimization

Element Finder or Manual?

Element Finder

Analyze
- Measure sample using a Fullframe in the Element Finder plug-in

Select
- Select the elements you would like to analyze

Import
- Import the results in to plasma optimization or directly into a LabBook

Manual

Method
- Create a basic method to measure within the software

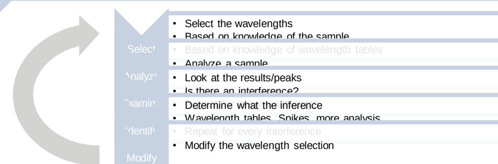
Select
- Select the wavelengths
- Based on knowledge of the sample
- Based on knowledge of wavelength tables

Analyze
- Analyze a sample

Examine
- Look at the results/peaks
- Is there an interference?
- Repeat for every wavelength

Identify
- Determine what the inference
- Wavelength tables, Spikes, more analysis
- Repeat for every interference

Modify
- Modify the wavelength selection



Use
- Use the wavelengths in a method and move on to manual plasma optimization

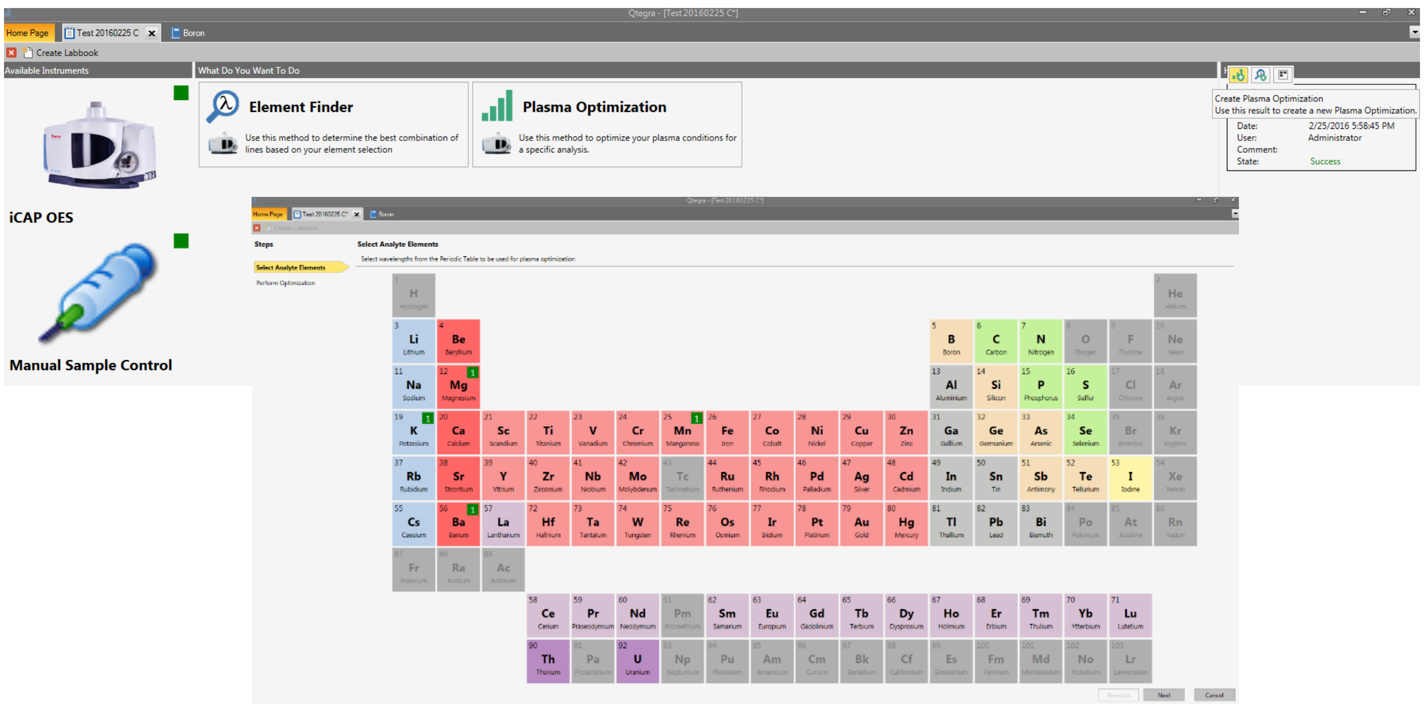
- **Less than 5 minutes and just 8ml of sample**

- **Multiple measurements, time and sample amount unknown!**

ThermoFisher SCIENTIFIC

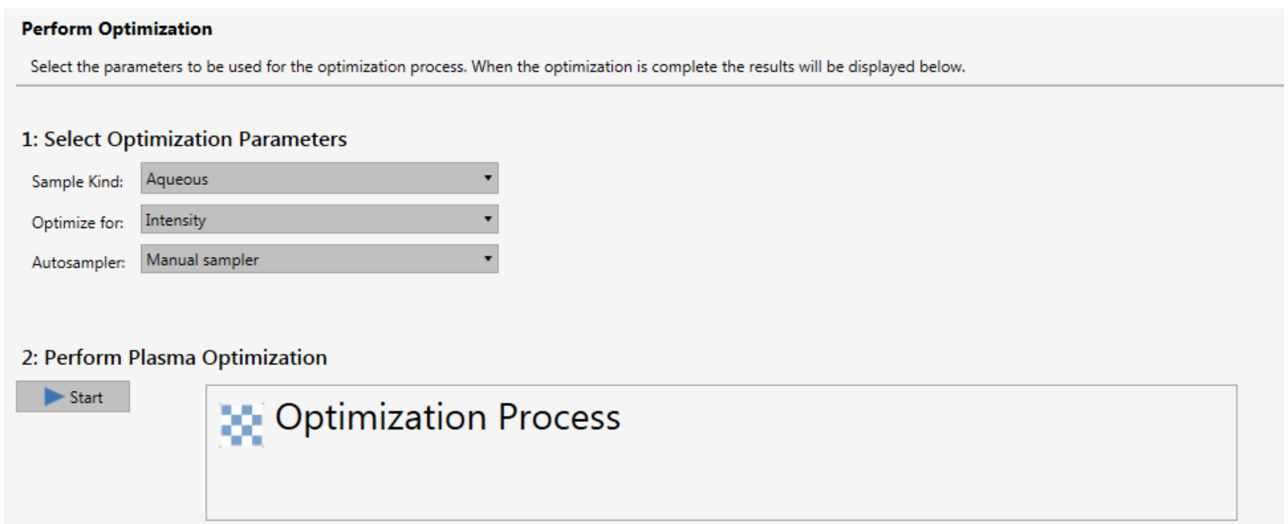
Plasma Optimization

- Plasma conditions can be optimized automatically, following wavelength selection
  - Different elements require different optimal conditions
  - A range of elements require a set of comprised conditions



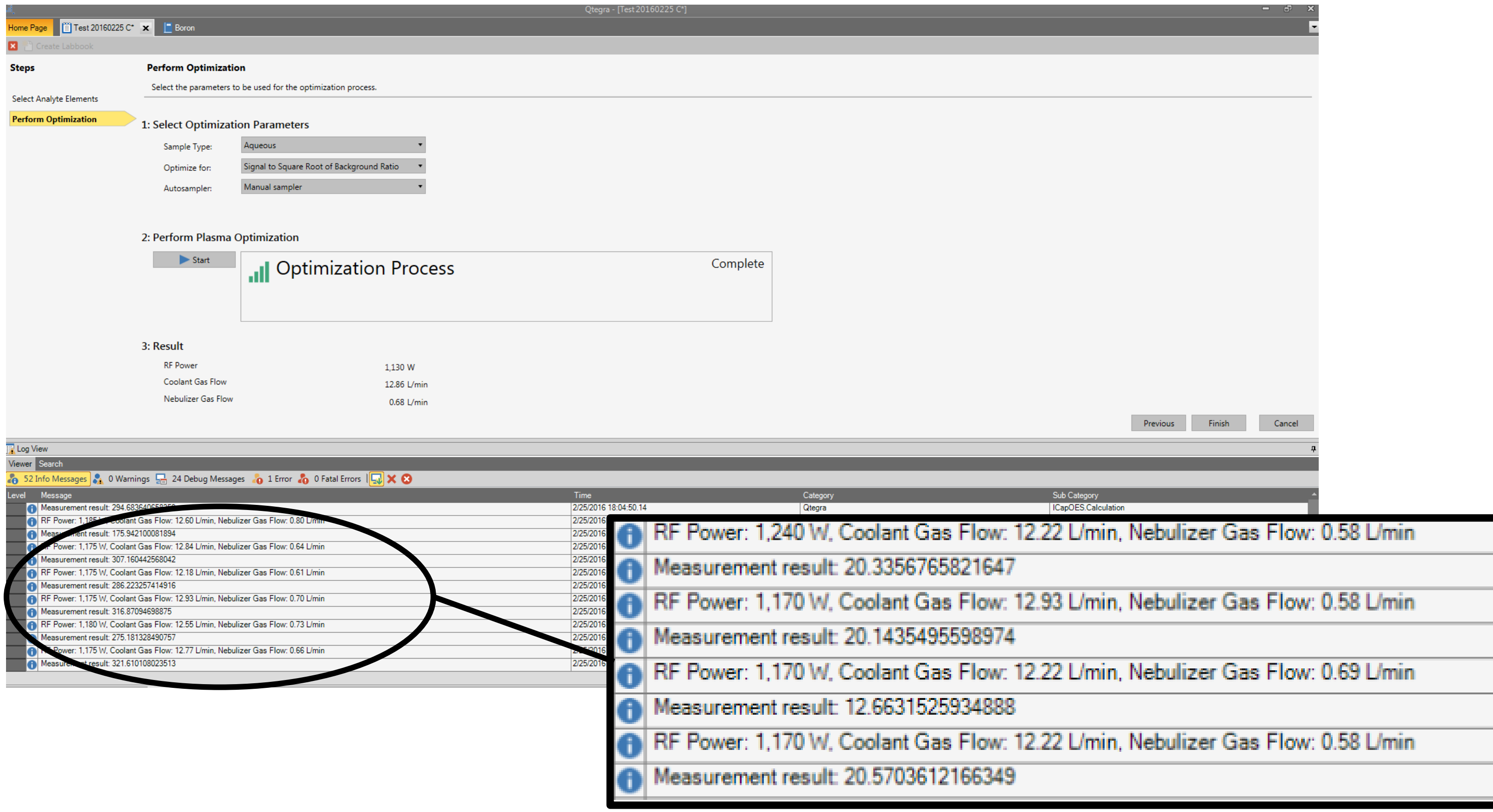
Plasma Optimization

- Select the wavelengths to optimize
  - Can use the wavelengths selected by Element Finder
  - Use a sub set of critical performance elements
- Select sample matrix: aqueous or organic
- Select the parameter you are optimizing for: intensity, signal-to-background ratio, detection limits
- A set of optimized values will automatically be returned



Plasma Optimization

- The optimization will take place based on a multi-component analysis
- Complete optimization process takes approximately ten minutes



Agilent

- No direct comparison within their software for Element Finder plug-in

- Expected response
  - FACT, may show the echellogram feature
    - **The echellogram just shows the wavelengths measured in the sample**
    - **<u>Fast Auotmated</u> Curve-fitting Technique requires lots of samples to be analyzed to bu ncludes: blanks, analytes, matri ts of time and effort**

Perkin Elmer

- No direct comparison within their software for Element Finder plug-in

- Expected response:
  - UDA and MSF
    - **UDA and MSF are both post processing tools (the data is collected and then corrected)**
    - **UDA requires users to analyze and then look at each sample and determine if there is an interference on the specific wavelength they are analyzing**
    - **UDA has not visual display of the wavelengths/spectrum, user has to manually search the wav 0+ lines/ only ca. 280 possible for PE)**
    - **MSF is matrix correction odels have to be created, time to analyze the differ**

Spectro

- No direct comparison within their software for Element Finder plug-in

- Expected response
  - As spectro can measure the most of the spectrum continuously they may also say they can “see/identify” every element in a sample, just a spectrum is displayed
    - **No tool for clear identification of elements**
    - **No suggestion of wavelengths for analysis**
    - **Lot of manual work required to identify elements**