# **MICAP-OES 1000** RIS USER MANUAL







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## **ABOUT MICAP-OES 1000**

The MICAP-OES 1000 (Microwave Inductively Coupled Atmospheric Plasma-Optical Emission Spectrometer) plasma operates on 99.99% nitrogen; this instrument does not require argon during operation. Utilizing state-of-the-art embedded electronics, commercial-grade microwave instrumentation, and custom-built optics, this instrument delivers performance, reliability, and high sample throughput.

MICAP-OES 1000 plasma source and high-resolution echelle spectrometer has wavelength coverage from 194-625 + 766 nm. Simultaneous multi-elemental analysis for most of the periodic table for applications ranging from mining, food, and petroleum. The 208-240 V power requirements together with nitrogen operation provide complete portable capabilities limited by only electricity and nitrogen. The MICAP-OES operates similarly to traditional ICP-OES instruments.

Our product is certified by analytical chemists and has unparalleled plasma characteristics that meet the most stringent operating requirements.

#### PORTABILITY AND SMALL FOOTPRINT

Weighing 34kg (19kg plasma source and 12 kg spectrometer module), [33×45 cm] allows sufficient space for an autosampler and associated chemistry needs.

#### **BETTER LOGISTICS**

No chiller or argon is needed for operation in standard laboratory environments.

#### **OPERATING COST SAVINGS**

Minimizes annual operating costs based on nitrogen consumption and infrastructure.

#### **BROAD MATRIX TOLERANCE**

Easily handles a broad array of sample types, including high concentrations of total dissolved solids and organic solvents.

#### **ELECTRICAL OUTLET COMPATIBILITY**

208V – 240V draws less than 2kW of power. It can also run on a portable generator.

MICAP-OES 1000 is a robust and intuitive system to use. Understanding the following key concepts and terminology is important for efficient operation of the instrument and the accompanying software.

## Definitions

**Radom Instruments Software (RIS):** RIS is the application software which controls the MICAP-OES 1000 hardware and all aspects of the elemental analysis.

**Method**: Data acquisition parameters including analyte wavelengths, instrument parameters, and calibration information.

**External Calibration**: Method type defined by the use of standards to create a calibration to which the sample intensities are then compared.



**Method of Standard Additions (MSA)**: Method type defined by the analysis of standards prepared within each sample to create an individual, matrix matched calibration per sample.

**Session**: The sequential list of sample analysis including which method used, and sample preparation details.

Line: Specific wavelength measured for a given element.

**Standards:** Standardization solutions of varying concentrations used to create a response curve for a given wavelength.

**Blank:** The calibration blank is defined as *Standard 1*. This is the sample spectrum subtracted from all session samples. When Internal Standards are used a separate Blank without internal standards is prepared to subtract from all samples.

**Internal standard**: An element added to all test solutions analyzed in a session to compensate for physical differences between standard solutions and test sample solutions.

**Exposure Time:** Time in ms represents the camera read time. The allowable range is 40ms to 10,000ms.

**# of Exposures:** The number of times the sample is exposed (of Exposure Time) to create an iterative response. These are averaged to define one Repeat.

**Repeats:** A set of individual measurements which constitute a single sample or standard, sometimes referred to as replicates.

Total measurement time = (Exposure Time)\*(# of Exposures)\*(# of Repeats)

**Sample Introduction Assembly (SIA):** Consists of the sample / drain tubing, peristaltic pump, nebulizer, spray chamber and torch.

**Limit of Detection (LOD):** The lowest concentration that can be accurately detected by the instrument.

**Limit of Quantitation (LOQ):** The lowest concentration that can be accurately quantified by the instrument. The LOQ = LOD value \* (10/3)

**Relative Standard Deviation (RSD):** Calculated value based on the average of a data set and the standard deviation of that data set. Represents the precision of the data set and is typically calculated in percentage.

## **Software Architecture**

#### **Methods and Sessions**

The two primary concepts relevant to the MICAP-OES software are Methods and Sessions. Methods define the target elements/wavelengths and the conditions for measurement including sample introduction, plasma power and accessory programming. Sessions define the sequence or order of the Test Solutions to be analyzed.



#### **Elements and Lines**

In Methods the target elements and corresponding wavelengths (lines) are selected. MICAP-OES captures the entire wavelength range between 194nm to 625nm for simultaneous data acquisition. Wavelengths not in the method can be added post-acquisition via the **Edit Method** icon in Data Analysis.

#### File Management

The directories for Methods and Sessions are organized by RIS. The two directories separate the Method files and Session files automatically. Each can easily be sorted, archived, or deleted from a drop-down menu.

#### NOTE:

**Archiving** is a storage function for methods and sessions. Using the archive feature will protect the methods and sessions from general editing. These can be recalled for use by locating the down arrow next to the Sessions or Methods icons. **Deleting** permanently removes the files from the computer. There is no recovery for deleted Methods or Sessions.



## Workflow

The basic workflow follows this outline:

- 1. Prepare samples
- 2. Prepare instrument
- 3. Create analytical method
- 4. Create session
- 5. Analyze and manage data

### **Prepare Samples**

Atomic spectroscopy analysis requires the sample to be in liquid form. The sample preparation is dictated either by the complexity of the sample matrix, the target element characteristics and/or the purpose of the analysis. The samples can be digested by adding acid and applying heat via hot plate/hot block or microwave digestion. In some cases, the samples may be soluble in a liquid matrix suitable for aspiration into the atomic spectrometer.



Once the sample preparation is defined, the standard solutions should be prepared in the same matrix. This practice creates a uniform matrix and minimizes aerosol formation differences between standards and sample solutions.

#### Prepare Instrument -refer to Operation Manual sections 9 through 11 for

Hardware Summary

- a. Ensure all gases are on and flowing at the desired pressure range.
- b. Turn on the exhaust system.
- c. Clamp pump tubing into peristaltic pump-make sure tubing is centered in the channel to prevent flow blockage. Pump tubing should be changed regularly, frequency depends on usage.

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#### Tech Tip – Peristaltic Pump

- With the plasma off, adjust pump tension by introducing air bubbles and increasing tension (thumb screw) until bubbles start flowing smoothly. Then add ½ turn. Too much tension can greatly shorten the usable lifespan.
- The tubing will wear from the friction it experiences during use. Check daily for flattened, discolored or torn sections. With 3-stop tubing, simply switch to a new section if available.
- Peristaltic pump tubing stretches during use, especially during its first 15-20 minutes of use. When changing pump tubing, make sure to allow the tubing time to stabilize before starting an analysis.
- Make sure the drain tubing is operating at a higher flow rate than the introduction tubing, to prevent flooding of the spray chamber.

If the plasma button on the instrument is red, this indicates that one or more of the interlocks are failing. If the plasma button is green, the system is ready to ignite. The instrument status in the top right corner should indicate ready. Refer to Table 11 in the Operation Guide if plasma does not initiate. For technical support and contact information, refer to the official Radom website: https://www.radominstuments.com .

#### **RIS Summary**

Locate the RIS software icon on the desktop labeled MICAP-OES





Open the software and click on the instrument button and plasma on button located in the top right of the window. This will begin the ignition sequence. Let the plasma/instrument stabilize for approximately 20 minutes. The spectrometer should be on for 60 minutes to stabilize. During stabilization the camera cools to the operational temperature of -10°Celsius. The instrument is ready for sample analysis.



## **Create Analytical Method**

From the Method menu select New or click New Method on the toolbar. This will open the New Method window.

#### General Tab

The method name is a required field. The fields labeled Matrix, Description and Notes are not mandatory but provide a way to share information among multiple users in the lab.



The Calibration Type box requires the user to select between External Calibration and Method of Standard Additions (MSA).



Elements tab – (External Calibration and MSA)

- Specify target analytes and wavelengths to be included in the Method. Target elements can be selected using the default Periodic Table view or Grid Sorted by Atomic Number. The selected element will be highlighted in pink, which indicates quantitative analyte.
- 2. To add an internal standard to the method, specify which analyte will function as the internal standard by accessing the drop-down menu in the column labeled "Type". The element that is chosen as the internal standard will be highlighted in green, which indicates it is an internal standard.



H																	He	lies	Damant	Crore Calibration	Pelativa Intentity	interferencer
11		1										B	C	N	0	F	Na	UN .	Caludin	Close Canada Non	sconn manual 2 can dia	uncentrenice).
		-										-	-	-					Co 345 350	Yol	267,500 1	
Na	M	9			_	_		_	_	_	_	AI	Si	Р	S	C	Ar	0	Co 240 725	You	153,740 1	1
ĸ	Ca	as	c T	V	Cr	Mn	Fe	Co	N	Cu	Zn	Ga	Ge	As	Se	В	Kr		Co 340.512	Xal	121,880 1	
Rb	S		Z	N	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Те	1	Xe	0	Co 350.228	Xcal	117.220 1	14
0.0		1	-	1 7.	Iw	Pa	00	10	D+		Ha	TI	Dh	0:	Pa		De	0	Co 237.863	Xcal	111.510 #	1
GS	0	1	n			I've	05		F1	Au	rig	п	PD	DI	PO	^	NO	D	Co 230.786	X Cal	100.230 0	14
Fr	R	9										_						0	Co 242,493	X Cal	93.780 1	1
		L	a Ce	P	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	L	1	0	Co 231,160	XCal	88.930 8	1
		A	c Th	P	U.	No	Pu	Am	Cm	Bk	Cf	Fs	Em	Md	No	1	-	0	Co 236.380	XCal	87.920 11	1
-			, I	11.		1	1	11	1	1	1	-		1	1.00			0	Co 241.158	Xcal	36,760 0	<b>1</b>
Ana	Anal	yte	_	-	-	in	iternal	Standa	ard	-	-	Eleme	nt Excl	uded	-	-			Co 399.531	Xcal	84.610 1	
Elen	ient	×	Line Type	щQ	xposur Froup	e	linter Stan	məl idard		Back	grouni	Corre	tion	æ	Peak							
C0 (	38.85	8	n.	A	1		Nor	e	1	inear				j,	rea							
0.4	25.43	5	í,	A			Non	e -	- 1	incar				-	rea							
Ni 3	52,45	4	(	A	L.		None	e	L	inear				1	rea							

Instruments and Sampling tab – (External Calibration and MSA)

1. Instrument Parameters: define the instrument parameters such as gas flows, power, and exposure time. The default parameters are recommended for most analyses. Exposure time refers to the amount of time the sCMOS camera will acquire a signal. If a parameter is entered which is outside the allowable range, an informational icon will appear and display the appropriate range.

Instrument Parameters San	npling Parameter	rs	
Coolant:	14	L/min	(12 - 20)
Auxiliary:	0.3	L/min	(0.2 - 2)
Nebulizer:	1	L/min	(0 - 2)
Power:	1000	w	(750 - 1000)
Multiple exposures:			
Exposure A:	1000	ms	(40 - 10000)

2. Sampling Parameters: Enter the desired pump speed, acquisition times, and stabilization times for sample uptake and rinses. Input values for # of Exposures which is the number of scans of a test solution and # of Repeats is the number of times the sample is measured. The total time for sample measurement is reflected under the Sampling Parameter section. This time is representative of (Exposure Time (ms)\*(# of exposures)\*(# of repeats).



Instrument Parameters Sampling	g Parameters		
Sample Uptake Delay:	50	s	(0 - 10000)
Speed:	100	rev/min	(0 - 100)
Stabilization Time:	20	S	(0 - 10000)
Speed:	25	rev/min	(0 - 100)
Data Acq. Speed:	25	rev/min	
Rinse Time 1:	1	s	(0 - 10000)
Autosampler location:	R1		
Speed:	0	rev/min	(0 - 100)
Rinse Time 2:	40	S	(0 - 10000)
Autosampler location:	R2	×	
Speed:	50	rev/min	(0 - 100)
Rinse Time 3:	0	s	(0 - 10000)
Autosampler location:			
Speed:	0	rev/min	(0 - 100)
Replicates			
# of Exposures:			
Exposure Group A:	10		(1 - 500)
Exposure Group B:	10		(1 - 500)
# of Replicates	3		(1 - 15)
Time per sample: 2 min 59 sec			
Pump			
Speed set point:		rev/min	(0 - 100)

- A. If an Autosampler is present, the default configuration can be programmed and stored in the method. The configuration options are the standard/sample rack size and position as well as the COM Port to MICAP.
- B. The Sampling Parameters tab can be used for instrument parameter optimization. The graphic display on the page reflects changes to signal with changes to gas and plasma power conditions. This capability also can be used to optimize the Sample Uptake Delay, Stabilization Time, and Rinse Time.





Standards tab - (External Calibration)

- 1. Add the number of standard solutions desired. The default number of standards is 5. To add or remove standards, right-click on the column description to see add or remove standard menu. Standard 1 must always have a concentration of zero (0.000); all other standards can have any desired concentration. An autofill function is available for ease of standard concentration setup.
- 2. Choose whether to force the calibration curve through the origin or not when calculating the calibration curve.
- 3. Define Correlation Coefficient Limit, Individual Standard Maximum Error, Linear Range and Internal Standards Limits for each analyte in the far-right columns.

r Method	Instrument	t and Sam	pling Standards	oc oc	Interia										-	u
Line	~ Ur	nit	Standard	Standard 2	Standard 3	Force Through Blank	Weighted	Weight	Fitting Method	Correlation Coefficient Limit	Individual Standard Max Error [N]	Cross Calibration Range	Upper Linear Range Limit	IS LOW Limit [94]	IS High Limit (N)	
Co 238.892	pp	an)	0.0000	5.0000	10.0000		-2	1.0000	Linear	0.9950	10.00		20,0000	10		130
Co 345.350	pp	in	0.000	5.0000	10.0000	0		1.0000	Linear	0.9950	10.00		20.0000	70		130
Fe 235.204	pp	100	0.0000	5.0000	10.0000	8		0.0000	Linear	0.9950	10.00		100.0000	70		13
Fe 259.940	pp	m	0.0000	5,0000	10.0000	0	0	0.0000	Linear	0.9950	10.00		100.0000	70		13
Mn 257.610	pp	m	0.0000	5.0000	10.0000	0		0.0000	Linear	0.9950	10.00		100.0000	70		13
Mn 259.372	pp	m	0.0000	5.0000	10.0000	D	0	0.0000	Linear	0.9950	10.00		100.0000	70		13
Ni 346.165	pp	m	0.0000	5.0000	10.0000	0		2.0000	Linear	0.9950	10.00		\$0.0000	70		13
Ni 352.454	pp	m	0.0000	5.0000	10.0000	0		0.0000	Linear	0.9950	10.00		50.0000	70		15



Additions Tab – (MSA)

- Add the number of additions desired. The default number is 3. To add or remove additions, right-click on the column description to see add or remove addition. Addition 0 is locked to a concentration of zero (0.000) since this is the sample matrix with no addition; all other additions can have any desired concentration. An autofill function is available by highlighting the desired rows and right-clicking.
- 2. Force through sample option is applied by default. This feature forces the calibration through addition zero. Weighting of the calibration can also be applied in this window by checking the box and assigning a weight value between 0-2.
- 3. Define Correlation Coefficient Limit, Linear Range and Internal Standards Limits for each analyte in the far-right columns.

1	Gene	eneral Elements Instrument and Sampling Additions														
		Line 🦯	Unit	Addition 0	Addition 1	Addition 2	Addition 3	Force Through Sample	Weighted	Weight	Fitting Method	Correlation Coefficient Limit	Upper Linear Range Limit	IS Low Limit [%]	IS High Limit [%]	
L		Cu 324.754	ppm	0.0000	0.2500	1.0000	2.5000			0.0000	Linear			70		130
		Fe 259.940	ppm	0.0000	0.2500	0.5000	0.7500			0.0000	Linear			70		130
		Mn 257.610	ppm	0.0000	0.2500	0.5000	0.7500			0.0000	Linear			70		130
		Ni 352.454	ppm	0.0000	0.2500	1.0000	2.5000			0.0000	Linear			70		130
	▶		ppm	0.0000	0.2000	0.6000	0.8000			0.0000	Linear					130

QC Tab - (External Calibration)

- 1. Apply quality control standards to method.
- 2. Assign failure sounds to quality control standards.
- 3. Choose failure actions for quality control standards.

Check	Use	Action Atter Falure	Pailure sound.	
teth Zanfardi				
- XXV rinitial Calibration Verification)		ignore and continue from the next sample		
CCV (Continuing Calibration Standard)		ignore and continue from the next usegle		
- CCV2		ignore and continue from the next sample		
LCS Baboratory Control Samplej		ignore and continue from the next sample		
KS (interference Check Standard)	D	ignore and continue from the next sample		
URS (Linear Range Sample)	D	ignore and continue from the next sample		
LFG (Lab Fortified Bank)	10	ignore and continue from the next sample		
etk Barka				
IC8 (milial Calibration Bank)		ignore and continue from the next sample		
CCE (Continuing Calibration Bank)		ignore and continue from the next sample		
M8 (Method Black)	0	ignore and cordinue from the next sample		
red Samules and Salkes				
DUP (Duplicate)	0	ignore and continue from the next cample		
MS Matrix Salker	0	lignore and continue from the next sample		
MSD (Metrix Space Duplicate)	. 10	ignore and continue from the next sample		
PDMS Post Orgention Matrix Spike)	D	ignore and continue from the next sample		
PDMSD Post Digestion Matrix Spike Duplicate)		ignore and continue from the next sample		

QC Criteria Tab – (External Calibration)

- 1. Define criteria for passing quality control standards.
- Different quality control standards will provide different criteria options such as concentration range and %RSD.

C Check: ICV (Chec	k Standa	rds)	Che Deta	ck Standard ult Recovery Range			90 % . 110 %
Analyte/Wavelength	Units	Concentration	Recovery Conc Low	Recovery Conc High	%R	D	Notes
AJ 396.152	ppm	10.000	9.000	11.000	3	10	
Au 242.795	ppm	10.000	9.000	11.000	N.	10	
Ag 328.068	ppm	10.000	9.000	11.000	5	10	
Ag 338.289	ppm	10.000	9.000	11.000	\$	10	
Pd 340.458	ppm	10.000	9,000	11.000	\$	10	
Pd 360.955	ppm	10.000	9.000	11.000	\$	10	
Pt 306.471	ppm	10.000	9,000	11.000	ż	10	
Pt 265.945	ppm	10.000	9.000	11.000	\$	10	
Rh 343.489	ppm	10.000	9.000	11.000	\$	10	
Rh 369.236	ppm	10.000	9.000	11.000	\$	10	
Ru 372.803	ppm	10.000	9.000	11.000	4	10	
Ru 349.894	ppm	10.000	9.000	11.000	5	10	



File       Session       Method       Instrument       Help         Session       New Session       Methods       New Method       Report       Add to Queue       Run       Instrument       Image: Comparison of the provided of the pr	New Method	2025/01/22 9:02:19 AM			Co, Fe, Mn, Ni, Y
File       Session       Method       Instrument       Help         Session       New Session       Methods       New Method       Report       Add to Queue       Run       Instrument       Image: Comparison of the comparison	٩	٩	٩	٩	٩
File       Session       Method       Instrument       Help         Instrument       Instrument       Help       Instrument       Instrument         Sessions       New Session       New Method       Report       Add to Queue       Run	Method Name	Created Date	V Matrix	Description	Elements
File Session Method Instrument Help	Sessions New Session Methods	New Method	eue Run		Instrument OFF Pump - Plasma Inst
Q MICAP-DES - D	Q MICAP-OES File Session Method Instrumer	nt Help			- 0

Save the method and close the window. A Method has been successfully created.

### **Create Session**

From the Session menu select New or click New Session on the toolbar. This will open the New Session window. Alternately one can choose "Create a Session with this Method" after a right click on the Method in the Method list.

The mandatory fields are Session Name and Method. Use the drop-down menu arrow to select a previously created method to apply to the session. The fields labeled Job ID, Customer Name, Matrix, Regulatory Information and Description are not mandatory but provide a way to share information among multiple users.

Q Edit Session: External Ca	alibration session									
Session name:	External Calibration session		Sequence Number	Rack:Tube	Sample Name	Sample Type	Initial [q]	Final [mL]	Dilution Factor	Overall Correction Factor
Method:	External Calibration method 1 (internal copy $\vee$	-	1	1:1	Blank	Standard 1				
Customer name:		-	2	1:2	1	Standard 2				
Matrix			111 <b>3</b>	1:3	2	Standard 3				
Regulatory Information			111 <b>4</b>	1:4	3	Standard 4				
Description:			5	1:15	Sample 1	Sample	1.0000	1.0000	1.0000	1.0000
Description:			<u>:::</u> 6	1:16	Sample 2	Sample	1.0000	1.0000	1.0000	1.0000
			111 <b>7</b>	1:17	Sample 3	Sample	1.0000	1.0000	1.0000	1.0000
			111 8	1:18	Sample 4	Sample	1.0000	1.0000	1.0000	1.0000
Sample Introduction:	O Manual									
	O Autosampler									
	Autosampler Configuration									

Choose between manual or autosampler sample introduction.

Selecting the autosampler option will automate the session. Double-clicking on the Rack: Tube cell will open the autosampler configuration. Double-clicking on a position will insert the position into the cell.

The Autosampler configuration button is active. the Autosampler configuration button to ensure the proper standard and sample rack configurations are present. Select the "edit" function to access the drop-down menu selections for rack types. Clicking on any sample positions will add a sample to the session list. Saving the configuration will update the autosampler graphic.



Session name:	External Calibration session		Sequence Number	Rack:Tube	Sample Name	Sample Type	Initial Igl	Final [mL]	Dilution Factor	Overall Correction Factor
Method:	External Calibration method 1 (internal conv. >	-	888 A	1et	Blank:	Standard 1				
	External canoration metrica i (internal copy	-	- 2	1:2	1	Standard			6	
ustomer name:			- 3	1:3	2	Stan	infiguration			
Aatrix:			4	1:4	3	Stan Click on any positi	on on the Au	tosampler	preview to ch	ange current rack:tube
legulatory Information:			.5	1:15	Sample 1	Sami 0	G	) (		00
Description:			6	1:16	Sample 2	Sam	C		2)	3 4
			7	1:17	Sample 3	Sami	_			
			8	1:18	Sample 4	Samj 1	_		2	
Sample Introduction:	Manuaj     Autosampler     Autosampler Configuration						8 9 10 11 12	15 16 17 18 19	1 2 3 4 5	9 10 11 12

Note: If configured with an ESI autosampler, the image above will display the appropriate rack layout.

The number of standards that will populate in the session is determined by the number of standards defined in the method.

If an internal standard is used in the selected method, another sample type Blank without Internal Standard will populate at the top of the sequence. This standard is used for the internal standard recovery calculation.

To add samples to the session, follow these steps:

- 1. Right click in the empty space under the sequence list to the right and click insert row below to begin adding samples to the session.
- 2. Insert enough rows for all samples and the relevant number of QC samples that are needed for analysis.
- 3. Double clicking in the sample name column allows naming functionality for all items. Fill in the sample weights, final volumes, and dilution factors (if applicable) for all samples. Right-clicking on the multiple highlighted sample rows will provide an auto-fill feature for sample preparation information.
- 4. Fill in the sample weights, final volumes, and dilution factors (if applicable) for all samples. Right-clicking on the multiple highlighted sample rows will provide an auto-fill feature for sample preparation information.
- 5. These three columns will determine the overall correction factor that is applied to the instrument result value to determine the final concentration of the samples.
- Autosampler rack positions can be automatically populated in multiple highlighted rows by right clicking anywhere in the highlighted area and selecting Fill Rack:Tube sequentially.



Session name:	External Calibration session	Sequence Number	Rack:Tube	Sample Name	Sample Typ	e		Initial [g]	Final [mL]	Dilution Factor	Overall Correction Factor
Method:	External Calibration method 1 (internal conv. >>	111	1:1	Blank	Standard 1						
	External cambration metrical r (metrial copy -	<u>::::</u> 2	1:2	1	Standard 2						
Customer name:		111 <b>3</b>	1:3	2	Standard 3						
Matrix:		<u> </u>	1:4	3	Standard 4						
Regulatory Information:		111 5	1:15	Sample 1	Sample			1.0000	1.0000	1.0000	1.0000
Description:		6	1:16	Sample 2	Sample			1.0000	1.0000	1.0000	1.0000
		111 <b>7</b>	1:17	Sample 3	Sample			1.0000	1.0000	1.0000	1.0000
		8	1:18	Sample 4	Sample			1 0000	1 0000	1 0000	1.0000
							Insert Row	Above Below			
Sample Introduction:	O Manual						Insert Samp	ples Below			
	<ul> <li>Autosampler</li> </ul>						Delete Sele	cted Row(s)			
	Autosampler Configuration						Fill Rack#T	ube Sequent	ially		
							Fill Sample	Name Seque	ntially		
							Fill Sample	Туре			
							Fill Initial				
							Fill Final				
							Fill Dilution	n Factor			

7. Sample information can also be automatically imported from with the Import Sample Information from the file button at the bottom of the screen. Upon clicking this, a new window will appear to select the file location, data separator type, and rack autofill. The file type used in this import is .CSV. The CSV file will require five columns: sample name, sample type, initial, final, and dilution factor to properly import.

ielect File:				
Jata separator: , (comma)				
iutofill Rack:Tube positions: O No O Yes				
mported samples will be added below last selected	tow.			
		amp	ort	Cancel
_		Imp	ort	Cancel
_	_	Tanp	ort	Cancel

8. Click the Save button at the bottom right and close the session window.

Session name:	PGM CRMs		Sequence	Back:Tube	Sample Name	Sample Type	Initial	Final	Dilution	Overall Correction
Job ID:			Number					<u>fmL1</u>	Factor	Factor
Method:	PMG Method	× \Xi	翌 1	1	Blank witho	Blank without IS				
Customer name:			111 <b>2</b>	2	Standard 1	Standard 1				
Matrix	Aqua Regia		333 <b>3</b>	3	Standard 2	Standard 2				
Regulatory Information:			111 <b>4</b>	4	Standard 3	Standard 3				
Description:	Precious Metal Group analysis		111 <b>5</b>	5	Standard 4	Standard 4				
			111 <b>6</b>	6	ICV1	ICV	1.0000	1.0000	1.0000	1.000
		_	111 <b>7</b>	7	ICB1	ICB	1.0000	1.0000	1.0000	1.000
Sample Introduction:	<ul> <li>Manual</li> <li>Autosampler</li> </ul>		111 <b>8</b>	1:1	890134	Sample	0.9987	100.0000	1.0000	100.130
	Autosampler Configuration		111 <b>9</b>	1:2	890135	Sample	0.9955	100.0000	1.0000	100.4520
Plasma off after Sessi	on		111	1:3	890136	Sample	1.0023	100.0000	1.0000	99.770
Stop MICAP pump wh	nen collection is finished or stopped		333 <b>11</b>	1:4	890137	Sample	0.9994	100.0000	1.0000	100.060
			112 E	1:5	890138	Sample	1.1230	100.0000	1.0000	89.047
			11 <b>13</b>	1:6	890139	Sample	1.5000	100.0000	1.0000	66.666
			111	1:7	890140	Sample	1.0033	100.0000	1.0000	99.671
			111 15	1:8	890141	Sample	1.0094	100.0000	1.0000	99.068
			111 16	1:9	890142	Sample	0.9456	100.0000	1.0000	105.7530
			117	1:10	890143	Sample	0.9857	100.0000	1.0000	101.450
			111 18	8	CCV1	ccv	1.0000	1.0000	1.0000	1.000
			111.40			ccp.				

The Session has been successfully created.



## Analyze and Manage Data

- A. Prior to initializing the Data Analysis, ensure the SIA (sample introduction assembly) is thoroughly rinsed with blank diluent to eliminate potential elemental contribution to the blank due to carryover from residual elements in the pump tubing or SIA.
- B. To analyze test solutions, either highlight the Session name and press the Run button or press the Add to Queue button. Alternatively, you can right-click on the Session name and click add to queue. When no sessions are present in the queue, the run button will add the highlighted session and begin the queue. When sessions are present, the run button will begin analysis of the queue.

Pile Session Metho	rd inst	rument Help		1						1.00	- 17 8
Sessions New Session	Metr	nods New Method	REPORT IN	ear to Queser	<b>.</b>				Instrument OFF	Pump -	Plasma Instrumen
Session Name	Crea	ated Date	Job ID		Method		Customer Name		Matro	Sess	ion Status
P	p	)	P		P		Q		(p	P	
New Session 2	2025	5/01/22 9:28:32 AM	1		New Method (internal copy)			_		Not	started
New Session	2025	501/22 9:19:13 AM			New Method Jin	ternal coshi				Not	started.
Session Queue		Acquire Esterence C	NUME.								
Session Name		Session Status		Sequence Progre	55	Runtime		Curren	at Action	Use Re	ference Blank
New Session		Not started		0 of 4							
End of Queue Actions	Plaima		Pump Saver								

C. The dropdown arrow next to the run button allows for a delayed start to the queue.





D. After Run Queue is selected, choose whether to use an initial reference image for queued session and whether to use original wavelength calibration when resuming paused sessions. Using the same reference image for all sessions in the queue for a 12-hour period will take a reference image on the first session in the queue and prevent the reference image from being taken at the beginning of each subsequent session. A paused session can be resumed with its original wavelength calibration or with a new wavelength calibration at that time.



- E. Following the selections above, either Acquiring reference spectrum or Running wavelength calibration will begin.
- F. After the wavelength calibration this real-time status window will update information regarding the data analysis progress.
- G. Behind this status window is the Data Analysis window where the results of the session will appear.

		Acc	luiring re	eference	spectrum				1	Running wavele	ength calibration
Seque	Rack:T	Overall correct factor	Sample Name	Sample Type	Final Conc. [	Pause	- Mg 279.	553 (ppm) Intensity RS	Init Conc. (p	ISR (%)	Pause
1 +	2:15	1	Blank wit	Blank with	-0.689	-0.1	0.000	29,886,514,0	-0.689	0.000	
2 +	2:17		blank wit	Standard 1	-0.689	-0.1	0.184	71.6	-0.689	100.000	
6.11	2:11		0.500	Standard S	0.109	5.4	226.036	0.7	0.109	101.450	
7 (+)	2:5		1.00	Standard 6	0.912	1.5	453.103	0.9	0.912	101.563	
8.0	2:13		5.00	Standard 7	7.051	0.5	2,190.353	0.5	7.051	100.659	
9 +	2:7		10.0	Standard 8	12.958	0.5	3,861.865	0.5	12.958	101.367	
10 ±	2:19		20.0	Standard 9	18.034	0.2	5,298.293	0.2	18.034	98.864	
11.9	1	1.0000	RINSE	Sample	-0.687	-0.1	0.767	29.0	-0.687	0.230	
			mining	Parrieta	0 699	.0.1	0.261	65.7	-0.689	0.182	
12 :+	1	1.0000	RUNDE	Sample	-0.005						
12 +	1	2497.5025	256b 1/100	Sample	18,537.775	0.8	2,295.524	0.7	7.423	102.283	



- H. Expanding rows allows you to exclude any number of replicates from an item in the sequence. As the example above, the first replicate can be removed as the sample was not present in the SIA. The recalculate button must be clicked to apply any changes.
- Expanding columns will display more information in addition to the final concentration of each item in the sequence. Similarly, the Internal Standard can be applied by toggling the ISR button to the right.



J. The Profiles button can be clicked to open the line viewer window, which displays intensity data of all method analytes for any selected sample/standard. You can also see any desired wavelengths using the custom option in the select line drop down menu. After clicking the profiles button, the following window will provide an option of which samples to display.

Q Viev	v Data	a Analys	sis: M0016PS00	02_STABILITY	(_9_27_23_RL	in5						//
O	0	F	F	13	13	<b>BBB</b>	<b>B</b>	8	17		14	
Resume	Stop	Report	Copy Data Sheet	Expand Rows	Collapse Rows	Expand Columns	Collapse Columns	ISR	Recalculate	Edit Method	Profiles	View Session

K. When viewing data from an external calibration, each sequence line will have a sequence number, rack position, concentration, etc. Data from an MSA session will have all of these for the additions, but the final sample results will be displayed on their own line due to that concentration being a calculated value.

Sequence Number	Rack:Tube	Overall Correction Factor	Sample Name	Sample Type	Ag 328.068 [ppm] IS: Co 238.892 + Group A
1 🕂	3:15		Blank witho	Blank without IS	-0.004
2 🕂	3:9		Blank IS	Standard 1	0.000
3 +	3:17		50	Standard 2	50.428
4 🛨	3:11		100	Standard 3	102.738
5 +	3:19		500	Standard 4	482.033
6 🕂	3:13		MA3	Standard 5	not used
7 +	3:21	1.0000	rinse	Sample	0.062
8 +	3:21	1.0000	rinse	Sample	0.009

L. MSA Data Analysis window example:

:	Sequence Number	Rack:Tube	Overall Correction Factor	Sample Name	Sample Type	Al 396.152 [ppm] IS: Y 371.029 🕀 Group A
	1 +	1:15		Blank	Blank	
			1.0000	s1a —	MSA Sample	0.237
	2 +	1:1		s1a	Addition 0	-0.001
	3 +	1:9		sta	Addition 1	0.250
	4 +	1:17		s1a	Addition 2	0.500
	5 +	1:3		sta	Addition 3	0.753
	6 +	1:11		s1a	Addition 4	0.998



<b>Q</b> Select Samples	-		×
CAL BLANK			1.
CAL 1 ppm			
CAL 5 ppm			
CAL 10 ppm			
CAL 20 ppm			
20 ppm 1			
○ 20 1			
Select all	ОК	Cance	el

Integration parameters should be set for each analyte for both standards and samples. This is done by clicking and dragging the vertical, dotted lines on the graph and placing them in the appropriate location. This can also be done by entering numerical values in the Left, Right, and Center start/stop boxes. A six-line background correction can be used also. The default integration parameters can be activated by clicking the Reset button. The Merge button reduces the background to a two-point background. By holding the shift key and left clicking on a line the 3 lines can be separated to the right. The average of left start and stop defines the Left baseline and the average of right start and stop defines the right baseline. The baseline shape is defined by the correction drop- down box as linear, gaussian and exponential. Clicking Save will save the integration parameters to the method.









M. Modifying the method.

From Data Analysis the Edit Method button can be selected to add or remove analytical lines, change calibration specifications or QC criteria as previously described in the Method creation.

contraction and a second contraction and a sec	Resume	O	Report	Copy Data Sheet	Expand Rows	Collapse Rows	Expand Columns	Collapse Columns	ISR:	Recalculate	Edit Method	Profiles	View Session
--	--------	---	--------	-----------------	-------------	---------------	----------------	------------------	------	-------------	-------------	----------	--------------



#### N. Generating a Report and Exporting Data

A custom report format can be created to print the results.

Use the Report icon located at the top of the page to open the Report Configuration window. This window allows the user to create a custom PDF report or data export with select elements from the session.

Q View [ Resume S	Data Analysis: M	10016PS(	2002_STABILITY_9_27	23_Run5	Columns Collapse Columns	ISR Recalculate	Edit Method Profiles View S	Session
Ω         Report Config           PODF Report         Data           Report Section         Report Section           Φ Standard         Basic           O Standard         Basic           Custom         Custom	juration Derport Analyte Solection n	De	Layout Orientation Dentrait Andrespet Wavelength Columns Orien Dentrait Markhetical Wavelength Selection Dentrait Markhetical Wavelength Selection Dentrait Columns Orient Dentrait Den			×		
RIS Section Method Session Autosampler Data Analysis	Location <u>Method Details</u> Elements and Wavelengths Instrument and Sampling Standards Calibration Guality Control Quality Control Criteria	Options Method Name Matrix Method Descr Method Notes	PDF Report Data Export Analyte Select Export Options CSV Export Column Separator: Decimal Separator: Sample Orientation: R	tion formma oint ows	XML Export     Export 1D spectra data			
Preset Name: Output file:	AReport.pdf			Measurement Time Rack/Tube Position Initial/Final wt/vol. Sample Name Units Overall Correction Factor Final Concentration Diktion Factor Exposure Group Final RSD Net Intensity RSD [%]	Order  By Wavelength  Alphabetical Wavelength Selection  Individual  Cross Calibration  Show Replicates			
				Initial Concentration Calibration curve equebion Internal Standard Internal Standard Recover R*2 Value Estimated LOD S/N Estimated LOD S/N Correction Correction Std Blank Intensity Blank Intensity Std	Q Report Configuration PDF Report Data Export An	alyte Selection		
			Load Preset Configuration: New Preset Name Output file Chreport.csv		Analyte/Wavelength Al 394.401 Al 396.152 Ba 413.065 Ba 553.548 Co 238.892 Co 240.725 Cr 283.563 Cr 283.563	PDF Report	Data Export	
					K 766,490 Mn 259,372 Mn 403,076 Na 588,995 Na 589,592 Pb 405,781			



## Menus

## File Menu

File	
	Import
	Export
	Open Log Folder
	Settings
	Exit

**Import** Allows the user to import a previously exported (from another computer for example) Session or Method. A file dialog directory of ZIP files (.zip extension) will appear to select the files. Software will automatically detect if it is importing a Method or a Session.

**Export** Allows the user to export currently selected Method or Session to a ZIP file (.zip extension) for future capability to import to another MICAP-OES application residing on another computer.

**Open Log Folder** Opens the folder containing log files which can be useful for diagnosing issues with software or hardware. Logs are text files that can be easily copied or sent via email.

**Settings** Thes settings window consists of General Settings, Global Sounds, and Warmup Settings. General Settings includes significant figures options, profile window default span, a plasma shut off option, and custom wavelength addition. Global sounds are where the mp3 and wav files are displayed. Warmup settings are the instrument parameters that are applied directly after plasma ignition .

Exit Use it to exit MICAP-OES application.

## **Method Menu**

Metho	d
Vi	ew Methods
N	ew
Ec	dit
Vi	ew
Ar	rchive
D	elete Permamently

**View Methods** Changes the display mode of the Main Window to show the list of Methods. **New** Opens the Add Method Window allowing to create a new Method.



**Edit** Opens the Method Window for the specific method allowing the user to edit currently selected Method.

**View** Opens a "view only" version of the Edit Method Window.

**Archive / Unarchive** Allows the user to archive or unarchive a Method. Archiving provides a means to store Methods outside the main directory so that editing or deletion is not possible. To view/use archived Methods, click the drop-down to the right of the Method icon on the toolbar in the Main Window and select an appropriate option.



**Delete permanently:** Permanently deletes currently selected Method from the list and all data associated with it. **NOTE - This operation cannot be undone!** 

Sess	sion
	View Sessions
	New
	Edit
	View
	Import Spectrum Files
	Data Analysis
	Add to Session Queue
	Remove Session from Queue
	Report
	Archive
	Delete Permanently

## **Session Menu**

View Sessions Changes the display mode of the Main Window to show the list of Sessions.

New Opens the Add Session Window allowing the user to create a new Session.

Edit Opens the Edit Session Window for the highlighted session, allowing editing.

View Opens a "view only" version of the Edit Session Window.

**Import Spectrum Files** Imports spectral files from previously completed Sessions. This import function provides the capability to process measured sample results with a different method with different wavelengths.

**Data Analysis** If the selected session has run any number of items in its sequence, this option will be available to open the data analysis window for the session.



**Add to Session Queue** Adds the highlighted session from the sessions list to the end of the session queue. This session in the session list will now be highlighted grey.

Remove From Session Queue Removes the highlighted session from the session queue.

**Report** Opens the Report Configuration Window which allows the user to create a custom PDF report or data export with select elements from the session.

**Archive / Unarchive** Allows the user to archive or unarchive a Session. Archiving provides a means to store Sessions outside the main directory so that editing or deletion is not possible. To toggle between viewing Sessions that have been archived, unarchived or both, click the triangle to the right of the Session icon on the toolbar in the Main Window and select appropriate option.



**Delete Permanently: Permanently deletes** currently selected Session from the list and all data associated with it. **NOTE - This operation cannot be undone!** 

### **Instrument Menu**

Instr	ument	
	System	Status
	Autosar	npler Setup

System Status Opens the System Status Window.

**Autosampler Setup** Opens the Autosampler Setup Window. This is where default autosampler configurations are propagated from. If a session has an autosampler configuration that does not match the Autosampler Setup Window, a message will prompt the user to either continue using the session configuration or change it to match the configuration in the Autosampler Setup Window.



## Help Menu

Help	
F	lequest help
A	bout

**Request help:** Opens the Report Issue window where the user can submit software issues directly to Radom Instruments.

**About:** Opens the About Window which displays software version.

		0 8
0		
	0	9

## Windows

## Main Window

This window gives access to all functions and features of the system. It is the first window that opens when you start the MICAP-OES application.

Menus - Refer to the Menus section.

**Toolbar** – Toolbar buttons are simply shortcuts to the commands available in menus.



#### Plasma Status

On the right side of the toolbar, system status information is displayed as a combination of text messages and icons. Clicking the **Plasma** icon will initiate the ignition sequence if the Instrument icon is blue.



#### Instrument OFF

Indicates that system is turned off. Click the MICAP Instrument power icon to turn the system on. The Instrument icon will then turn blue.

#### **Blue Blinking Plasma Icon**

Indicates that the MICAP system is still warming up or the camera has not yet cooled to specified temperature.





Pump

Plasma

Green Plasma Icon and Blue Instrument Indicates that everything is working properly, and system is ready for

#### **Orange Plasma Icon**

Indicates that the system is in an error state. Click the text message to open the System Status Window for more information.

#### **Status Messages**

Camera temperature: 0.0°C

Plasma Error

**Instrument OFF** Instrument is turned off, no measurements can be performed, nor can parameters be changed. However, you can still use the software to manage and analyze data, create/modify Methods and/or Sessions.

Instrument

Camera OFF Camera is turned off. The camera must be turned on manually on the back of the Spectrometer.

Camera Error Camera is in an error state.

**Camera cooling** [°C] Camera is still cooling and has not yet reached the set temperature.

Camera temperature: [°C] Camera has reached the desired temperature and is ready for operation.

**Plasma OFF** Plasma is turned off. You can turn it on with the Plasma button on the main menu.

Plasma Error Plasma is in error state.

**MICAP warming up** MICAP systems including Plasma are still warming up. It takes about 20 minutes for the systems to reach ready states from the moment the plasma was turned on. The spectrometer should be on for at least 60 minutes.

MICAP warmed up MICAP systems including Plasma are ready but still waiting for camera to reach set temperature.

System ready System is ready for measurements.

Double-click on the message text or from the Instrument menu select System Status to open the System Status Window where you can see more information related to the abovementioned messages and change system parameters.



#### **Sessions / Methods Table**

The table displays all the Sessions and Methods with the most recent ones on top.

Q MICAP-OES						- 0 ×
File Session Meth	nod Instrument Help					
Sessions New Session	n Methods New Method	Report Add to Que	ue Run •		Instrume O	nt Dump - Diasma (1) Pump - Plasma
Session Name	Created Date	Job ID	Method	Customer Name	Matrix	Session Status
Q	Q	R	٩	Q	Q	Q
New Session 2	2025/01/22 9:28:32 AM		New Method (inter	nal copy)		Not started
New Session	2025/01/22 9:19:13 AM		New Method (inter	nal copy)		Not started

#### Filter / Sort

Over time, the Sessions and Methods directory will increase in size. To help navigate the items, the file names can be sorted by clicking the column header. A sorted column will have an up or down pointing arrow to indicate the direction of sorting. Click the column header again to reverse the sort order.

To filter the list, click in the top row of the column (next to the magnifying glass symbol), type filter criteria and press ENTER. Multiple columns can be filtered at the same time. The filtering logic uses AND operator which means that all filter criteria must be met for a row to be displayed.

#### **Delete Data**

To delete a Session or a Method from the Session or Method menu, right-click and select **Delete permanently**.

#### NOTE - This operation cannot be undone!



## New / Edit Method Window

#### **General Tab**

Allows the user to enter basic information such as Method Name, Matrix (diluent, acid concentration and type), Description and Notes.

### **Elements Tab**

#### Periodic Table / Elements

Provides visual representation of the Elements in the form of a Periodic Table or a list that can be sorted by atomic number, element symbol, or element name. Analytes that have been selected for quantitation are highlighted in pink. Analytes selected as Internal Standard are highlighted in green. Unused Analytes are highlighted in blue. Elements that cannot be analyzed by a MICAP-OES are highlighted in grey.

#### Wavelengths

Click on the element in the periodic table to show the available wavelengths. Lists all the wavelengths for the selected Element. This is a custom library developed on the nitrogen MICAP plasma.

**Use:** Select checkbox to include in the Method.

Element: Symbol and the wavelength.

Cross Calibration: Click to pair calibration to other wavelengths for extended linearity

Intensity: Relative Intensity of this wavelength.

**Ion** I: for atomic, II for ionic

**Interferences:** Click icon to see a graph showing nearby interferences and corresponding relative intensities in relation to the wavelength of the selected Element.

Analytes: Lists all the wavelengths that were selected for this Method.

**Element:** Indicates the Element and the wavelength.

Ion I: for atomic, II, III, etc. for ionic.

**Internal Standard:** Select any elements in the method from the drop-down menu. Any wavelengths selected as an internal standard are unable to have another internal standard applied to them, and the column will automatically populate with "none".

Background Correction: Expand to see selection for Type, Positions, and Peak

Type Open the drop-down menu to select the type of background correction. Options include Linear, Exp1, Exp2, Gauss1, with Linear as the standard setting. NOTE – If using less than six integration points, Exp2 and Gauss1 are not applicable. Positions Left, Center, and Right Define the integration of the selected analyte wavelength.



- Two-point integration is when both Left points = Center Left and both Right points = Center Right.
- Four-point integration is when Left point 1 = Left point 2 < Center Left and Right point 1 = Right point 2 > Center Right
- Six-point integration is when Left point 1 < Left point 2 < Center Left and Center Right < Right point 1 < Right point 2

**Peak:** Open the drop-down menu to select the type of peak integration

**Profiles:** Clicking this button opens a new window that prompts the user to select files to be imported to view the peaks that have been generated by either a previously run Session, or text files that were generated by a python script. You can select files individually from a specified Session folder or import an entire Session's files chronologically. Once the intended files are selected, click **Import** to load data into the **Profiles window**.



Profiles Button

#### **Instrument and Sampling Tab**

#### **Instrument Parameters tab**

The user inputs the instrument parameters such as gas flows, power, and exposure time. The default parameters are recommended for most analyses. Exposure time refers to the amount of time the CMOS Camera will acquire a signal. If a parameter is entered which is outside the allowable range, an informational icon will appear and display the appropriate range.

**Multiple Exposures:** Select this option to run a second set of exposures with settings of exposure time, # of exposures, and # of repeats. Be aware this will increase analysis time and require more sample volume.

#### Sampling Parameters tab

This section allows the user to input time values for sample uptake delay, stabilization time, and rinse times, as well as control the pump speed for each of those times. The rinse location as well as rinse time can be programmed with the capability of up to three different rinse solutions.

**# of Exposures:** Define the number of exposures (number of pictures taken within the exposure time defined on the Instrument Parameters tab) per replicate.

# of Repeats: Specify how many replicates will be read per sample/standard.

#### Time Scan

Click **Start** button at the bottom of the tab to initiate continuous scanning by the instrument. This function allows the user to visualize signal data displayed in the graph in real-time. Clicking Start will trigger the ignition sequence if the plasma is off. If the plasma is already on, the automatic scan function will begin. Parameters for both the instrument and sampling



can be changed to visualize changes in real-time. The two blue icons at the top of the time scan function allow to toggle between the raw data graph and a normalized data graph. The freeze toggle stops automatically snapping to full view when a new data point appears. Once all relevant data has been acquired, you can click **Stop** to end sample measurement. The **Clear** button will delete all data that was previously populated in the graph. The Graph display can be customized by selecting **Show all** or **Show last** via the radio buttons in the lower left corner. The Show last option allows customer definition of the recent data collected shown in minutes. Select/deselect clicking of the analyte/wavelength (respective check boxes on the right) includes/excludes the view in the graph. If an autosampler is being used, clicking on the **Autosampler Config** button allows the user to select which tube/rack to take solution from.

#### **Standards Tab**

Provides the ability to add/remove standards, define concentration per analyte/wavelength, set flag limits for correlation coefficients, set individual standard max error, set fitting methods, specify forcing the curve though origin, weighting factor and internal standard criteria.

Selecting the rows and right clicking allows to fill values based on the first selected row's value. Rows can be sorted alphabetically by element symbol, unit, and fitting method. Rows can be numerically sorted by standard concentrations, correlation coefficients, and individual standard max errors.

**Standards:** Standard 1 must always have a concentration of **ZERO (0.0000)**, as it is considered the blank in any Session or Method. All other standards concentrations can be unique to the method requirement. To add or remove a standard, right-click anywhere in the standards column and select add or remove standard.

Units: Define the units that will be used for each analyte. Options include ppm, ppb, and %.

**Correlation Coefficient Limit:** This value is the criterion for the minimum acceptable  $R^2$  value to which the calibration curve is assessed. Any correlation coefficient ( $R^2$ ) that is less than the specified criterion will be flagged in the data analysis section.

**Linear Range:** This overrides the high calibration standard for the "Error code E1: Calculated concentration exceeds highest standard concentration" in Data Analysis. The maximum concentration value at which the calibration curve remains linear. Any concentration larger than the specified value will be flagged in the Data Analysis section with a corresponding message.

**Individual standard max error:** The maximum % max error criterion can be entered for each Individual standard. This error is associated with the error from the actual measurement to the defined concentration on the standards page. Any standards with percent errors larger than the specified value will be flagged in the Data Analysis section with a corresponding message.

**Cross Calibration Range:** the range designated to a wavelength in a cross-calibration group to connect linear range with other wavelengths in this group.

Fitting Method: Linear function is the only available option currently.



**Internal Standard Limit:** The minimum/maximum allowed values for internal standard recovery in percent. Internal standard recoveries outside the specified range will be flagged in the Data Analysis section with a corresponding message.

**Force Through Blank:** Specify if the calibration curve algorithm for any analyte should be forced through the calibration blank.

**Weighted:** Choose whether to apply weight to any lines by checking their respective box. Weight can only be applied for calibration curves of three points or more.

**Weight:** A calculated modification to the data to allow data collection for low intensity analytes. Specify weight factor by entering a value between 0-2.

Weight equation: 
$$\sum_{i} \frac{(\Delta y_i)^2}{x^a}$$

where:

- y = the Δ between the data point and the calibration curve
- a = user specified weight
- x = concentration
- i = index

The impact of selecting this weighting option is that the lower calibration points gain more significance in the plotting of the calibration plot (with reduced weight to higher concentration standards). This selection results in improved recoveries on low concentration analytes.

**Note:** Selecting multiple rows and right clicking allows to fill values based on the first selected row's value. Rows can be sorted alphabetically by element symbol, unit, and fitting method. Rows can be numerically sorted by standard concentrations, correlation coefficients, linear ranges, Internal standard limits, weight values, and individual standard max errors.

#### Additions Tab (MSA only)

Assign concentration values to MSA additions. Addition 0 is locked to a value of zero since this is the sample matrix with no analyte addition. Force through sample is also selected by default. All other definitions for the tab can be found above in Standards Tab section.



#### QC Tab

IC Check		Use	Action After Failure	Failure sound
Check Standards				
	+		Ignore and continue from the next sample	
- CCV (Continuing Calibration Standard)			Ignore and continue from the next sample	
LCS (Laboratory Control Sample)			Ignore and continue from the next sample	
— ICS (Interference Check Standard)	+		Ignore and continue from the next sample	
— LRS (Linear Range Sample)			Ignore and continue from the next sample	
LFB (Lab Fortified Blank)			ignore and continue from the next sample	
Check Blanks				
ICB (Initial Calibration Blank)			Ignore and continue from the next sample	
- CCB (Continuing Calibration Blank)			Ignore and continue from the next sample	
— MB (Method Blank)	+		Ignore and continue from the next sample	
Paired Samples and Spikes				
- DUP (Duplicate)			Ignore and continue from the next sample	
— MS (Matrix Spike)			Ignore and continue from the next sample	
— MSD (Matrix Spike Duplicate)			Ignore and continue from the next sample	
- PDMS (Post Digestion Matrix Spike)			Ignore and continue from the next sample	
PDMSD (Post Digestion Matrix Spike Duplicate)		0	Ignore and continue from the next sample	

Selection of quality control functions to be included in the method.

**QC Check:** Types of QC available for use. Clicking + icon creates a repeat of that type followed by a number.

÷

Use: Click the box in this column to turn on specific QC Types.

Action After Use: Choose what action should be taken by the software if defined criteria (described in QC Criteria tab) are not met. Actions after QC failure include:

*Ignore and continue from the next sample*: will let the session continue with no changes regardless of QC failure.

*Rinse and repeat test*: will automatically populate a duplicate line in the session immediately following the QC that failed. The repeat line will have a sample name identical to the failed QC with the addition of (2) at the end.

*Pause the session and pause the queue*: will automatically pause the session and queue immediately following the QC that failed.

*Pause the session and continue with the next queue action*: will automatically pause the session and continue analysis with the next session in the queue.

**Failure Sound:** Select sound for software to play when QC failure occurs. Users can add new sounds from the File > Settings on the main window.

<b>Q</b> Select sound file	-		×
Sound			2
cannonroundwav-14480.mp3			
engine-helicopter-47189.mp3			
sample-9s.wav			
sample-9s.wav			
		-	
	Save	Ca	incel



#### **QC Types**

**ICV (Initial Calibration Verification):** A check standard that confirms the accuracy of the calibration. Usually tested immediately after calibration is complete.

**CCV (Continuing Calibration Verification):** A check standard that confirms the accuracy of the calibration after a certain number of samples have been measured. Commonly performed every 10 samples.

**LCS (Laboratory Control Sample):** A preparation check standard with a known concentration to confirm the viability of the preparation method.

**ICS (Interference Check Standard):** A check standard that confirms the existence of interference from one analyte to another at a given concentration.

**LRS (Linear Range Sample):** A check standard that determines the extent to which a calibration curve remains linear.

**LFB (Lab Fortified Blank):** A blank that is prepared under the same conditions as the samples being measured with the addition of a known concentration to confirm the accuracy of sample measurement and sample preparation method.

**ICB (Initial Calibration Blank):** A check blank that is measured immediately after calibration/ICV.

**CCB (Continuing Calibration Blank):** A check blank that is measured multiple times throughout a session.

**MB (Method Blank):** A blank that is prepared under the same conditions as the samples being measured to confirm that no contamination occurs during preparation.

**DUP (Duplicate):** A quality control measure that determines the precision of sample measurement. A second preparation of a sample that is being measured.

**MS (Matrix Spike):** A quality control measure that confirms the accuracy of sample measurement as well as the quality of preparation. A sample with the addition of a known concentration.

**MSD (Matrix Spike Duplicate):** A quality control measure that confirms the precision and accuracy of sample measurement as well as the quality of preparation. A sample that is identical in preparation to the Matrix Spike.

**PDMS (Post Digestion Matrix Spike):** A quality control measure that confirms the accuracy of sample measurement. A sample that has already been digested followed by the addition of a known concentration.

**PDMSD (Post Digestion Matrix Spike Duplicate):** A quality control measure that confirms the precision and accuracy of sample measurement. A sample that is identical in preparation to the Post Digestion Spike.



#### QC Criteria Tab

Specify the concentrations and passing criteria of all the QC functions that were selected for the method in the QC tab. Check standards have the option to define recovery ranges which are automatically calculated based on the concentration specified. Check standards also have a %RSD criteria that is user specified. Any check standards with %RSD larger than the specified value, and/or a concentration outside of specified range will be flagged in the Data Analysis section with a corresponding message. Wavelengths that are selected as internal standards will not appear in this menu.

(	General Elements Ins	trument a	ind Sampling Stan	dards QC Q	C Criteria								
	QC Check: CCV (Check Standards) Check Standard Default Recovery Range: 80 % - 120 %												
	Analyte/Wavelength	Units	Concentration	Recovery Conc Low	Recovery Conc High	%RS	D	Notes					
	AI 396.152	ppm	5.000	4.000	6.000	≤	10						
	AI 394.401	ppm	5.000	4.000	6.000	≤	10						

Blanks are required to have a zero (0.000) concentration and cannot be changed. The criteria options for passing/failing blanks are  $\pm$ LOD or  $\pm$ LOQ.

(	General Eler	ments Ins	trument a	and Sampling Stan	dards QC C	C Criteria	
	QC Check:	CCB (Chec	k Blanks)		↓ Che Def	ck Blank ault Recovery Range	: ± LOD ∨
	Analyte/Wa	velength	Units	Concentration	Recovery Conc Low	Recovery Conc High	Notes
	AI 396.152		ppm	0.000	-LOD	+LOD	
	AI 394.401		ppm	0.000	-LOD	+LOD	



## New / Edit Session Window

Sessions specify the sequence in which samples/standards defined in the Method are measured as well as the type of sample introduction and Plasma status after analysis.

Session Name, Method, and Sample Introduction are required fields while Job ID, Customer name, Matrix, Regulatory Information, and Description are optional fields.

Once a Method is selected, the sequence table to the right is pre-filled with all the standards (or additions for MSA) as defined in the Method.

of demail       Demail <thdemail< th="">       Demail       Demail</thdemail<>	Series       Image: Standard 1       Image: Standard 2       Image: Standard 2 <thimage: 2<="" standard="" th="">       Image: Standar</thimage:>	n name:	External Calibration session		Sequence Number	RackTube	Sample Name	Sample Type		inits 101	at 1	Final	Dilution Factor	Overall Correction Factor					
C Manual       2       12       1       Manual         C Minual       2       1       Manual       1.000       1.000       1.000         C Minual       C Manual       2       1.000       1.000       1.000       1.000         C Manual       C Manual       C Manual       C Manual       0       1.000       1.000       1.000         C Manual       C Manual       C Manual       C Manual       0       1.000       1.000       1.000         C Manual       C Manual       C Manual       C Manual       0       1.000       1.000       1.000         C Manual       Manual       C Manual       C Manual       0       0       0.000       1.000         C Manual       Manual       Manual       0       Manual       0       0       0.000       1.000       1.000         C Manual       Manual       Manual       0       Manual       0 <th>•••••••••••••••••••••••••••••</th> <th></th> <th>Edimal Calibration method 1 per</th> <th></th> <th>111 v</th> <th>191</th> <th>Bank</th> <th>Standard 1</th> <th></th>	•••••••••••••••••••••••••••••		Edimal Calibration method 1 per		111 v	191	Bank	Standard 1											
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atory (of of matching)                4             4	Atomistice         4         4         3         Standard 4         1000         10	mer name:			111.3	1:3	2	Standard 3											
Mary Promission.         Sample 1         Sample 2         Sample 1         Sample 2         Sample 1         Sample 2         Sample 1         Sample 2         Sample 1	Status         Sample 1         Sample 2         Sample 2         Sample 1         Sample 1         Sample 2         Sample 1         Sample 1         Sample 1         Sample 2         Sample 1         <	r.			84	1.4	3	Standard 4		1									
intro       6       1:6       Sample 2	Advasampier Configuration         Semple 1 intervalution         Semple 2 intervaluti	atory information:			5	1:15	Sample 1	Sample			1.0000	1.0000	1.0000	1,0000					
V         117         Sample 3         Sample 4         10000 <th< th=""><th>Interduction         7         17         Sample &amp; Sample &amp; Sample &amp; 1000         10000</th><th>ptiont</th><th></th><th></th><th>116</th><th>1:16</th><th>Sample 2</th><th>Sample</th><th></th><th></th><th>1.0000</th><th>1.0000</th><th>1.0000</th><th>1.0000</th><th></th><th></th><th></th><th></th><th></th></th<>	Interduction         7         17         Sample & Sample & Sample & 1000         10000	ptiont			116	1:16	Sample 2	Sample			1.0000	1.0000	1.0000	1.0000					
e Intreduction:	Introduction				117	1:17	Sample 3	Sample		1.1	1.0000	1.0000	1.0000	1.0000					
e introduction: Minual Mariad Mariad Mariad Sample introduction: Sample introduc	etereduction				8	1:18	Sample 4	Sample			1.0000	1.0000	1.0000	1.0000					
Settion name:         MSA #20100           Job ID:         Mathod         MSA method 1 (internal coop)         Image:         Im	Autosampier Configuention       Satistion name:       MSA #85800       Satistion       Sample 100	e introduction:	O Manual O Autosampier	Q Edit Season M	Asession							_							- 0
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Curtomer name:       2       1.2       Salt       Audiion 0       1.0000	Cuttorer name       2       12       Sp11       Austion 0       1.0000			Method	MO	method 1 lint	ternal comi	~	_	111 o	191	Bla	nk	Bank					
Maine:       13       13       501       Addition 1       0	Sample introduction:       13       13       5al       4adtion 1       0       0       0         Bestription:       Description:       14       14       591       4adtion 2       0			Cutterrane					-	1152	1:2	Spl	1	Addition 0	1.0000	1.0000	1.0000	1.0000	
Regulatory information:       4       14       Sp1       Addition 2       0       0       0         Description:       Description:       15       Sp13       Addition 5       0       0       1.000	Regulatory information:			Mature	-					111.3	1:3	Spi	1	Addition 1					
Description:       3       1.5       Sp1       Addition 3       0       0         0       Description:       6       1.6       Sp1       Addition 0       1.000       1.000       1.000       1.000         7       1.7       Sp1       Addition 1       0       0       0       0         8       1.8       Sp1       Addition 1       0       0       0       0         9       1.9       Sp1       Addition 1       0       0       0       0	Sample Introduction       Minual         Addosampler Configuration       Addosampler Configuration			Regulatory Inform	nation			_		田4	1:4	Spl	1	Addition 2					
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Sample Introduction:  Autosampler	Image: Sample Introduction     Image: Manual Sample Introduction     Image: Manual Sample Introduction     Image: Sample I			WESCOPOLOTE.						116	1:6	Spl	2	Addition 0	1.0000	1.0000	1,0000	1.0000	
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	Autosampler: Configuration			Sample Introduct		tanual utosampier													

#### **Sample Introduction**

Select between Manual and Autosampler (if Autosampler is available)

If Autosampler is selected, clicking the **Autosampler configuration** button allows the user to select the type of rack and tube size for each of the four tray slots of the autosampler.



#### Table

**Sequence number:** Shows the order by which the respective line will be run in each session. Clicking on the 3x3 dot pattern and dragging the label changes the analysis order of the Session to reorder the Test Solution measurement. Multiple sequence items can be moved at once by highlighting the relevant rows before clicking one the 3x3 dot pattern. This capability provides RUSH sample priority to a Session.

**Rack/tube:** Displays the autosampler location for the respective sample or standard in the sequence. Double-clicking this cell open the Autosampler Setup Window which allows the user to select a new autosampler rack/tube location by double-clicking the intended location number.

Sample Name: Double-click to edit the name of the sample.

**Sample Type:** Double-click to select from a drop-down between QC functions, standards, blank without internal standard (if applied method utilizes an internal standard), and samples.

Note - If QC types DUP, MSD, and/or PDMSD are selected, a dialogue box will prompt the user to select a parent sequence number to calculate %RPD from.

**Initial:** Input the initial weight/volume of sample used in grams or milliliters respectively. Clicking the blue unit in the column header allows the user to switch between g/mL units.

**Final Vol:** Input the final weight/volume of sample in grams or milliliters respectively. Clicking the blue unit in the column header allows the user to switch between g/mL units.

NOTE – Accepted configurations include (w/w), (w/v), and (v/v). (v/w) is invalid and will not allow the user to save the method.

Dilution Factor: Input any dilution factors if applicable.

**Overall correction factor:** Automatically calculated based on the initial sample weight/volume, final sample weight/volume, and dilution factor.

#### **Buttons**

**Import Sample Information from File:** Provides ability to import sample ID and dilution information.

Save: Saves configuration and closes Edit Session window.

Cancel: Closes window. Prompts user to save if changes were made.



## **Data Analysis Window**

To access this window, open any completed/paused/stopped session by double clicking on the session in the session list or clicking on Data Analysis in the drop-down Session list from the Main Menu. Alternatively, this window will open automatically upon starting/resuming a session that is not completed. This is where all sample/standard measurement data is accessible.

#### Toolbar

0	F	Ē	1E				0	5		1	
Resume	Report	Copy Data Sheet	Expand Rows	Collapse Rows	Expand Columns	Collapse Columns	ISR	Recalculate	Edit Method	Profiles	View Session

**Resume:** For paused sessions continues the Session from the last unmeasured sample in the Session.

**Report:** Opens the Report Configuration Window which allows the user to create a custom PDF report or data export with select elements from the session.

**Copy data sheet:** Copies all displayed data in Data Analysis including expanded rows/columns to be pasted into any Excel-like program.

**Expand Rows:** Expands all rows for any samples/standards that have been measured in the Session to show all replicate data.

Collapse Rows: Collapses all open rows in the Session.

**Expand Columns:** Expands all columns to show other data in addition to final concentration.

**Collapse Columns:** Collapses all open columns in the Session to show final concentrations exclusively.

**ISR:** Toggle to apply/remove internal standard corrections.

**Recalculate:** This icon will apply any changes made in Data Analysis e.g.: excluded replicates, excluded standards, ISR correction, preparation parameters and Sample Type.

NOTE - Data will not be affected until the Recalculate icon is clicked.

**Edit Method:** Allows the user to access a limited version of the method editor that contains only the Elements, Standards, and QC Criteria tabs.

**View Session:** Opens a "view only" version of the Edit Session window that allows the user to reference the details of the session while collecting data. In this is a view only version of the acquisition Method parameters.

**Profiles:** Clicking the Profiles icon opens the Profiles window to inspect full spectral information for all solutions measured in the Session. Here changes can be made to the integration parameters.

Prior to the Profiles window appearing, this window will require the user to select what they would like to view. In external calibration, everything can be viewed at the same time while in MSA, each sample set will be viewed individually.





Select MSA sample						
Please select which MSA sample you would like to see in Profiles window.						
◙ s1a						
⊖ s1b						
⊖ s1c						
⊖ s1d						
🔿 s1e						
⊖ s1f						
	ОК					

Once the changes are complete, click the save button. The session will provide save options as changes to the local copy of the Method (only affects current Session being viewed), a new global Method (only makes a new Method with the changed parameters, would not affect current session being viewed), or both the local copy and a new global Method (affects session currently being viewed and makes a new Method that can be applied to a different/new Session).

#### **Data Analysis Table**

Sequence	Overall					— AI 394.	401 [ppm]			
Number	Correction Factor	Sample Name	Sample Type	Final Conc. [ppm]	Final RSD [%]	Intensity	Intensity RSD [%]	Init Conc. [ppm]	ISR [%]	4
4 —	1.0000	IV-RADOM S	Sample	5.036	0.3	220.270	0.3	5.036		
			🕝 Replicate 1	5.018		219.486		5.018		
			🗹 Replicate 2	5.051		220.940		5.051		
			🕗 Replicate 3	5.039		220.383		5.039		

The default display will show columns for Sequence Number, Rack/Tube (if autosampler was used), Overall Correction Factor, Sample Name, Sample Type, and a column for concentration for each analyte/wavelength selected in the method.

Right-clicking in any cell on the data analysis view provides the option to sort analytes alphabetically by chemical symbol or numerically by wavelength, as well as displaying/hiding information about the session.

MSA sessions will include another line per sample prior to the additions. This line is for the calculated result and has a sample type of MSA Sample.

Sequence Number	Rack:Tube	Overall Correction Factor	Sample Name	Sample Type	AI 396.152 [ppm] IS: Y 371.029 🛨 Group A
1 🛨	1:15		Blank	Blank	
		1.0000	s1a —	MSA Sample	0.237
2 +	1:1		s1a	Addition 0	-0.001
3 +	1:9		s1a	Addition 1	0.250
4 +	1:17		s1a	Addition 2	0.500
5 ±	1:3		s1a	Addition 3	0.753
6 +	1:11		s1a	Addition 4	0.998





#### **Exclude / Include Replicates**

Right-clicking on any data cell will provide the option to exclude all replicates for that analyte. This will cause the data in that cell to have a slash through it as well as change its color to grey for clear data representation. Replicates can also be excluded/included individually by clicking their respective checkboxes.

Sample Type	Al 394.401 [ppm] 🛨	Al 396.152 [ppb] 🕂
Standard 1	0.000	0.000
Standard 2	5:000	5.000

#### **Flags and Errors**

Blue or red triangles in the lower corners of a cell indicate warnings or errors that are associated with that value or line. Click on either triangle to see details.







#### Graphs

To the right of the data columns, **Intensity plot** and the **Calibration Curve** graphs are visible.

Left-click-and-drag: move the graph in any direction.

Mouse wheel: zoom in and out.

Right-clicking-and-dragging: stretch/shrink the graph.

**Right-click:** brings a menu which allows you to copy and save an image of the graphs or reset zoom to fit data.

**Double-click and mouse wheel click:** reset the view of the graph back to default.

A combination of these functions can be used in tandem to see intricacies in the graphs.

**Intensity Graph:** The top display is a graph of intensity values for any selected data cell of a given line, centered on the wavelength.

**Calibration Curve Graph:** The bottom display is the calibration curve graph, which also shows the correlation coefficient along with the corresponding estimated LOD for the selected analyte in ppb. Right-clicking near a data point without dragging in this graph allows to **exclude/include** individual calibration standards from the curve. The nearest data point to the mouse cursor will be circled in red.





R<sup>2</sup> without weight is calculated by the equation:  $R^2 = 1 - \frac{\sum (\Delta y_i)^2}{\sum (z - \bar{z})}$ 

where:

- Z = average intensity
- i = index
- y = the Δ between the data point and the calibration curve

R<sup>2</sup> with weight is calculated by the equation: 
$$R^{2} = 1 - \frac{\sum_{i \neq B} \left(\frac{(\Delta y_{i})^{2}}{(x)^{a}}\right) + \frac{(\Delta y_{0})^{2}}{1}}{\sum \left(\frac{z}{x^{a}} - \left(\frac{\overline{z}}{x^{a}}\right)\right)}$$

where:

- B = blank
- a = user specified weight
- Z = average intensity
- X = concentration
- i = index
- y = the Δ between the data point and the calibration curve

Estimated LOD is calculated by the equation: 
$$LOD = \frac{3xy}{z}$$

where:

- y = standard deviation of the intensity of standard 1
- z = average intensity of highest standard average intensity of standard 1
- x = average calculated concentration of highest standard

#### **MSA Sample Calculation**

The concentration shown on the MSA sample line in the data analysis window:

$$x = \left|\frac{y - b}{m}\right|$$

- m = slope acquired from calibration of sample additions
- x = concentration at intercept
- y = 0 at x intercept
- b = y intercept from calibration of sample additions





## **Settings Window**

The setting window is used to define the number of decimal places to be shown on the Data Analysis window, as well as the default range of the Profiles data display in nanometers. The user can also choose to keep the plasma on when RIS is closed. The second tab is used to view, add, and remove global sound files. The third tab, warmup settings, has the settings for the instrument parameters that take effect directly after plasma ignition.

Q Settings	- 1	3 8	Q Settings X	Q Settings		_	- 🗆 🗙
General Global sounds Warm up			General Global sounds Warm up	General Global sounds	Warm up		
Number of decimal places used on Data Analysis			Sound	Coolant:	14	L/min	(8 - 20)
Final Concentration:	3			Auxiliary:	0.4	L/min	(0.2 - 2)
Final RSD:	1		cannonroundwav-14480.mp3	Nebulizer:	0.3	L/min	(0 - 2)
intensity:	3		engine-helicopter-47189.mp3	Power:	1000	w	(750 - 1000)
Intensity RSD:	1		mixkit-sad-game-over-trombone-471.wav				
Initial Concentration:	4		▶ sample-9s.wav	Pump	10	rou/min	(0. 100)
158:	3			speed set point.		Tev/IIII	(0 - 100)
LOD:	4						
Profiles window							
Default span value:	0.Z	nm					
RIS shutdown			Add Remove				
Say		Cancel	Save Cancel			Save	Cancel

On the General tab, the option to add/edit wavelengths will open a new window. Here, the user is able to select the element, wavelength and line type for a wavelength to add to the line library. Once added, this wavelength can be used in the method editor.

Q Add/Edit	Wavelenghts			- 0	X
	Element:	Ac	Y		
	Wavelength:	000.000	_	nm (194	- 625) 🕖
	Line Type:	none	×.		
	Add				
Element	Wavelength	Line Type		Dele	te
Liement	wavelength	T the type		Dele	LC



## System Status Window

Provides the ability to review and change several features regarding the hardware of the instrument. In the **Overview** tab, only readouts are available for informational purposes. The **Interlocks** tab shows all the instrument interlocks with a color-coded circle next to each one. Green indicates that the interlock is passing, red indicates that the interlock is failing, and grey indicates that the instrument is not connected. In the event of a problem, the user may contact Radom to access the password protected **Advanced** tab to assist with troubleshooting.

#### Camera

The status of the spectrometer is viewed in this section.

Status Shows status of the camera.

- Not detected system cannot communicate with the camera.
- **OFF** camera is turned off.
- **ON** camera is turned on and working properly.

Temperature Displays current camera temperature.

#### **Autosampler**

This section informs the user whether the autosampler is connected.

#### **Plasma Source**

Status Shows "Not Detected" or "Connected" – indicates if plasma is on or off.

#### Plasma

Plasma light: Green indicates the Plasma is Lit; red indicates the Plasma is off.

**Power:** Displays current power setting in Watts.

**Gas Pressure**: This section monitors the current input pressures of Nitrogen, Argon, and Air, and displays the pressure ranges for which each of these gases needs to be to allow the instrument to function correctly.

Units: Allows units to be selected for gas pressures. Options include psi, kPa, and bar.

A green light indicates pressures in range and red indicates pressures out of range.



#### **Gas Flow Rates**

This section allows the user to input desired flow rates within a given range for the Coolant, Auxiliary, and Nebulizer gases. It also displays the real-time flow rates of these three gases.

A green light indicates flow rates that are in range and red indicates flow rates that are out of range.

#### Pump

This section shows the current speed of the pump.

#### Temperatures

This section monitors the current temperatures of the Magnetron, Exhaust, and Microwave Cavity inside the instrument.

#### Wavelength calibration

Displays when the last calibration was completed, as well as the axis shift and order data from that calibration.

#### **Buttons**

Apply: Immediately initiates the settings displayed.

**Close:** Exits without saving changes.



## **Autosampler Setup Window**

This window allows the user to select the appropriate autosampler model and tray assembly type as well as specify what kind of racks will be used in each rack position.



Note: Cetac ASX-560 and ESI 2DX pictured above.

Autosampler Model: Choose from ESI-SC 2DX, ESI SC-4 DX, Cetac ASX-560, Cetac Oils 7400, and Cetac Oils 7600.

**Tray Assembly Type and Racks**: These dropdown menus are used to sort and select racks depending on the autosampler model.

**Control Mode:** Allows the user to have full access to the position of the autosampler probe. This mode must be activated to move the probe and must be turned off before saving the configuration.

**Home:** Click to remove the probe from any position it is currently in and move it directly above the rinse station.

**R Position:** Double-clicking the R position will initiate a rinse sequence and will continue to rinse until the user clicks on another position.

**Rack Positions:** Double-click any rack position shown to initiate the probe's movement and descent into that position.

Save: Saves the Tray and Rack changes and closes the window.

Close: Closes the window without saving changes.

#### **Autosampler Operation:**

ESI SC-2 DX and ESI SC-4 DX: ESI SC software will open alongside RIS. Users are not required to interact with this software unless certain hardware is added that requires it.

Cetac ASX-560: No additional software required for use. ASX Dashboard software included at install.

Cetac Oils 7400/7600: ASX Dashboard will open alongside RIS. Users are not required to interact with this software. Certain autosampler settings exclusive to the Oils 7400/7600 can be found here such as stir probe speed.



## **Profiles Window**

This is accessed through the **Profiles** icon in Data Analysis or in the Elements tab of the Edit Method window. In this window, the integration parameters for any analyte/ wavelength that has been included in the Method can be reviewed and altered. To change the integration parameters, click and drag the dashed vertical lines or enter the values directly in the **Background** section.



#### **Spectral Line Viewer Graph**

Displays the spectra, baseline correction and the integration area.

The legend on the right side of the graph allows the user to select which samples/standards are being shown, with the ability to look at multiple readings overlayed. The left radio buttons select which sample/standard's peak is highlighted in orange and whose integration data will be calculated in the fields below.

#### **Select Curves to Show**

**Sample minus blank:** Is the default display of all spectra except the Blank. The Blank is chosen after the Profile button is clicked. This can be any file in the Edit Method Profile tab but is typically the Blank without IS (Internal Standard). In Data Analysis only the Blank without IS or Blank with IS are possible choices.

Sample rep: Selecting Avg shows average of all replicates; All shows all replicates values.

Blank: Selecting Avg shows average of all replicates, selecting; All shows all replicate values.



#### Wavelength

**Select Line:** When you select a Line, the spectral line viewer graph will zoom in on the spectrum to the wavelength associated with that Line. Alternatively, you can select **Custom** and enter wavelength in the **Enter number** box.

**Enter number:** This box becomes active if you select Custom in the **Select Line** drop-down and allows the user to enter custom wavelength at which to display the spectral data.

**Span:** Allows the user to select how much data will be shown from the spectrum. The default view is 0.1 nanometers, showing 50 picometers to the left of the selected wavelength and 50 picometers to the right of the selected wavelength.

Default: Click to reset Span to the default view.

#### Background

This section shows the numerical values for the placement of the dashed vertical lines that determine the integration of the selected analyte wavelength. The position of the dashed vertical lines can be changed by entering custom numerical values (in picometers) in the left, center, and right text boxes. Default settings define the left points as equal to the center left point, and right points as equal to the center right point.

**Shift-click and drag** dashed vertical lines to separate the right and left points lines from their corresponding center point.

Reset: Clicking this button will separate all integration points for a six-point integration.

**Merge lines:** Checking this box will combine left points with the center left point and all right points with the center right point for a two-point integration.

**Undo/Redo:** These buttons are available after making any changes to the integration points. The counterclockwise arrow will undo any changes made in chronological order. The Clockwise arrow will redo any changes undone by the previous button in chronological order.

**Correction:** Select what type of correction to apply. If a six-point integration is applied, correction options include Linear, Exp1, Exp2, and Gauss1. If an integration of less than six points is applied, only Linear and Exp1 are available to choose from. Exp and Gauss need the nearby waveform encompassed by the left or right background points.

#### Areas under the curves

This section shows the calculations of **Peak area** defined by the selected integration parameters. Data is shown as an average (**Avg**), along with its corresponding standard deviation (**Std**) value. This section also displays the relative standard deviation (**RSD**) of the replicates, and the signal to noise ratio (**S/N**) of the selected analyte wavelength.

#### **Buttons**

Save and Exit: Saves Changes and closes Profiles window.



## **Report Configuration Window**

This window allows the user to select or design a PDF report or CSV/XML export for their RIS session data.

#### PDF Report





**Report Types:** The user can select basic, standard, detailed, or custom. Each report type has a different set of report information found in the selected category to the right side of the window. To create a custom report type, the user can modify the selected category by double clicking additions in and out of the area and then saving the preset at bottom of the window.

**Report Graphic:** This allows the user to add an image to their PDF report. By default, the MICAP logo will be added. This can be changed to no image or a custom image imported by the user.

Layout: This section has the following options for users to customize.

Orientation- select between portrait and landscape

Wavelength- select between rows and columns for displaying data tables

**Order**- select display order of wavelengths to be either alphabetical (by analyte name) or by wavelength (number)

**Wavelength selection-** select to report all wavelengths with the individual option or select to report cross calibration groups, if cross calibration is in use, as one column/row in report

**Calibration graphs per page-** select how many graphs should print per page if Display Calibration Graphs option is selected.



Data font size- select font size for tables in report

Page break after each sample- selecting this will start each sample on its own page

**Generate Report:** After choosing the output file location, this button will generate the PDF report. Upon generation, RIS will ask the user if they would like to open the save location folder for immediate access to the report.

#### **Data Export**



**Export Options:** Data can either be exported in CSV or XML format. Column separator allows the user to define what separator to use in CSV format. This separator can be a comma, tab, semicolon, or space. Decimal separator can be either a comma or a point for both CSV and XML. Sample orientation allows the user to export data in either rows or columns. Export 1D spectra data can be selected to export additional raw data.

**Data Options Selected:** This field contains all export details selected by the user from the data options available field. By default, all options are selected.

Additional options for data export include Order, Wavelength Selection, and Show Replicates. (MSA methods will also have an option to show additions)

**Order**- select display order of wavelengths to be either alphabetical (by analyte name) or by wavelength (number)

**Wavelength Selection-** select to export all wavelengths with the individual option or select to report cross calibration groups as one column/row in report

Show Replicated- select to export replicate data



**Custom Preset:** Save custom preset by providing a name and clicking save preset. This will save the current configuration. To load a saved configuration, select preset from dropdown menu. Deleting a template is also available from this dropdown.

**Generate Report:** After choosing the output file location, this button will generate the Data Export report. Upon generation, RIS will ask the user if they would like to open the save location folder for immediate access to the file.

#### **Analyte Selection**

<b>Q</b> Report Confi	Q Report Configuration							
PDF Report Dat	ta Export Anal	yte Selection						
Analyte/W	avelength	PDF Report	Data Export					
AI 394	4.401	$\sim$						
AI 396	5.152	<u>~</u>						
Ba 413	3.065	<u>~</u>						
Ba 553	3.548	$\sim$						
Co 23	8.892	$\sim$						
Co 24	0.725	$\sim$						
Cr 283	3.563	$\sim$						
Cr 360	0.534	$\sim$						
K 766	5.490	$\sim$						
Mn 25	9.372	$\sim$						
Mn 40	3.076	$\checkmark$						
Na 58	8.995	$\checkmark$						
Na 58	9.592	$\sim$						
Pb 405	5.781	$\sim$						

In the Analyte Selection tab of the Report Configuration window, the user can define which analytes/wavelengths will be included in the PDF report or Data Export.



## **ESI Autosampler Compatibility**

## **ESI Autosampler:**

MICAP-OES 1000 units may be equipped with an Elemental Scientific (ESI) autosampler. Models currently available are the 2DXe/4DXe and the 2DXCi/4DXCi.

#### **2DX Autosampler:**

Dimensions and Weight: Height: 460mm (18") Width: 540mm (21") Depth: 295mm (11.5") Weight: 8.2kg (18 lbs.)



#### 4DX Autosampler:

Dimensions and Weight: Height: 460mm (18") Width: 770mm (30.3") Depth: 295mm (11.5") Weight: 14.97kg (33 lbs.)





Both autosampler models share the same power requirements and electrical connections.

Power Requirements:

24 V DC switching power supply, 6 A (included) Input power: 100-240 VAC ± 10%, 50-60 Hz, 2.8A

**Electrical Connections:** 

1x USB 2x RS485 4x I/O

ESI SC/FAST

The ESI autosampler software will be pre-installed on the instrument computer when an ESI autosampler is purchased with the MICAP-OES 1000.

This software will work in the background behind RIS and will open automatically with RIS.

#### ESI SC software with 2DX autosampler:

File Calibrate Manual Configure Diagnosis Communication FAST Security About 🚝 Language

This is the window that will open with RIS when using an ESI autosampler. Autosampler will initialize upon opening RIS and no action is needed in this window.

×





Autosampler Setup Window with 2DX autosampler:



The autosampler control will be done within RIS in the Autosampler Setup window. Here, the user can select and save autosampler, tray assembly, and rack setup.



### **ESI Fast Valve:**



The Fast Valve module is controlled through a combination of the ESI SC software and RIS.

In the ESI SC software a Fast Method must be selected. This is done by opening the FAST menu at the top of the window.

ESI SC/FAST		- 🗆 X
File Calibrate Manual Configure Diagnosis	Communication FAST Security Abo	ut 🚝 Language
FAST Method File: Fast-with-LoopRinse-SS.txt	Enable FAST Control     Loop Size(mL)     Early Retract     Probe Rinse     Extra Rinse After Analysis	Rinse     Refill       Time     Time       Rinse 1     10     15       Rinse 2     10     15       Max Rinse     999999       Rinse On     Rinse Off
Initialize	Move Next <u>Suggested Instrument Settings</u> Advanced	



In this window, click on File at the top and open one of the pre-programmed Fast Methods.

Open		
< > < 1	]≪ Local Disk (C:) → ProgramData → ES	I → ESI SC → Methods → FAST
Organize 🔻 New fold	er	
> 🚞 MICAP -OES - I	Name	Date modified
🗸 📮 This PC	FAST-with-Rinse-SS_2	10/27/2023 9:53 AM
Local Disk (C:)	Fast-with-LoopRinse-SS	10/30/2023 1:35 PM
V 🔰 Network	Align_Method	11/7/2023 1:02 PM

This will populate the FAST Method Control window with the chosen fast method.

<b>F</b>	AST Method Contro							- 0
File								
	Event	Action	Parameter	Parameter Units	Event Paramete	FAST Control	Rins	seTime (s) se1 5
► 1	On Probe Down	Vacuum1 On				Method File Name:	Rin	se2 -1
2	On Probe Down	Load1				Fast-with-LoopRinse-SS.txt		
3	Probe In Sample	Monitor Inject1	1-25	start(s)-end(s)			IV	ax vacuum Time (
4	On Monitor Inject	Timer A	.1	seconds				300
5	Timer A Expires	Move Into(rrvv)	R1	mvv		Events & Actions FAST Control	Syringe Dilution Peripump	Sample Sense 4
6	Timer A Expires	Timer H	6	seconds		Events	Actions	
7	Timer H Expires	Trigger Instrument				Host Instrument	Autosampler Mayo Binos	Valve
8	On Monitor Inject	Timer F	.1	seconds		On Probe Up	Move Next	Load0/Inject0
9	Timer F Expires	Move Into(mvv)	R1	nvv		On Rinse On Rinse Type2	Probe Up/Down Move To(rrvv)	Load1/Inject1 Load2/Inject2
1	Timer F Expires	Timer I	5	seconds		On RRVV	Move Into Next	Load3/Inject3
1	Timer I Expires	Trigger Instrument				On Receive Sample Location	Flick	Load5/Inject5 Load6/Inject6 Toggle Valve FIAS Toggle M1/M2/M3/M4
1	Timer H Expires	Timer B	6	seconds		FACT	Probe Stir FAST Timer [] Sub-Method Stop FAST Read Barcode	
1	Timer I Expires	Timer B	6	seconds		Proho lo Samolo		
1	Timer H Expires	Vacuum1 On				Rinse Completed		
1	Timer I Expires	Vacuum1 On				Move Into Next Complete Timer [] Expires		Vacuum
1	Timer B Expires	Load1				On Monitor Volume True	Run Batch File	Vacuum1 On/Off
1	Timer B Expires	Timer C	2	seconds			Monitor Volume	Vacuum2 On/Off
1	Timer C Expires	Probe Up				Syringe	Syringe	Vacuum On/Off Vacuum0 On/Off
1	Timer C Expires	Timer D	3	seconds		Fill Syringe # Complete Dispense Syringe # Complete	Fill S# Fill S# Continuously	Peripump
2	Timer C Expires	Timer E	0.2	seconds		Start prepFAST Offline	Dispense S#	Peripump10n/Of
2	Timer D Expires	Vacuum1 Off				Didle Sample Complete	Stop S#	Peripump2 On/Of Peripump3 On/Of
2	Timer E Expires	Move Next				Value	S# Valve Position S# Vacuum State	Peripump4 On/Off Peripump5 On/Off
2						On Monitor Load # True	Dilute Sample	Gradient Method
						On Monitor Load # False	Dilute X	Gas Flow
						On Monitor Inject # True On Monitor Inject # False	Send X SV1 Fill/Dispense Timed Gradient Method	Set Gas Rate[] Gas Flow Off[]
							Output/Special	Rack
							A# On/Off DIW On/Off AuxOut Monitor Input Set Output	Mix Sample Heated Tray On Heated Tray Off PC3x
							Send Position Text	PC3x On PC3x Off

Here the user can edit their methods as needed. When this window is closed, the Fast Method chosen will be displayed on the ESI SC/FAST main window:



	ES	I SC/FAST							
F	ile	Calibrate	Manual	Configure	Diagnosis	Communication	FAST	Security	Abo
						Enable FAST Cor	ntrol		
	FA	AST Method F	ile: Fast-with	-Loop Rinse-SS	.txt		arly Retr	act	
							Probe Rins	se	
						🔽 E	Extra Rins	e After Analy	/sis
					~	Suggested Inst	Nove Next rument Se	t ettings	
		Initialize				<ul> <li>Advanced</li> </ul>			

With a Fast Method selected the user can finish the Fast Valve setup in RIS. The user must have either the 2DX or 4DX selected in the autosampler setup window.



In the Edit Session window, there is a check box to use the Fast Valve.

		Sample Introduction: O Manual
		<ul> <li>Autosampler</li> </ul>
Sample Introduction:	O Manual	Autosampler Configuration
	O Autosampler	Measure with FAST
	Automatics Configuration	Measure with Sample Sense
	Autosampler Configuration	ESI In-Series Automation

The user must select Autosampler under Sample Introduction to view the options: Measure with FAST, Measure with Sample Sense, and ESI In-Series Automation. Select Measure with FAST to complete the Fast Valve setup. Selecting ESI In-Series Automation will allow use of fast methods that utilize pre-stirring of next sample cup.



### **ESI SampleSense Valve:**

SampleSense is an optional component with the FAST valve and 2DX/4DX autosamplers. This component adds a sensor to the Fast valve that signals when the sample loop is full.





When using a valve with SampleSense, the user must also check the box: Measure with Sample Sense in the Session Editor window.

Sample Introduction:	<ul> <li>Manual</li> <li>Autosampler</li> </ul>
	Autosampler Configuration
Measure with FAST	
Measure with Sample Sense	
ESI In-Series Automation	



## K 766.490 Enabled Spectrometer:

The potassium enabled MICAP-OES 1000 Spectrometer pair has an added window of detection to quantify potassium at the 766.490nm wavelength. When validating this spectrometer, the user must add a K standard to the IV-Radom-Solution 2 for K recovery data.

IV-Radom-Solution 2 is a mixed element solution containing a concentration of 5 ppm for the following elements: Al, Ba, Co, Cr, Mn, Na, and Pb. By following the chart below, 20 ppm of K can be added to this solution while retaining 99.8% of the original 5 ppm mixed element concentration. \*Updated versions of this solution now automatically contain K at the required concentration.

Total Vol. (mL)	K 10,000 ppm Stock (mL)	K Concentration (ppm)
50	0.1	20
100	0.2	20
500	1	20
1000	2	20

To prepare this solution, add K 10,000 ppm stock solution and bring to corresponding volume with IV-Radom-Solution 2. Shake well for 10-20 seconds. This solution is now ready for instrument validation.

Aside from the validation solution modification, the K 766.490 Enabled Spectrometer does not require any unique setup or maintenance.

Here are some tips to get the most out of your K enabled spectrometer:

Recommended calibration range for K 766.490:
Aqueous matrix 0 ppm – 100 ppm

(1 sec exposure time)

Organic matrix 0 ppm – 500 ppm

(0.5 sec exposure time)

Changes in method parameters will influence calibration range.

A High standard must be at least 1 ppm for K calibration to function correctly.
Using K 766.490 for low level analysis and either K 404.721 or K 404.414 for high level analysis is recommended for best results.



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## **Getting More Help**

For more help, you can contact us via telephone or email. You can also find additional resources on our website.



