

The world leader in serving science

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 autooptimization 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





iCAP 7000 RF Generator MK III performance prove





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	
λRange	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
AI	167.079	0.12*
AI	308.215	4.1
As	189.042	1.43
As	193.759	2.14
Ba	455.403	0.03
Be	311.107	0.017
Са	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
К	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
Мо	202.030	0.38
Na	589.592	0.37
Ni	231.604	0.36
Р	177.495	1.55
Р	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
ТІ	190.856	1.16
ТІ	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 3o model)



Element	Wavelength (nm)	DL (15s integrations) ug/L
Ag	328.068	2.46
AI	167.079	1.51
As	189.042	4.74
Ва	455.403	0.17
Ве	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
к	766.490	5.10
Li	670.784	0.83
Mg	279.553	0.04

Element	Wavelength (nm)	DL (15s integrations) ug/L		
Mn	257.610	0.21		
Мо	202.030	1.11		
Na	589.592	1.80		
Ni	231.604	2.29		
Р	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		
ТІ	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





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 °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







ThermoFisher SCIENTIFIC

Improving robustness for ICP-OES analysis

Proprietary & Confidential

The world leader in serving science

- 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

25

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







- Nebulisers
 - Parallel path Burgener
 - Large capillary concentric devices (e.g. SeaSpray)
 - V-groove

26

- Resistant to blocking
- Spray chamber
 - Baffled cyclonic type
 - Reduced sample loading on plasma





- 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
- Burged radial view window (iCAP 7000 Buo)
 - 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





















- 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







Example application 1: Analysis of 25% NaCl samples

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

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



- 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)





Measurement without sheath gas adaptor

- Without sheath gas
 - Completely blocked injector tube after < 2h, signal lost
 - If sheathiggs network and the lab leader gon hum set is in a correction







25% NaCl analysis results summary

Element and wavelength (nm)	R²	Internal standard wavelength (nm)	Known spike concentration (μg·L ⁻¹)	Measured spike concentration (µg∙L⁻¹)	Recovery (%)	MDL (µg∙L⁻¹)
AI 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



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




Engine lubrication oils analysis results

Element and wavelength	New oil	Intermediate oil	Old oil	Element and wavelength	New oil	Intermediate oil	Old oil
Ag 338.389 nm	0.76	0.87	0.94	Mo 281.615 nm	ND	0.16	0.38
Al 308.215 nm	0.09	0.05	0.05	Na 589.592 nm	5.71	5.2	3.71
B 208.959 nm	2.14	1.63	2.46	Ni 231.604 nm	0.73	0.59	0.48
Ba 223.527 nm	ND	0.46	0.82	P 178.284 nm	972.4	1045	984.1
Ca 184.006 nm	1103	2293	3014	Pb 220.353 nm	16	12.1	8
Cd 214.438 nm	0.15	0.17	0.27	S 180.731 nm	5731	5776	5134
Cr 267.716 nm	0.12	1.15	2.54	Si 212.412 nm	7.15	10.3	10.8
Cu 324.754 nm	0.58	2.03	3.49	Sn 283.999 nm	7.7	4.58	2.53
Fe 238.204 nm	2.76	23.2	30.8	Ti 334.941 nm	0.4	0.48	0.51
Mg 279.553 nm	870.8	631.2	323.4	V 309.311 nm	2.2	1.46	0.7
Mn 293.930 nm	0.21	0.63	0.89	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





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







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 431
MAN	
2.11.12	A SI II
Pa	
3	
*	
Shrint analyeie	of lubricating oils using the
	or rubridating the
Thermo Scient	fic iCAP 7000 Plus Series ICP-OF
Thermo Scient	fic iCAP 7000 Plus Series ICP-O
Thermo Scient	fic iCAP 7000 Plus Series ICP-OL
Thermo Scient	fic iCAP 7000 Plus Series ICP-O
Authors Nora Bartsch,	fic iCAP 7000 Plus Series ICP-OE Introduction The analysis of lubricating oils is a powerful tool in preventative maintenance
Authors Nora Bartsch, Application Specialist, Thermo Elarge Scientific	fic iCAP 7000 Plus Series ICP-OE Introduction The analysis of lubricating cits is a powerful tool in preventative maintenance of engines and machinery. Regular oil sampling and trend analysis will are process information about the table of a porty captor among and the
Authors Nora Bartsch, Application Specialist, Thermo Fisher Scientific, Brenen, Germany	Introduction The analysis of lubricating cities 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 machanical part, and signify the need for maintenance before critical failure
Authors Nora Bartsch, Application Specialist, Thermon Fisher Scientific, Bremen, Germany Keywords	fic iCAP 7000 Plus Series ICP-08 Introduction The analysis of lubricating oils is a powerful tool in preventative maintenance of engines and machinery. Regular oil sampling and trand analysis wil give precious information about the state of a motor, gear transmission or machanical part, and signify the need for maintenance before critical failure in particular, elemental analysis by Inductively Coupled Plasma Optical Errission Sectometry (IPC-05) is used to determine the concentration
Authors Nora Bartsch, Application Specialist, Thermon Fisher Scientific, Bremen, Germany Keywords High throughput,	fic iCAP 7000 Plus Series ICP-OE Introduction The analysis of lubricating oils is a powerful tool in preventative maintenance of engines and machinery. Regular oil sampling and trend analysis wil give precious information about the state of a motor, gave transmission or machanical part, and signily the need for maintenance before critical failure in particular, elemental analysis by Inductively Coupled Flatema Optical Emission Spectrometry (ICP-OES) a used to determine the concentration of ware metales, contaminants and additives present in used to list at an
Authors Nora Bartach, Application Specialist, Therror Flaher Scientific, Bremen, Germany Keywords High throughput; Labroating ol, Sprint Valve,	fic iCAP 7000 Plus Series ICP-OE Introduction The analysis of lubricating oils is a powerful tool in preventative maintenance of engines and machiney. Regular via sampling and trend analysis will give procious information about the state of a monte, gear transmission or mechanical part, and signify the need for maintenance before critical failure in particular, elemental analysis by Inductively Coxpled Plasma Optical Errisation Spactrometry (ICP-OES) is used to determine the concentration of wave melands, contaminate and additives prevent in used oils that can be sampled from car to train fleets, or even large construction or mining
Authors Nora Bartsch, Application Specialist, Thermo Fisher Scientific, Bremen, Germany Keywords High throughput, Lubricating ol, Sprint Valve, Used oil, Wear metals	fic iCAP 7000 Plus Series ICP-OF The analysis of lubricating oils is a powerful tool in preventative maintenance of engines and machinery. Regular oil sampling and trend analysis wil give procious information about the state of a month, gene transmission or mechanical part, and signify the read for maintenance before critical failure in particular, elemental analysis by Inductively Coxpled Plasma Optical Ernission Spactrometry (ICP-OES) is used to determine the concentration of ware metals, contaminants and additives present in used oils that can be sampled from ar to train fleets, or even large construction or mining machines. Wear metals are elements auch as Fe, Ou and Ni, and their presence may indicate wave of metallic parts. Other elements mug give
Authors Nora Bartsch, Application Specialist, Thermor Faiber Scientific, Bremen, Germany Neywords High throughput, Lubricating of Sprint Valve, Used oil, Wear metals	fic iCAP 7000 Plus Series ICP-OE 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 procious information about the state of a motor, gear transmission or machanical part, and signity the read for maintenance before critical failure in particular, elemental analysis by Inductively Coupled Plasma Optical Errisation 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 intests, or even large construction or mining machines. Wear metals are elements auch as Fe, Qu and Ni, and their presence may indicate wear or metallic parts. Other elements may give evidence of contamination from foreign matter, for example Si and dirt reterience the inite rise of the large additives, the the metal of the Ter-
Authors Nora Bartsch, Application Specialist, Thermor Flark Scientific, Bremen, Germany Keywords High throughput, Lubencating oil, Sprint Valve, Used oil, Wear metals	In the production of the second of the secon
Authors Nors Bartsch, Application Specialist, Therror Fisher Scientific, Bremen, Germany Keywords High throughput, Lubricating of, Sprint Valve, Used oil, Wear metals Coal This application note describes how the Thermo Scientific	Fit CAP 7000 Plus Series ICP-OF
Authors Nora Bartsch, Application Specialist, Thermo Fisher Scientific, Bremen, Germany Keywords High throughput, Lubricating ol, Sprint Valve, Used oil, Wear metals Coal This application note describes how the Thermo Scientific ICAP 7600 (CP-OES Readil and	fic iCAP 7000 Plus Series ICP-OF 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 procious information about the state of a motor, gear transmission or mechanical part, and signify the read for maintenance before critical failure in particular, elemental analysis by Inductively Coxpled Plasma Optical Errission Spactrometry (ICP-OES) is used to determine the concentration of ware metala, 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, Qu and Ni, and their presence may indicate ware of metallic parts. Other elements muy give evidence of contamination from foreign matter, for example Si and dirt entering the engine via a faultifier. Additives thick are typical Qa, P or Zh based compounds are added artificially to the oil to improve lubricating properties. Monitoring the deplation of these elements may threatore hep in identifying optimum conditions and maintenance scheduling.
Authors Nora Bartsch, Application Spocialist, Thermor Flaver Scientific, Bremen, Germany Negwords High throughput, Lubricating oil, Sprint Valve, Used oil, Wear metals Caol This application note describes how the Thermo Scientific ICAP 7600 ICP-OSEs Radial and its Integrated Sprint Valve offer	In the second se
Authors Nors Bartsch, Application Specialist, Thermo Fisher Scientific, Bremen, Germany Keywords High throughput, Lubricating oil, Sprint Valve, Used oil, Wear metals Coal This application note describes how the Thermo Scientific ICAP 7800 ICP-OES Radial and the Integrated Sprint Valve offer high throughput capabilities to becarding eaching Metricination	fic iCAP 7000 Plus Series ICP-OI manual series of the ser
Authors Nora Bartach, Application Specialist, Thermo Flaher Scientific, Bremen, Germany Keywords High throughput; Lubricating oil, Sprint Valve, Used oil, Wear metals Coal This application nots describes how the Thermo Scientific (CAP 7600 ICP-OES Redial and its integrated Sprint Valve offer high throughput capabilities to laboratories analyzing Ukricating oil samples. The instrument	fic iCAP 7000 Plus Series ICP-OI Plus Series ICP-OI Bandward Stran
Authors Nora Bartsch, Application Specialist, Thermor Faiber Scientific, Bernen, Germany Keywords High throughput, Lubricating od, Sprint Valve, Used oil, Wear metals Change The application note describes how the Thermo Scientific CAP 7600 (CP-OSE Radial and tish throughput capabilities to laboratories analyzing lubricating ornhine fast analysis time with	In the second se



Automated sample preparation and intelligent dilution



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



Auto-dilution systems – Prescriptive dilution



- 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}



Prescriptive dilution – building a calibration curve



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



	D	ilution of (one sto	ck star	ndard	1
2	Label ⊽₽	Sample Type ⊽+⊐	Stanc and ⊽⊀	Rack ⊽+¤	Vial 🖓 🗗	prepFAST DF マ무
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



- 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













Intelligent Scientific Data Solution™



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



- Start-up
- 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'

		Qtegra - [Home Page]	
neter			
		Interlocks	
923.0	W	Get Ready	
0.000	L/min	iCAP, Manual Sampling	
0.000	L/min		
0.000	L/min	The following Options are available: iCAP OES Spectrometer	
0.000	L/min	✓ ✓ Spectrometer Optimization 5 min	
05505		Run Performance Checks 30 min	
00030	rpm	✓ Use Manual Sampling	
		Wash time (s) 30 Uptake time (s) 30	
		Total time (estimated) 5 min	
		Warm up 1 Minutes OK Cancel	









- Prepares system for analysis
 - Confirms performance
- Improves quality of results
- Saves time
- Reduces requirement for training
- Improves productivity



Workflow - Qtegra LabBook

Experiment Editor - [H	ome Page]	
Dashboard	Analysis	
Analysis	Create LabBook Create a new LabBook based on an existing Template or LabBook	
Templates	Name US EPA METHOD 200.8 (FAST)_1 Enter a Name for the Labbook	,
Results	Location LabBooks	
Manage Files	Create a new LabBook from an existing Template Template Name US EPA METHOD 200.8 (FAST)	
Help	Samples 75 Import from CSV	_
	CSV name	
	Mapping Name	
	Create a new LabBook from an existing LabBook	
	LabBook Name FinalDVT_HighMatrixSingleElement_Suppression_QUICK MASTER v	
	Create a new LabBook from a blank Template	
	Evaluation	
	Create LabBook	_
and water	Open LabBook Open an unit ting 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

Create a new Lab	Book based on an existing Template or LabBook	
eme EPA 200.	8	
cation LabBooks		
Create a new Lab	Book from an existing Template	
Template Name	EPA 200.8	~
Samples	100 Import from CSV	
CSV name		~
Mapping Name		~
Create a new Lab	Book from an existing LabBook	
LabBook Name	EPA 200.8	~
Create a new Lab	Book from a blank Template	
Evaluation	eQuant	

- 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

	open										-
				(Qtegra - [eQuan	nt - 004*]				-	
Page 🛛 📚 eQuant - 004 - [Complete	d] 🗙										
K 🕨 Create • 🔪 🔭 👫	😽 Add 🕶	🔄 Delete 🕥 Print	sample layout	- 🐁 Comm	ents 🕼 Options	• Eta Copy 1	🕄 Paste 🛛 😽 Insert	Lo Append			
t	Sample	elist estimated runtime: 2	2 minutes 30 s	econds / 14 minute	es 30 seconds remai	ning					
Summary	团	Label ⊽ ₽	Status ⊽+	Repeats ⊽-¤	Comments ⊽+¤	Evaluate ⊽+Þ	Sample Type ∵⊽⊀	Standard ⊽-Þ	Dilution Factor ⊽⊀	⊐ Amount ⊽+⊧	1
iCAP OES	1	Blank	0	3	<comment></comment>	~	BLK		1	1	Г
Method Parameters	2	Standard 10 ppm	0	3	<comment></comment>	~	STD	OES Test Solution	10	0	T
- Measure Modes	3	Standard 100 ppm	•	3	<comment></comment>	~	STD 🗸	OES Test Solution	1	1	t
Acquisition Parameters	4	Tap water	•	3	<comment></comment>	~	UNKNOWN		1	1	t
Standards	5	Diluted tap water	•	3	<comment></comment>	~	UNKNOWN		1	1	t
Ratios	6	Standard No 1	0	3	<comment></comment>	~	UNKNOWN		1	1	t
Evaluation Results	7	Sample 103	0	1	<comment></comment>	~	UNKNOWN -	1	1	1	t
Concentrations	8	Sample 104	0	1	<comment></comment>	~	UNKNOWN	-	1	1	t
Intensities	9	Sample 105	0	1	<comment></comment>	~	UNKNOWN		1	1	t
- Intensity Ratios	10	Sample 106	0	1	<comment></comment>	~	UNKNOWN		1	1	t
Spectra View	11	Sample 107	0	1	<comment></comment>	~	UNKNOWN		1	1	t
Sample List	12	Sample 108	0	1	<comment></comment>	~	UNKNOWN		1	1	t
Log Messages	13	Sample 109	0	1	<comment></comment>	~	UNKNOWN		1	1	t
Signing	14	Sample 110	0	1	<comment></comment>	~	UNKNOWN		1	1	t
Query	15	Sample 111	0	1	<comment></comment>	~	UNKNOWN		1	1	t
	16	Sample 112	0	1	<comment></comment>	~	UNKNOWN		1	1	t
	17	Sample 113	0	1	<comment></comment>	~	UNKNOWN		1	1	t
	18	Sample 114	0	1	<comment></comment>	~	UNKNOWN		1	1	t
	19	Sample 115	0	1	<comment></comment>	~	UNKNOWN		1	1	t
	20	Sample 116	0	1	<comment></comment>	~	UNKNOWN		1	1	t
	21	Sample 117	0	1	<comment></comment>	~	UNKNOWN		1	1	t
	22	Sample 118	0	1	<comment></comment>	~	UNKNOWN		1	1	t
	23	Sample 119	0	1	<comment></comment>	~	UNKNOWN		1	1	t
	24	Sample 120	0	1	<comment></comment>	~	UNKNOWN		1	1	t
	25	Sample 121	0	1	<comment></comment>	~	UNKNOWN		1	1	t
	26	Sample 122	0	1	<comment></comment>		UNKNOWN		1	1	t
	27	Sample 123	0	1	<comment></comment>	~	UNKNOWN		1	1	t
	28	Sample 124	0	1	<comment></comment>	~	UNKNOWN		1	1	t
	29	Sample 125	0	1	<comment></comment>	~	UNKNOWN		1	1	t
	30	Sample 126	0	1	<comment></comment>	~	UNKNOWN		1	1	t
	31	Sample 127	0	1	<comment></comment>	~	UNKNOWN		1	1	t
	32	Sample 128	0	1	<comment></comment>	~	UNKNOWN		1	1	t
	33	Sample 129	0	1	<comment></comment>	~	UNKNOWN		1	1	+
	34	Sample 130	0	1	<comment></comment>	~	UNKNOWN		1	1	t
						•					ir.



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)



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

Con	centrat	tions							
	2	No	Time	Sample Type ▽	Label V	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	48.87 8%)	49.280 (98.6%)	50.201 (100.4%)	508.572 (101.7%)
Ð		14	2/24/2012 3:12:49 PM	QC - ICB	ICB			0.001	0.462
•		15	2/24/2012 3:13:48 PM	UNKNOWN	TW	The in	itial diam		3.971
l 🖬 🖓		16	2/24/2012 3:14:45 PM	UNKNOWN	TW	i ne in	illai disp	nay 👔	7.298
÷.		17	2/24/2012 3:15:42 PM	UNKNOWN	TWS	foour	on tha m	voot	209.094
		18	2/24/2012 3:16:38 PM	UNKNOWN	TWS	locus	on the n	iosi	210.532
•		19	2/24/2012 3:17:34 PM	UNKNOWN	TW	mnortar	st voluee	tha	3.851
•		20	2/24/2012 3:18:32 PM	UNKNOWN	TW	пропаг	it values	- uie	6.779
•		21	2/24/2012 3:19:30 PM	UNKNOWN	TWS	final co	ncontrat	ione 📕	215.145
• •		22	2/24/2012 3:20:27 PM	UNKNOWN	TWS	iniai co	ncentiat	.10115	211.552
•		23	2/24/2012 3:21:24 PM	UNKNOWN	TW			208	3.480
• •	_	24	2/24/2012 3:22:23 PM	UNKNOWN	TW	0.030	0.039	0.191	7.003
l 🗐 🖓		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
l 🖬 🖓		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
i i		_ 37	2/24/2012 3:37:16 PM	LINKNOWN .	TW	0.030	0.037	0.212	



Workflow – LabBook Data presentation

Con	icentra	tions									
	2	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	
k		2	2/24/2012 3:01:20 PM	STD							
13					0.111.0						
	+				Calibrate	on					
		2	2/24/2012 3:01:20 PM	STD	CALIBRA	TI	1.015 (1.000)	1.054 (1.000)	1.061 (1.000)	10.351 (10.000)	1.0
	.	3	2/24/2012 3:02:18 PM	STD	CALIBRA	TI	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	CALIBRA	TI	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	CALIBRA	TI	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	CALIBRA	TI	100.296 (100.000	99.618 (100.000)	99.473 (100.000)	996.019 (1,000.00	100.57
					Calibrati	on	and the second s	en e	es e	ar a for	
	2	No		Sample Tupe V	Label	∇	51V (KED) [ppb] +	52Cr (KED) [ppb] +	55Mn (KED) [ppb] +	56Fe (KED) [ppb] +	59Co (Ki
						-	0.010	0.007	0.011	0.027	
		M	ore detaile	ed info	rmat	ic	on 0.7%)	50.330 (100.7%)	51.018 (102.0%)	519.533 (103.9%)	49.7
							0.001	0.000	0.005	-0.074	
÷		IS	available	by click	kina	tł	1e 0.190	0.933	0.630	200,019.137	
•			1.1.6				2.057	182.555	197.997	194,072.929	
•			'+' for ea	ch ana	Iysis	5	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	2/24/2012 3.12.43111	QC-ICD	ICD		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	1
•		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	1
•		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	40.01



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





LabBook Results

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





Qtegra: Data presentation

Cor	centra	tions								
	1	No	Time	Sample Type	7 Label ∇	103Rh (KED) - 🕫	103Rh (STD) +=	185Re (KED) - 🕫		
		3	6/21/2012 12:25:48 PM	BLK		100.0%	100.0%	100.0%		
	•	4	6/21/2012 12:28:06 PM	STD						
÷.		22	6/21/2012 1:08:47 PM	UNKNOWN	Sample 2 200x	103.2%	104.9%	109.0%		
		23	6/21/2012 1:11:04 PM	UNKNOWN	Sam Longoo	40.4.000	104.2%	106.2%		
Ð		24	6/21/2012 1:13:22 PM	UNKNOWN			.0%	107.8%		
		25	6/21/2012 1:15:39 PM	UNKNOWN	Manua	ally modif	Ied 🤋%	109.9%		
÷.		26	6/21/2012 1:17:57 PM	UNKNOWN	1 - 1 - 1 - 1 -		.0%	110.5%		
		27	6/21/2012 1:20:14 PM	UNKNOWN	data is	s nigniign	ted 2%	106.8%		=
÷.		28	6/21/2012 1:22:32 PM	UNKNOWN		0 0	5.9%	110.4%		-
÷		31	6/21/2012 1:29:23 PM	UNKNOWN	Sample 1 400x	100	107.1%	111.4%		-
Ð		32	6/21/2012 1:31:41 PM	UNKNOWN	Sample 1 400x	105.02	109.6%	111.5%		-
÷		33	6/21/2012 1:33:59 PM	UNKNOWN	Sample 1 400x	109.1%	107.9%	109.5%		
Ð		34	6/21/2012 1:36:17 PM	UNKNOWN	Sample 1 400x	108.4%	111.0%	112.5%		
÷		35	6/21/2012 1:38:35 PM	UNKNOWN	Sample 1 400x	109.1%	110.7%	114.7%		
Ð		36	6/21/2012 1:40:53 PM	UNKNOWN	Sample 1 400x	110.3%	111.1%	116.6%		
•		37	6/21/2012 1:43:11 PM	UNKNOWN	Sample 1 400x	113.1%	112.4%	115.5%		
Ð		43	6/21/2012 1:56:59 PM	UNKNOWN	Sample 1 200x	131.9%	134.2%	138.7%		
÷.		44	6/21/2012 1:59:17 PM	UNKNOWN	Sample 1 200x	131.4%	132.0%	139.1%		
•		45	6/21/2012_2:01:36 PM	UNKNOWN	Sample 1 200x	133.9%	132.9%	137.6%		
L.					Sample 1 200x	132.7%	132.9%	136.4%		
De	ails	Or	nline moni	toring of		Sample list line 4				-
4			tornal ata	ndarda		Add Comm	ient			
F		 "	itemai sta	nuarus						
	200					Status: Suc				
		-				Creation: Wit	🖌 Qu	alitv cont	rol 🔪	
		1				Description:				
	450	+				Comment:	warnır	id and fa	Ilures	1
	150	1	· · · · · · · · · · · · //		20aca09	Start time: 6/2	2			
₅		+			8000800	Stop time: 6/2	easil	/ Identifie	ed by	
5		1			30		í		í 📕	
	100	00000	•	30000000 · 00000			COL	our colai	ng 🖉	1
8		1							-	-
"		+								
	50	1								
		+								
		1	- i - i -							1
	•	1								
	U	0	10 20	30	40 5	10				
		-	20 Ça	mple Number						
				inpre Autorer						-



Customizable reports for tailored data presentation

tensities A oncentrations	Intensities △ Concentrations	Water samples 01. March 2013	EPA 200.7 3		Page 1/5			QTEGRA
leader ample name 🖉 🛆 cquisition date	Sample identifier 🛛 🛆 Acquisition date	Sample 345-12-96-20 Acquisition date: 01. N	12 Narch 2013 – 12	37:54		0	perator: Holger Je	eglinski
er name	Operator		Ва	<u>Ca</u>	<u>Ce</u>	К	La	Mg
ment		Concentration Run 1	16.567 ppm	7.620 ppm	4.075 ppm	4.054 ppm	24.367 ppm	5.262 ppm
on Factor Int		Concentration Run 2	16.669 ppm	7.847 ppm	3.741 ppm	3.934 ppm	24.632 ppm	5.460 ppm
Quantity		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
\V \$		Concentration RSD	0.74 %	2.70 %	2.13 %	4.95 %	1.01 %	2.153 %
35.353 {63} (radial) △ 57.863 {126} (radial)	Ba 455.403 {74} (Axial) △ Ca 393.366 {86} (Axial) △		Mn.	Ni	Cu	Zn	Al	Р
).358 {78} (radial)	K 766.490 {44} (Axial)	Concentration Run 1	47.988 ppm	25.902 ppm	17.992 ppm	18.042 ppm	54.433 ppm	9.564 ppm
5.109 {83} (radiai)	Mg 279.553 {120} (Axial)	Concentration Run 2	48.429 ppm	25.835 ppm	18.277 ppm	17.837 ppm	54.811 ppm	9.401 ppm
	Mn 257.610 {131} (Axial) Ni 221.647 {452} (Axial)	Concentration Run 3	48.034 ppm	25.338 ppm	18.021 ppm	17.707 ppm	53.612 ppm	9.687 ppm
	Cu 324.754 {104} (Axial) Zn 213.856 {457} (Axial)	Concentration Average	48.150 ppm	25.691 ppm	18.097 ppm	17.862 ppm	54.285 ppm	9.550 ppm
~	Al 167.079 {502} (Axial) P 177.495 {490} (Axial)	Concentration RSD	0.50 %	1.19 %	0.86 %	0.94 %	1.12 %	1.50 %
umns centration SD △ nsity per Run nsity average nsity SD nsity RSD nsity per Run	Concentration per Run Concentration average Concentration RSD	Sample 346-12-96-201 Acquisition date: 01. N	L 2 March 2013 – 12	38:56		0	perator: Ho	WYSIWYG report generation
relation coefficient		Easy drag ar	nd drop rep	oort	4.075 ppm	4.054 ppm	24.367 ppm	g



Free customizable data exports

Exporter: Excel Export Preview Multiple export formats	
Preview Multiple export formats	
Towards of TETRAL and TETRAL	
allow to adapt onto most	
Image of the state of the s	
Image 24 Columbia Colu	
And parts 10 Notices 10 Not	
Image: Constraint of the	
1 March and 10 March 2004 March 2004 <td></td>	
Image of the construction (ID) Distribution (ID) <thdistribution (id)<="" th=""> Distribution (ID</thdistribution>	
export generation	
Export Cancel	





ThermoFisher SCIENTIFIC

Element Finder plug-in Applications and Competition

Proprietary & Confidential

The world leader in serving science

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











Element Finder – Analysis of an unknown sample

Takes less than 5 minutes and uses just 8mL of sample!

Home Page 🞽 20160301 test 3		1160302 test 1* 🗙	Qtegra - [20160302 test 1*]								- 7 ×		
Create Labbook													
Steps	Element Finder Element Finder performs Fullfram	ne measurements to identify elements in your sample.											
Select Matrix Elements	Element Finder Measurement				Elements found in your sample								
Element Finder	1: Select Analysis Paramet	ers			5 1	.4	15 2 B	6	29 48	C 1			
Result	Sample Type: Autosampler:	Aqueous • Manual sampler •			B Boron Matrix	Silicon Analyte	Phosphorus Analyte	Fe Iron Matrix	CU Copper Analyte	Cadmium Matrix			
	2: Run Element Finder	💥 Measure Fullframe											
		Processing Fullframe	2	Complete									
Г	3: Element Finder Result	76	Elements Scanned										
	Additional Elements Found: Added to matrix selection:		Elements Found		calculate	Clean			Prev	ious Next	Cancel		
			Additional Matrix Eleme	ents									



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)





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

Home Page 📋 20160301 test 3	🗎 20160301 test 4 📋 20160302 test 1* 🗶											
🗙 👕 Create Labbook												
Steps												
Select Analyte Elements	The elements tound by Element Finder and those selected in previous screens are displayed below. The element type, wavelengths and Measure Modes that ha	ve been suggested for your analysis can be modified here.										
Select Matrix Elements	Elements originally selected as Matrix or Analyte	Elements found by Element Finder										
Element Finder	15 14 29	5 14 15 26 29 48										
Result	P Si Cu Phosphorus Mastre Silicon Mastre Cu Copper Mastre User defined Elements	Boron Paralyte Prosphorus Iron Matrix Element Paralyte Robins Analyte Robins Prosphorus Iron Matrix Analyte Robins Prosphorus Iron Matrix Analyte Robins Prosphorus Iron Matrix Robins Prosphorus Iron Prospho										
	Wavelengths suggested for Analyte Elements that are suited to your analysis											
	14 Wavelength Y Order Y Intensity Y Preference Y Available for analysis Y Measure Mode Y Remarks Y 15 Image Vavelength Y Order Y Intensity Y Preference Y Available for analysis Y Measure Mode Y Remarks Y 15 Wavelength Y Order Y Intensity Y Preference Y Available for analysis Y Measure Mode Y Remarks Y 10 Image 177.495 489 150.000 Automatic Yes Radial 29 Image Wavelength Y Order Y Intensity Y Preference Y Available for analysis Y Measure Mode Y Remarks Y 29 Image Wavelength Y Order Y Intensity Y Preference Y Available for analysis Y Measure Mode Y Remarks Y 20 Cu 223.008 451 1,250,000 Automatic Yes Radial Image	Cadmium 2.5*10^4 2.0*10^4 1.5*10^4 1.0*10^4 5.0*10^3 214.438										
	Apply Changes Show More Lines	vravelengtn (nm) Previous Finish Cancel										



Element Finder – Analysis of an unknown sample

	_					Qtegra - [20160301 test 2]		ъ ×
Home Page 📋 20160301 test 1	20160301 tes	at 2* 🗙						Ŀ
🗙 💾 Create Labbook								
Steps	Result							
Select Analyte Elements Select Matrix Elements Element Finder Result	The elements fou Elements originally	und by Element Finder and selected as Matrix or An No	d those selected ir alyte USEr de	n previous screens are o	displayed below. The element	ype, wavelengths and Measure Modes that h	It have been suggested for your analysis can be modified here.	-
	Wavelengths sugge	ested for Analyte Elemen	ts that are suited to	to your analysis	Available Measure	Bematr		
	R	Wavelength Orde	12E 4.00		for analysis Mode	Leterformer with Ex. 240,782, Interfer	Boron	
	Boron Analyte	249.678 208.999 208.893 182.641 182.591 181.837	135 4,00 135 2,00 461 1,50 461 75 484 66 484 25 485 7	00000 Automatic 00,000 Automatic 00,000 Automatic 50,000 Automatic 60,000 Automatic 90,000 Automatic 73,000 Automatic	No Radial No Radial Ves Radial No Radial No Radial No Radial	Interference with: Fe, 249./62; Interfer Interference with: Fe, 249.653; Interfer Interference with: Fe, 208.412;	fre 6.0 2002 5.0 10/3 5.0 10/3 3.0 10/3 2.0 10/3 1.0 10/3 2.0 10/3 1.0 10/3 2.0 10/3 1.0 10/3 Wavelength (nm)	
	Apply Changes	Show Less Lines					Previous Finish (Cancel



Element Finder – Analysis of an unknown sample

đ							Qtegra - [20160301 test 2]							- 5 ×
Home Page 📋 20160301 test 1	20160301 tes	st 2* 🗙												!
🗙 শ Create Labbook														
Steps	Result													
Select Analyte Elements Select Matrix Elements Element Finder Result	The elements for	und by Element Finder a	and those sele	ected in previous screens a	re displayed below.	The element type	, wavelengths and Measure Modes that har	es that have been suggested for your analysis can be modified here. Elements found by Element Finder Elements found by Element Finder Fe Boron Iron Matrix						
	Wavelengths sugg	ested for Analyte Eleme	ents that are s	uited to your analysis										
	₅ B	Wavelength Y Or 249.773	rder T Int 135	tensity Y Preference 4,000,000 Automatic	Available for analysis No	Measure Mode Radial	Remarks Interference with: Fe, 249.782; Interfer				Boron			
	Boron Analyte	249.678 208.959 208.993 182.641 182.591 181.837	135 461 461 484 484 484	2,000,000 Automatic 1,500,000 Automatic 750,000 Automatic 290,000 Automatic 73,000 Automatic 73,000 Automatic	No Yes No No No No	Radial Radial Radial Radial Radial Radial	Interference with: Fe, 249.653; Interfer	3.0°10^3 20°10^3 2.0°10^3 1.5°10^3 1.0°10^3			249.678 Wavelength (nm)			
		Show Less Lines										Previous	Finish	Cancel


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

â,			_	_	_		Qtegra - [20160301 test 2]		×						
Home Page 📋 20160301 test 1	20160301 tes	t 2* 🗙													
🗙 瞥 Create Labbook															
Steps	Result														
Select Analyte Elements Select Matrix Elements Element Finder Result	The elements fou	ind by Element Finder and i selected as Matrix or Analy	those selected in p /te	evious screens are o	Jisplayed below. The e	element type, w	avelengths and Measure Modes that ha	have been suggested for your analysis can be modified here. Elements found by Element Finder B B Boron Analyte Iron Matrix	_						
	Wavelengths sugge	ested for Analyte Elements	that are suited to y	our analysis			_								
	5	Wavelength T Order	T Intensity	Preference	Available for analysis	Measure Mode	Remarks	Boron	Boron						
	В	249.773	135 4,000,	00 Automatic	No	Radial	Interference with: Fe, 249.782; Interfer								
	Boron	249.678	135 2,000,	00 Automatic	No	Radial	Interference with: Fe, 249.653; Interfer	1 4*1002							
	Analyte	208.959	461 1,500,	00 Automatic	Yes	Radial									
		208.893	461 750,	00 Automatic	No	Radial	Interference with: Fe, 208.412;	1.2*10^3							
		182.041	484 660,	00 Automatic	No	Radial									
		181.837	485 73	00 Automatic	No	Radial		10*10^3							
		•					•	► ^E 80*10^2							
								6.0°10^2 4.0°10^2 208.959 Wavelength (nm)							
		Show Less Lines						Previous Finish	Cancel						



Methods of element input and selection

Home Page 20160301 test 1 Create Labbook Steps Select Analyte Elements Select Matrix Elements Element Finder Result	Home Page 20160301 test 1 Create Labbook Steps Select Analyte Elements Select Matrix Elements Element Finder Result	Home Page 20160301 test 1 Center Labbook Center Labbook Steps Select Analyte Elements Select Matrix Elements Element Finder Result	Home Page 20160301 test 1 Create Labbook Steps Select Analyte Elements Select Matrix Elements Element Finder Result
 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!!











Manual Wavelength Selection (without Element



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



Use

Element Finder or Manual?

Element Finder Manual · Create a basic method to measure within the software • Measure sample using a Fullframe in the Element Finder plug-in Select the wavelengths · Based on knowledge of the sample Based on knowledge of wavelength tables · Select the elements you would like to Analyze a sample analyze Look at the results/peaks Is there an interference? · Repeat for every wavelength Import the results in to plasma Determine what the inference · Wavelength tables, Spikes, more analysis optimization or directly into a LabBook · Repeat for every interference Modify the wavelength selection Select the wavelengths Based on knowledge of the sample Analyze a sample Look at the results/peaks Is there an interference? Determine what the inference Wavelength tables Spikes more an

• 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!



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

a,															
Home Page Test 20160225 C 🗙 📘 Boron															
🔀 한 Create Labbook															
Available Instruments What Do Y	/ou Want To Do												H	8 B E	
n • 🔊	Element Finder		Plasm	a Optimizatio	on								Crea	te Plasma Optimi this result to crea	ization ate a new Plasma Optimization.
	Use this method to determine	the best combination of	Use this me	had to optimize your	plasma conditions for									Date: User	2/25/2016 5:58:45 PM Administrator
	lines based on your element s	election	a specific ar	alysis.									L	Comment: State:	Success
iCAP OES	Home Page Test 20160225 C* 🗶	E Seen			Qtegra - [Test 2016	2225 C·]								1	
	Steps S	elect Analyte Elements													
	Select Analyte Elements	Select wavelengths from the Periodic Table t	o be used for plasma optimizat	ion											
61	Perform Optimization	1. H Hydrogen										2	He		
		3 4 Li Be Lithium Benylium						5	B C Boron Carbon	7 N Nitrogen	8 S Oxygen	F Fluorine	Ne		
Manual Sample Control		11 12 1						13	3 14	15	16	17 18			
		Na Mg Sodium Magnesium						4	Al Si Aluminium Silicon	P Phosphorus	S Sulfor	Cl Chlorine	Ar Argon		
		¹⁹ 1 ²⁰ Ca	21 22 Sc Ti	23 24 V Cr	25 <u>1</u> 26 Mn Fe	27 28 Co	8 29 Ni Cu	30 31 Zn	Ga Ge	33 As	34 Se	35 36 Br	Kr		
		Potassium Caldium	Scandium Titanium	Vanadium Chromium	Manganese Iron	Cobalt	Nickel Copper	Zinc	Gallium Germaniu	n Arsonic	Solerium	Bromine K	rypton		
		37 38 Rb Sr Rubidium Strontium	39 40 Y Zr Yttrium Zirconium	41 42 Nb Mo Nicolum Molybdenu	43 44 Tc Ru Technetum Rutherium	45 48 Rh n Rhodium 1	5 47 Pd Ag Palladium Silver	48 49 Cd Cadmium	In Sn Indium Tin	51 Sb Antimony	52 52 Te Tellutum	53 54 I Iodine	Xe Kenon		
		55 56 1	57 72	73 74	75 76	77 78	8 79	80 81	1 82	83	84 8	85 86			
		Cs Ba Caesium Barium	La Ht Lantharum Hafnium	Tantalum Tungsten	Re Os Rhenium Osmium	1r Iridiam	Pt Au Platinum Gold	Hg Mercury	Thallium Lead	Bi Eismuth	Polonium	At Astatine	Radon		
		87 88 Fr Ra Francium Radium	89 Ac Activium												
			58 Ce Cerium	59 60 Pr Nd Praseodymium Neodymium	61 62 Pm Sm Promethum Samarium	63 64 Eu Europium C	Gd Tb Sacolinium Terbium	66 67 Dy Dysprosium	7 68 Ho Er Holmium Erbium	69 Tm Thulium	70 T The Yb	71 Lu Lutetium			
			90 Th Thorium	91 92 Pa U Protectinium	93 94 Np Pu Nepturium Plutorium	95 96 Am Americium	5 97 Cm Bk Curium Berkelium	98 99 Cf Californium E	9 100 Es Fm insteirium Fermium	101 Mendelevium	102 : No Nobelium	103 Lr Lawrencium			
											Pr	evitus Ne	t Cancel	i	



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-tobackground ratio, detection limits
- A set of optimized values will automatically be returned

Perform Opti	mization
Select the para	meters to be used for the optimization process. When the optimization is complete the results will be displayed below.
1: Select Op	timization Parameters
Sample Kind:	Aqueous 🔹
Optimize for:	Intensity •
Autosampler:	Manual sampler 🔹
2: Perform F	Plasma Optimization
► Start	Optimization Process



Plasma Optimization

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

			Qtegra - [Test20160225 C"] — 🗇 X
ne Page 📋 Test 20160225	C* 🗙 📘 Boron		
aps.	Perform Optimization		
	Select the parameters to be used for the	optimization process	
ect Analyte Elements	Select the parameters to be used for the	optimization process.	
form Optimization	1. Salast Optimization Decemate		
	1: Select Optimization Paramete	ers	
	Sample Type: Aqueous	-	
	Optimize for: Signal to Squar	re Root of Background Ratio 🔹	
	Autosampler: Manual sample	er 🔫	
	2: Perform Plasma Optimization	1	
	► Start	timization Process	Complete
	3: Result		
	RF Power	1,130 W	
	Coolant Gas Flow	12.86 L/min	
	Nebulizer Gas Flow	0.68 L/min	
			Previous Finish Cancel
og View			a
ver Search			
52 Info Messages 🤱 0 Wa	arnings 🔚 24 Debug Messages 🛛 👌 1 Error	🖧 O Fatal Errors 🛛 🗔 🗙 🔕	
el Message	000000000000000000000000000000000000000		Time Category Sub-Category *
 RF Power: 1,1851 Cool 	Tant Gas Flow: 12.60 L/min, Nebulizer Gas Flow: 0.8	80 L/mm	2222 00 19 10 49 00 14 000 14 000 14 000 14 000 12 22200 16 10 14 000 14 000 14 000 14 000 14 000 14 000 14 000
Measument result: 175.	.942100081894		222016 1 RF Power: 1,240 W, Coolant Gas Flow: 12.22 L/min, Nebulizer Gas Flow: 0.58 L/min
Measurement result: 307.	lant Gas Flow: 12.84 L/min, Nebulizer Gas Flow: 0.6 160442568042	64 Umin	2252016
RF Power: 1,175 W, Cool	lant Gas Flow: 12.18 L/min, Nebulizer Gas Flow: 0.6	61 L/min	2222216 Measurement result: 20.3356765821647
Measurement result: 286.	223257414916	201/min	
Measurement result: 316.	887094698875		223016 TRE Power: 1,170 W, Coolant Gas Flow: 12.93 Lmin, Nebulizer Gas Flow: 0.58 Lmin
RF Power: 1,180 W, Cool	lant Gas Flow: 12.55 L/min, Nebulizer Gas Flow: 0.7	73 Umin	
Measurement result: 275.	i.181328490757 Jant Gas Elow: 12 77 L/min: Nabulizar Gas Elow: 0.6	66 L/min	2252016 (1) Measurement result: 20.1430450598974
Measurem of result 321.	.610108023513		225015 DE Deuren 1 170 M/ Contract Care Eleve 12 221 /aria Naturiane Care Eleve 0.001 /aria
			TRE Fower: 1,170 W, Coolant Gas Flow: 12.22 Dmin, Nebulizer Gas Flow: 0.69 Dmin
			Measurement result: 12 6621525924999
			measurement result 12.0031525554000
			PE Power: 1 170 W. Coolant Gas Elow: 12 22 L/min. Nebulizer Gas Elow: 0.58 L/min.
			The Fower, 1, 170 W, Coolant Gas How, 12.22 Dhill, Nebulizer Gas How, 0.36 Dhill
			Measurement result: 20 5703612166349



- 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 Auotmate</u>d Curve-fitting Technique requires lots of samples to be analyzed to bu analytes, matri
 <u>Includes</u>: blanks, ts of time and effort





- 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 wavelengths/spectrum, user has to 0+ lines/ only ca. 280
 possible for PE)
 - MSF is matrix correction time to analyze the differ



odels have to be created,



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



