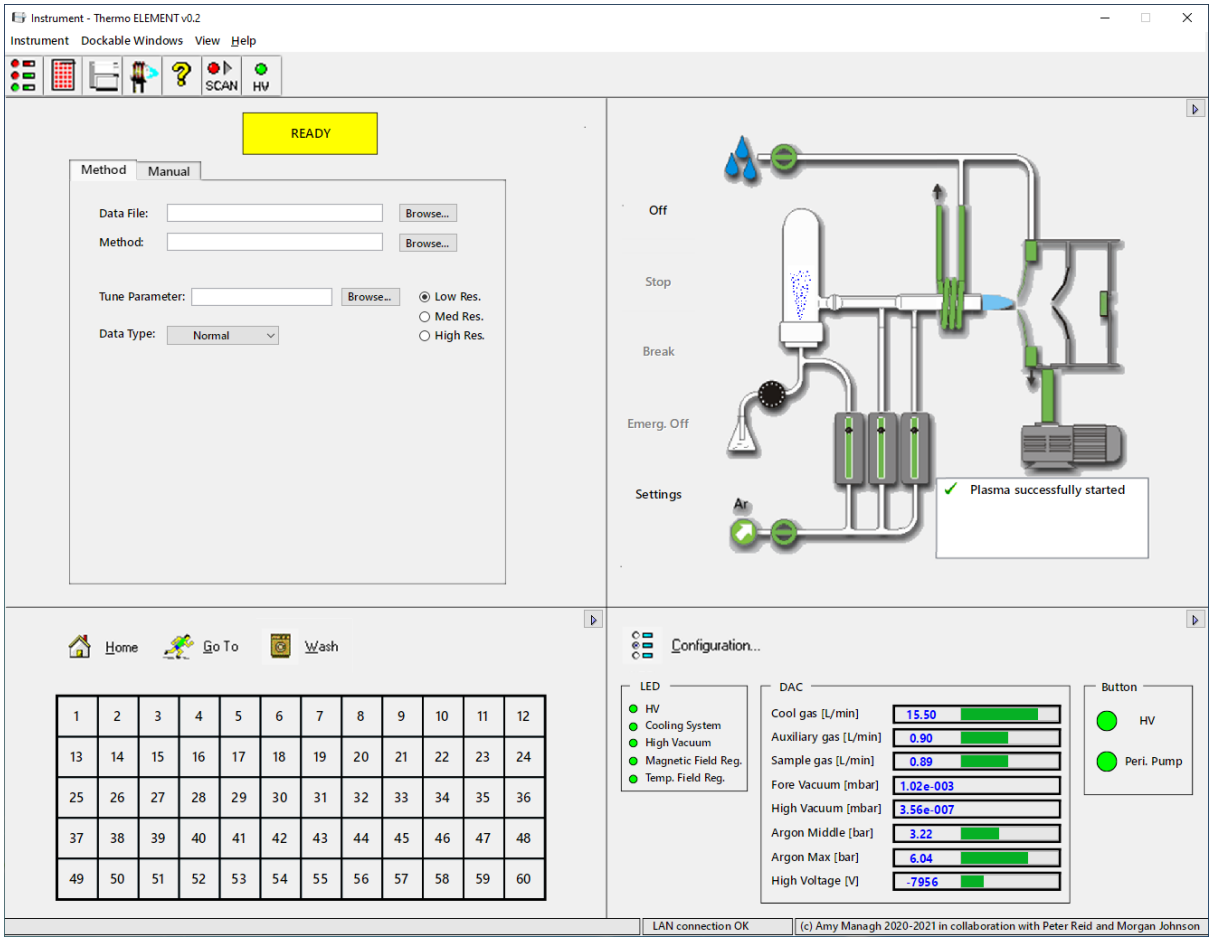
ICP-MS Instrument Simulator Basics

This app doesn't require any special installer or uninstaller. Simply unzip the archive you've downloaded and place the folder on your desktop. The app uses associated support files to control the facilities and behaviour of the app. These files must remain in the folder alongside the app itself (*.exe or *.app).

Open the file Instrument.exe. The program will initially appear as shown below:



1	2	3	4	5	6	7	8	9	10	11	12
13	14	15	16	17	18	19	20	21	22	23	24
25	26	27	28	29	30	31	32	33	34	35	36
37	38	39	40	41	42	43	44	45	46	47	48
49	50	51	52	53	54	55	56	57	58	59	60

The main screen contains four main panels: the analysis panel (top left), the plasma start-up panel (top right), the autosampler panel (bottom left) and the watch parameters panel (bottom right). In this simulation, the instrument has already been switched on for you and is ready to start analysis. There are two scan modes available: *method scan* and *manual scan*.

A range of samples have been loaded into the autosampler rack, as detailed overleaf.

1. Quantification of selenium in a nutritional supplement

This experiment involves quantification of the selenium content of a nutritional supplement. Samples of the supplement were prepared by dissolving a 0.1g portion of the 0.5g tablet in 10 ml of concentrated HNO_3, followed by a 100-fold dilution of the solution with DI water. Samples of three tablets were prepared and are loaded into positions 6-8 of the autosampler rack. Calibration standards containing 0, 25, 50, 75, 100 ppb Se in 1% HNO_3 are loaded into positions 1-5 of the rack (in order of lowest concentration to highest concentration). A 5 ppb gallium internal standard was added to all solutions.

2. Cellular uptake of a gadolinium-based MRI contrast agent

This experiment involves comparison of the cellular uptake of two Gd-based MRI contrast agents by T cells *in vitro*. CD4+ T cells were cultured in 2ml of RPMI 1640 medium, supplemented with 10% human albumin, penicillin, streptomycin and glutamine, plus 1×10^5 U/mL human recombinant IL-2. Each well also received a 50 µl volume of either Gd-DTPA (Omniscan®) or Gd-DOTA (Dotarem®). The cells were incubated overnight (~16 h) at 37°C in 95% air/5% CO_2. Following the incubation period, the cells were washed extensively in PBS/2% FCS to remove any unbound label. Prior to analysis, the cell pellets (~$9x10^5$ cells) were digested using a mixture of concentrated HNO_3 and H_2O_2. Following digestion, the samples were evaporated to dryness under a stream of nitrogen and reconstituted in 1.5 mL of 2% HNO_3. Further details on sample preparation and the background to this study can be found in the following publication: *Anal. Chem.* 2013, 85, 22, 10627–10634

A series of gadolinium calibration standards containing 0, 5, 10, 20, 30 and 40 ppb Gd in 2% HNO_3 are loaded in ascending order into positions 11-16 of the autosampler rack. Positions 17-19, 20-22 and 23-25 contain an unspiked control and cell samples doped with Gd-DOTA and Gd-DTPA respectively. A 5 ppb europium internal standard was added to all solutions.

3. Multivariate analysis of metals in fabrics

This experiment is designed to provide experience of multivariate analysis for an industrial application. Coloured cotton fragments (~1g) were fully submerged in 5 ml of concentrated nitric acid and heated at 60°C for 24 hours. The resulting solutions were filtered, then made up to 250ml using DI water. The samples are loaded into the following autosampler rack positions: method blank (32), black (33-35), white (36-38), red (39-41), blue (42-44), green (45-47). A series of standards containing 0, 5, 10, 25, 50 and 100 ppb of Cr, Mn, Co, Ni, Cu, Zn, As, Cd, Hg and Pb are loaded into positions 26-31 of the autosampler rack, in order of increasing concentration.

4. Qualitative analysis of gunshot residue

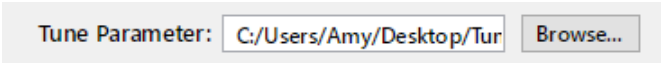
This experiment is designed to provide experience of qualitative analysis using manual scan mode and to demonstrate an application in forensic science. A student wearing latex gloves fired a starting pistol and the gloves were subsequently swabbed using a DI water wetted cotton bud. The swabs were transferred to a beaker containing 50mL of 2% HNO_3 and allowed to stand for 30 minutes. Finally, the solution was filtered using a Whatman GF/D 2.5 µm filter. The filtered sample has been placed into position 9 of the autosampler rack. Position 10 contains a pre-firing blank for comparison.

Method Scan

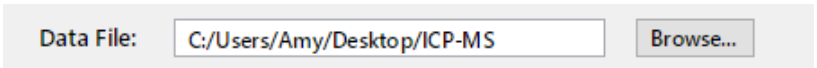
The method scan mode uses a pre-created method to measure specific isotopes. The result output will show a single average value for each of the isotopes of interest within the sample.

1. You have been provided with a method file, which will have the file extension ".met". This file specifies the isotopes to be measured and the conditions to be used. Load this method by clicking on Browse… and selecting the file that was provided to you.

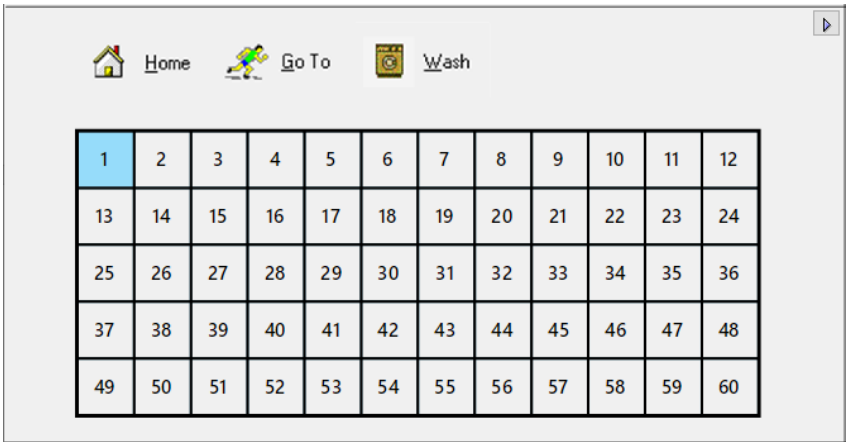
2. In the box marked Tune Parameter, click Browse… and select the tune file that you created earlier in the TuneSim (or the one that was provided to you). This file will have the extension ".tpf" (tune parameter file).



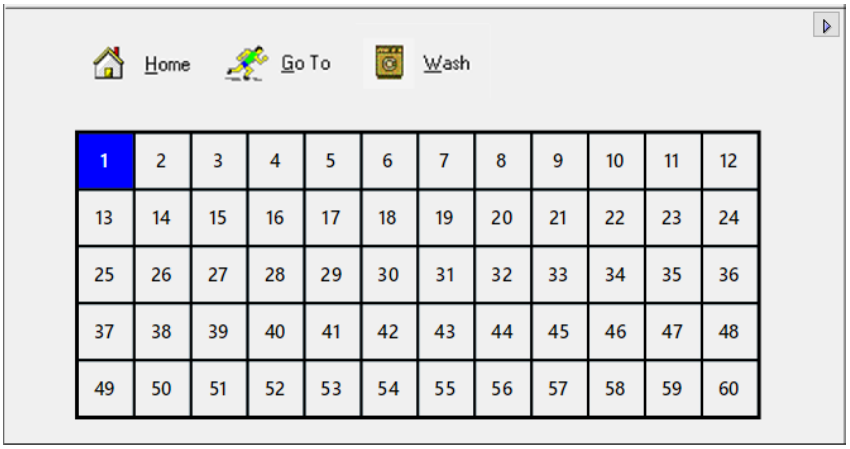
3. In the box marked Data File, click Browse.. and choose a location where you would like the data to be saved to e.g. you could create a folder on the desktop named ICP-MS.



4. Navigate to the autosampler panel. Select a position in the autosampler rack by clicking on it. The relevant box will turn light blue.



5. Click on the button marked Go To. The selected position will change colour to dark blue when the autosampler is in position.

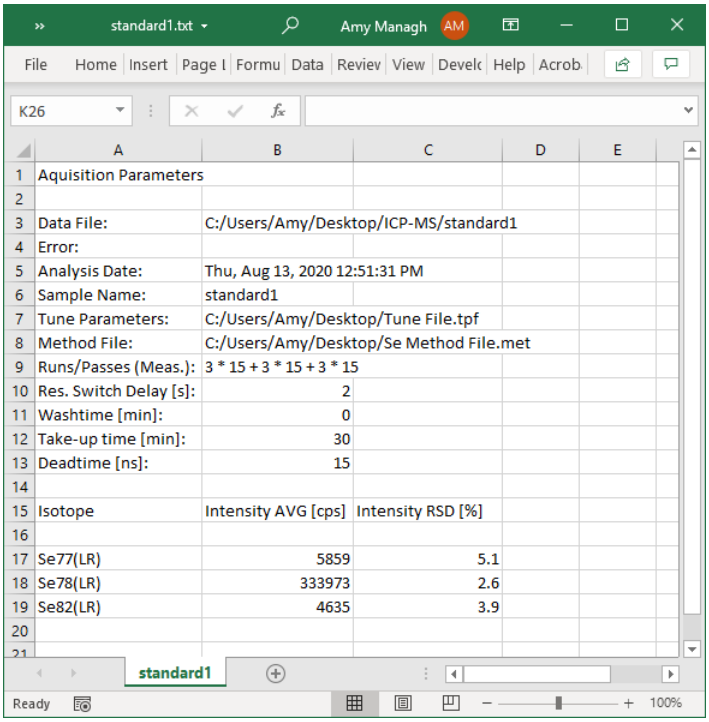


6. Return to the field marked Data File. After the file extension add a forward slash and a name for the sample being analysed e.g. "/standard1".

7. Click on the button marked Scan at the top of the window: 

The scan indicator will turn from yellow to green to indicate that the instrument is scanning and will return to yellow once the scan is complete:

8. Once the scan is complete, your data file can be found as a text file in the location that you specified. The data for the measured isotopes can be found at the bottom of the file. The intensity AVG [cps] column is the one to use when processing the data.



	A	B	C	D	E
1	Aquisition Parameters				
2					
3	Data File:	C:/Users/Amy/Desktop/ICP-MS/standard1			
4	Error:				
5	Analysis Date:	Thu, Aug 13, 2020 12:51:31 PM			
6	Sample Name:	standard1			
7	Tune Parameters:	C:/Users/Amy/Desktop/Tune File.tpf			
8	Method File:	C:/Users/Amy/Desktop/Se Method File.met			
9	Runs/Passes (Meas.):	3 * 15 + 3 * 15 + 3 * 15			
10	Res. Switch Delay [s]:	2			
11	Washtime [min]:	0			
12	Take-up time [min]:	30			
13	Deadtime [ns]:	15			
14					
15	Isotope	Intensity AVG [cps]	Intensity RSD [%]		
16					
17	Se77(LR)	5859	5.1		
18	Se78(LR)	333973	2.6		
19	Se82(LR)	4635	3.9		
20					

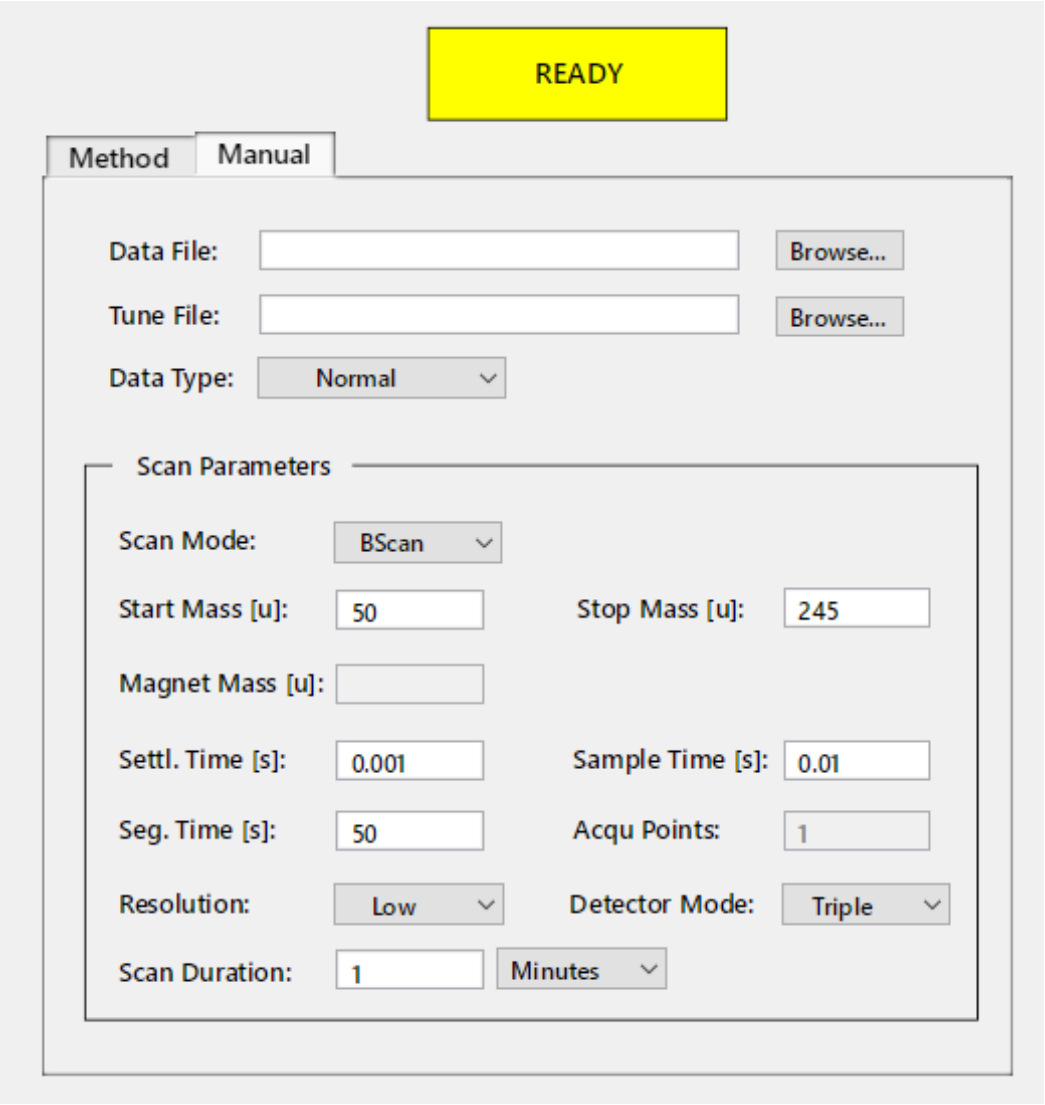
9. Repeat steps 4-7 to analyse the next sample. Be sure to give each sample a new name to prevent the files from overwriting each other.

10. When you have finished, you can exit the app by closing it in the usual way. If you wish, you can turn the plasma off first using the Off button in the plasma start-up panel.

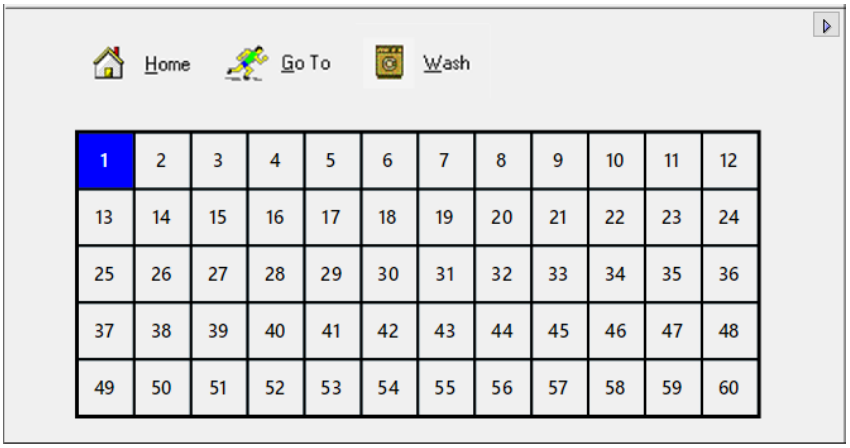
Manual Scan

The manual scan mode allows you to specify a mass range to analyse. The output will show a mass spectrum for the range being measured.

1. Navigate to the Manual scan window located to the left of the Method scan window. This will open the Manual scan page where you can specify different options as seen below.

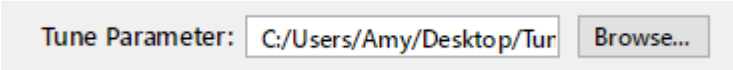


2. Click on a position in the autosampler rack and press Go To. The selected position will change colour to dark blue when the autosampler is in position.

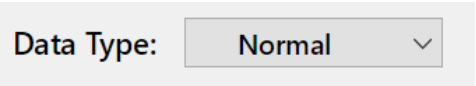


3. In the box marked Data File, click Browse.. and choose a location where you would like the data to be saved to e.g. the desktop.

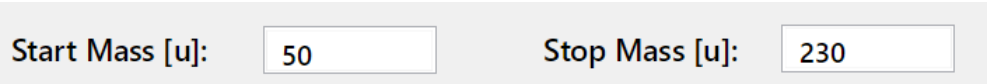
4. In the box marked Tune Parameter, click Browse… and select the tune file that you created earlier in the TuneSim (or the one that was provided to you) . This file will have the extension .tpf (tune parameter file).



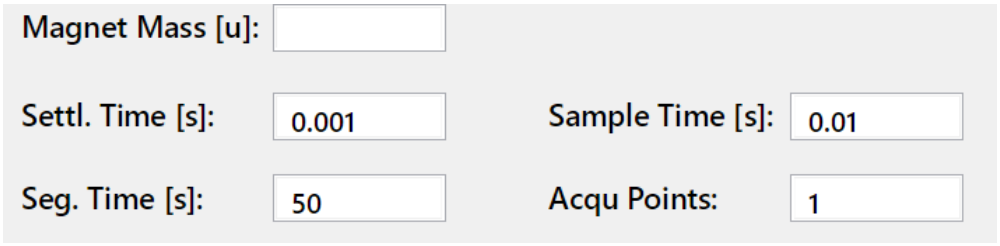
5. Select Normal from the Data Type dropdown menu.



6. The start and stop masses of the spectrum can be specified which will determine the mass range for your data. Enter values into the respective fields. The minimum Start Mass is 5 [u] and the maximum Stop Mass is 260 [u].

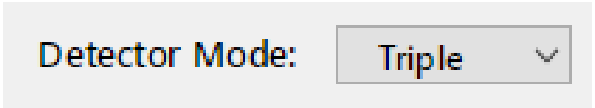


7. For the following variables, please enter these values into the field if they are not already present.

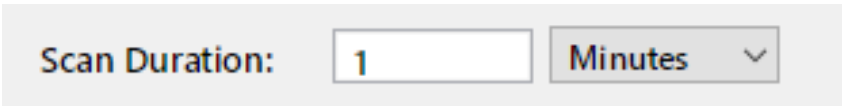


8. Choose the resolution required. Options are low, medium or high.

9. Choose the detector mode for the MS. These include modes such as: Triple, Faraday, Analog and Counting. Triple mode will ensure that high count rate signals that are outside the linear dynamic range of the SEM detector are deflected to the Faraday detector.



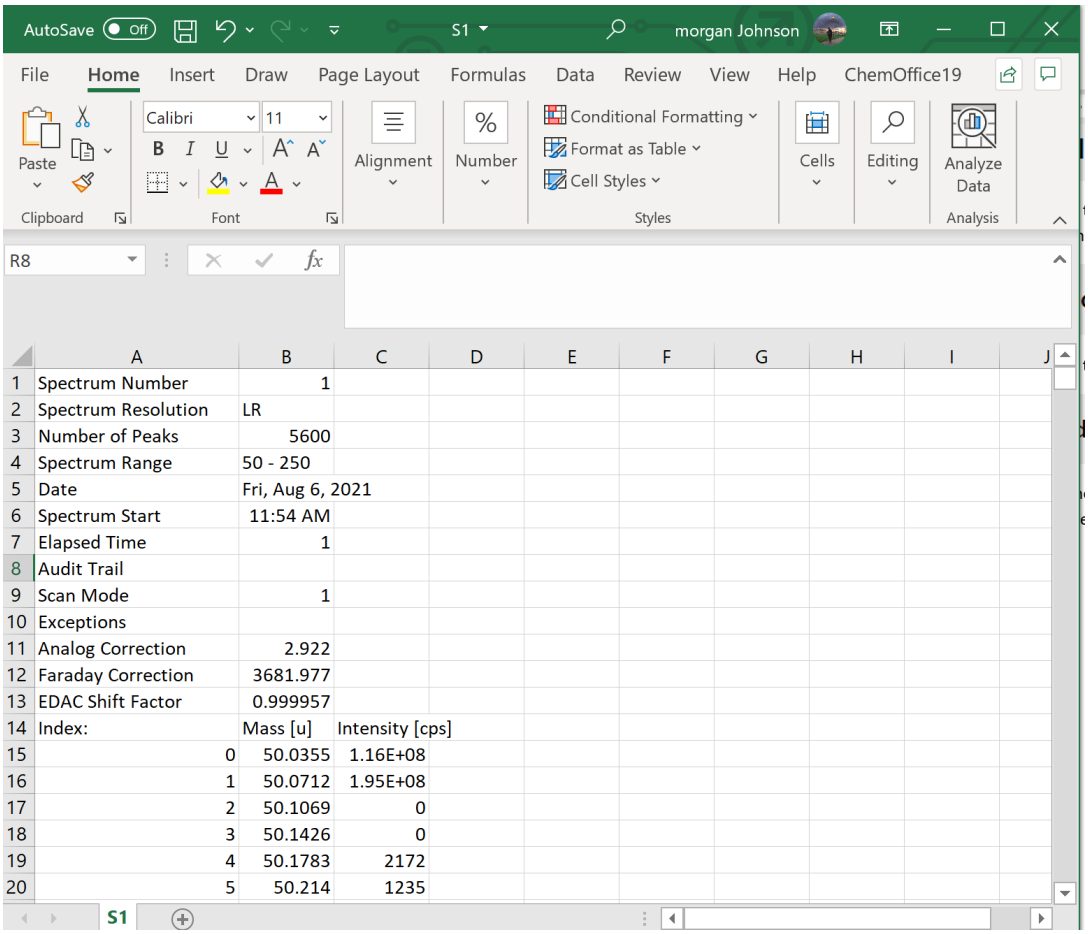
10. Choose the scan duration. This can be set to seconds, minutes or number of scans.



11. Click on the button marked Scan at the top of the window: 

The scan indicator will turn from yellow to green to indicate that the instrument is scanning and will return to yellow once the scan is complete:

12. Once the scan is complete, your data file can be found as a text file in the location that you specified. This .txt file can be opened via excel and will look like the example below. Your data is now ready to be analysed.



	A	B	C
1	Spectrum Number	1	
2	Spectrum Resolution	LR	
3	Number of Peaks	5600	
4	Spectrum Range	50 - 250	
5	Date	Fri, Aug 6, 2021	
6	Spectrum Start	11:54 AM	
7	Elapsed Time	1	
8	Audit Trail		
9	Scan Mode	1	
10	Exceptions		
11	Analog Correction	2.922	
12	Faraday Correction	3681.977	
13	EDAC Shift Factor	0.999957	
14	Index:	Mass [u]	Intensity [cps]
15	0	50.0355	1.16E+08
16	1	50.0712	1.95E+08
17	2	50.1069	0
18	3	50.1426	0
19	4	50.1783	2172
20	5	50.214	1235

13. Plot the data in columns B (mass, x-axis) and C (signal intensity, y-axis) to obtain the mass spectrum.

14. When you have finished, you can exit the app by closing it in the usual way. If you wish, you can turn the plasma off first using the Off button in the plasma start-up panel.

List of Samples in the Autosampler

Rack Position	Sample
1	1% nitric acid / blank, with (with 5 µg/L Ga internal standard)
2	25 µg/L Se standard (with 5 µg/L Ga internal standard)
3	50 µg/L Se standard (with 5 µg/L Ga internal standard)
4	75 µg/L Se standard (with 5 µg/L Ga internal standard)
5	100 µg/L Se standard (with 5 µg/L Ga internal standard)
6	Seleniuim supplement (with 5 µg/L Ga internal standard)
7	Seleniuim supplement (with 5 µg/L Ga internal standard)
8	Seleniuim supplement (with 5 µg/L Ga internal standard)
9	Gunshot residue sample
10	Pre-firing gunshot method blank
11	2% nitric acid / blank, with 5 µg/L Eu internal standard
12	5 µg/L Gd standard (with 5 µg/L Eu internal standard)
13	10 µg/L Gd standard (with 5 µg/L Eu internal standard)
14	20 µg/L Gd standard (with 5 µg/L Eu internal standard)
15	30 µg/L Gd standard (with 5 µg/L Eu internal standard)
16	40 µg/L Gd standard (with 5 µg/L Eu internal standard)
17	Unspiked cells / method blank (with 5 µg/L Eu internal standard)
18	Unspiked cells / method blank (with 5 µg/L Eu internal standard)
19	Unspiked cells / method blank (with 5 µg/L Eu internal standard)
20	Gd DOTA spiked cells (with 5 µg/L Eu internal standard)
21	Gd DOTA spiked cells (with 5 µg/L Eu internal standard)
22	Gd DOTA spiked cells (with 5 µg/L Eu internal standard)
23	Gd DPTA spiked cells (with 5 µg/L Eu internal standard)
24	Gd DPTA spiked cells (with 5 µg/L Eu internal standard)
25	Gd DPTA spiked cells (with 5 µg/L Eu internal standard)
26	1% nitric acid / blank (with 50 µg/L Sc internal standard)
27	Multi-element standard containing 5 µg/L Cr, Mn, Co, Ni, Cu, Zn, As, Cd, Hg, Pb and a 50 µg/L Sc internal standard
28	Multi-element standard containing 10 µg/L Cr, Mn, Co, Ni, Cu, Zn, As, Cd, Hg, Pb and a 50 µg/L Sc internal standard
29	Multi-element standard containing 25 µg/L Cr, Mn, Co, Ni, Cu, Zn, As, Cd, Hg, Pb and a 50 µg/L Sc internal standard
30	Multi-element standard containing 50 µg/L Cr, Mn, Co, Ni, Cu, Zn, As, Cd, Hg, Pb and a 50 µg/L Sc internal standard
31	Multi-element standard containing 100 µg/L Cr, Mn, Co, Ni, Cu, Zn, As, Cd, Hg, Pb and a 50 µg/L Sc internal standard
32	Fabric method blank (with 50 µg/L Sc internal standard)
33	Black fabric sample 1 (with 50 µg/L Sc internal standard)
34	Black fabric sample 2 (with 50 µg/L Sc internal standard)
35	Black fabric sample 3 (with 50 µg/L Sc internal standard)
36	White fabric sample 1 (with 50 µg/L Sc internal standard)
37	White fabric sample 2 (with 50 µg/L Sc internal standard)
38	White fabric sample 3 (with 50 µg/L Sc internal standard)
39	Red fabric sample 1 (with 50 µg/L Sc internal standard)
40	Red fabric sample 2 (with 50 µg/L Sc internal standard)
41	Red fabric sample 3 (with 50 µg/L Sc internal standard)
42	Blue fabric sample 1 (with 50 µg/L Sc internal standard)
43	Blue fabric sample 2 (with 50 µg/L Sc internal standard)
44	Blue fabric sample 3 (with 50 µg/L Sc internal standard)
45	Green fabric sample 1 (with 50 µg/L Sc internal standard)
46	Green fabric sample 2 (with 50 µg/L Sc internal standard)
47	Green fabric sample 3 (with 50 µg/L Sc internal standard)
48	Tuning/ mass calibration solution (Certipur® ICP Multi-element standard solution XXIII)
49	Empty
50	Empty
51	Empty
52	Empty
53	Empty
54	Empty
55	Empty
56	Empty
57	Empty
58	Empty
59	Empty
60	Empty