

# Software for Automated Speciation Analysis



# Xceleri Software

# **Software for Automated Speciation Analysis**

Xceleri is a simple but powerful tool that makes processing chromatographic data possible for any level of user.

#### **Data Processing**

- Data processing for transient signals
- Designed specifically for LC-ICP or LC-ICPMS measurements
- · Easy to build methods
- · Calibration curve building features

#### **Data Viewing**

- · Automated or manual peak selection and integration techniques
- · Visualization functions for easy comparisons of chromatograms for standards or samples

#### **Advanced Reporting Functions**

- · Automated read back functions for inline dilutions
- Report function offers a comprehensive overview of the results including calibration curves, raw intensities, calculated concentrations, and chromatograms
- QC exporting to a single Excel file

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Home Settings		
Calibration Sequences Report Charts		
Sequence Results	Data Analysis	
Arsenic Speciation Method 1 🗙		
Save Data Analysis 🔜 Save As		🧔 Refresh Data Analysis
Calibrations		
Elements Standards		
Element Measure Type: Mass   Wavelength		Equations
Analyte Configuration	<sup>1</sup> H	<sup>2</sup> He
33	Hydrogen 1	Helum 4
AS Arsenic 75	3 4 5 Li Be B Utimim Beylium Boylium Boylium	6 C N O F Nec Carbon Nitrogen Oxygen Fluorine Neon Add Remove
Available Analytes	11 12 13 13 1	14 15 16 17 18 10 10 10 10 10 10 10 10 10 10 10 10 10
75	Na         Mg         Al           Solum         Magnetum         Aluminum           23         24         22	SI P S CI Ar Silicon Phosphorus Sufur Chlorine Argon 28 31 32 35 40
Selected Analytes	<sup>19</sup> K <sup>20</sup> Ca <sup>21</sup> Sc <sup>21</sup> Ti <sup>22</sup> V <sup>24</sup> Cr <sup>25</sup> Mn <sup>26</sup> Fe <sup>27</sup> Co <sup>28</sup> Ni <sup>29</sup> Cu <sup>30</sup> Zn <sup>31</sup> Ga	<sup>32</sup> Ge <sup>33</sup> As <sup>34</sup> Se <sup>35</sup> Br <sup>36</sup> Kr
Mass Species Compound	roomaavuum cadoum saanduum itanuum vineduum chromium kanganese iron codeet nodee cooper 2,mc ceauum 39 40 45 46 51 52 56 56 59 58 50 56 51 50 64 81 37 38 39 40 41 42 43 44 45 46 47 48 49	50 51 52 53 54
75 AsB 75 As III	Rb         Sr         Y         Zr         Nb         Mo         Tc         Ru         Rh         Pd         Ag         Cd         In           Rubidum         Strontum         Yttrum         Zirconium         Noblum         Molybdenum         Technetium         Rubenlum         Paladium         Silver         Cadmium         Indum	Sn Sb Te I Xe Tin Antimony Tellurium Iodine Xenon
75 DMA	85 88 89 60 63 68 66 102 103 105 107 114 111 55 56 72 73 74 75 76 77 78 79 80 81 1	82 83 84 85 86 86 86
75 MMA	CS B2 57-71 HT 12 VV RC OS IF PT AU HG II Caestom Baltum Landronde Halfium Tantalum Tungstan Rhanium Osnium Iridum Platinum Gold Mierary Thallum 133 133 133 131 150 151 154 157 202 203	Lead Bismuth Polonium Astatine Radon 2011 202 2019 209 210 222
75 As V 75 AsC	87 88 104 105 106 107 108 109 110 111 112 113 Fr Ra 89-103 Rf Db Sg Bh Hs Mt Ds Rg Cn Nh	<sup>114</sup> FI Mc Lv Ts <sup>118</sup> Og
* Click here to add a new row	Francium Radium Activida Rutherfordium Dubnium Seaborgium Bohnium Hassium Metherium Damtstadium Roentgenium Copernicium Nhonum 223 226 267 268 271 272 270 276 281 280 286 287	Flerovium Moscovium Livermonium Tennessine Oganesson 289 288 293 292 294
Custom Configuration	E7 E9 E0 E0 E1 E2 E3 E4 EE EE	67 68 60 70 71
	Lanthanides La Ce Pr Nd Pm Sm Eu Gd Tb Dy	Ho Er Tm Yb Lu Helmum Ertium Thulium Ytterbium Ludetum
	159 140 141 142 145 152 153 158 159 169 169 89 90 91 92 93 94 95 96 97 98	99 100 101 102 103
	Actinides Ac Th Pa U Np Pu Am Cm Bk Cf Admium Thorium Protectnium Uranium Putonium Putonium Ameridum Curium Berkelum Californium	Es Fm Md No Lr Einsteinium Fermium Mendelevium Nobelium Lawrencium
	zer zaz zan 238 237 244 243 247 247 28	202 207 208 209 202
		Devel Calibration

**Figure 1**. Screen shot example of the arsenic speciation method. Element(s) of interest are selected then assigned the desired species that will be monitored. For example here AsB, As III, DMA, AsC, MMA, and As V have been selected for this method. More than one element can be selected if the method requires monitoring of multiple elements and species simultaneously.

### **Chromatogram Viewing**



Figure 2. An example arsenic species method (AsB, As III, DMA, AsC, MMA, and As V). Data from standards or samples can be easily overlaid for comparison purposes.



**Figure 3**. An example halogen species method (Br,  $BrO_3$ , I,  $IO_3$ , CI,  $CIO_2$ ,  $CIO_3$ , and  $CIO_4$ ). The example here shows how multiple elements being monitored can be displayed at one time.

#### **Report Function**

Calibration curves can be easily created and viewed using the Xceleri software. After transient peaks are identified, the software uses the integrated peak data along with the defined standards concentrations to create calibration curves for each species.

The report option has the ability to view each chromatogram individually, the integrated peak intensities, the calculated concentrations, and the calibration curves.

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Home Methods Settings												
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					Da	ta Analysis						
Arsenic Speciation Me	e As-	_								_	C Refresh	Data Analysis
Data Report											The second	outu ve tut jaa
Report Settings	) Å	Chromatogram	is Intens	ities Concentrations								
Analyte Column Ordering		Index	Arrived	Time	Description		75As (AsB)	75As (DMA)	75As (As III)	75As (MMA)	75As (As V	0
Analyte Column Filtering		1		9/18/2018 10:46:47 AM	Blank			0.0	0.0	0.0	0.0	0.0
Decimal Point Accuracy		2		9/18/2018 10:46:47 AM	Std-1			2.0	2.0	1.9	2.0	2.1
1	*	3		9/18/2018 10:46:47 AM	Std+2			10.3	10.1	10.1	9.9	10.0
Minimum Report Value		4		9/18/2018 10:46:47 AM	Std-3			19.9	20.0	19.9	20.1	20.0
Zero	*											
Automatic Scrolling												
Automatic Details												
Synchronize Reports	1											
		Sample Cor	ncentration I	Details								
		Calibration	Curves									
		75A 500000	s As8 - Standa	rds 500000 -	75As DMA - Standards	75As As III - Standards 1000000	75As MMA - :	Standards	75As As V	- Standards		^
			- 10.00		4 0 12 10		0 4 8	12 10 20	0 4	0 12 10 20		
Export Options		R = 0.999823	- 16.03	y = 42994 R = 0.9999	89 89	y = 60626.39 x - 131.82 R = 0.999964	y = 20772.83 x + 234.18 R = 0.99997		R = 0.999995			~

Figure 4. An example of how the calibration curves are displayed in the report function.

## **Export Function**

All data can be exported directly to a .csv or .xlsx. This excel file (.xlsx) option contains all of the data including the chromatograms, peak area intensities, concentrations, and calibration curves. This allows easy report generating when needing to send data off to customers, QC review, or lab managers.