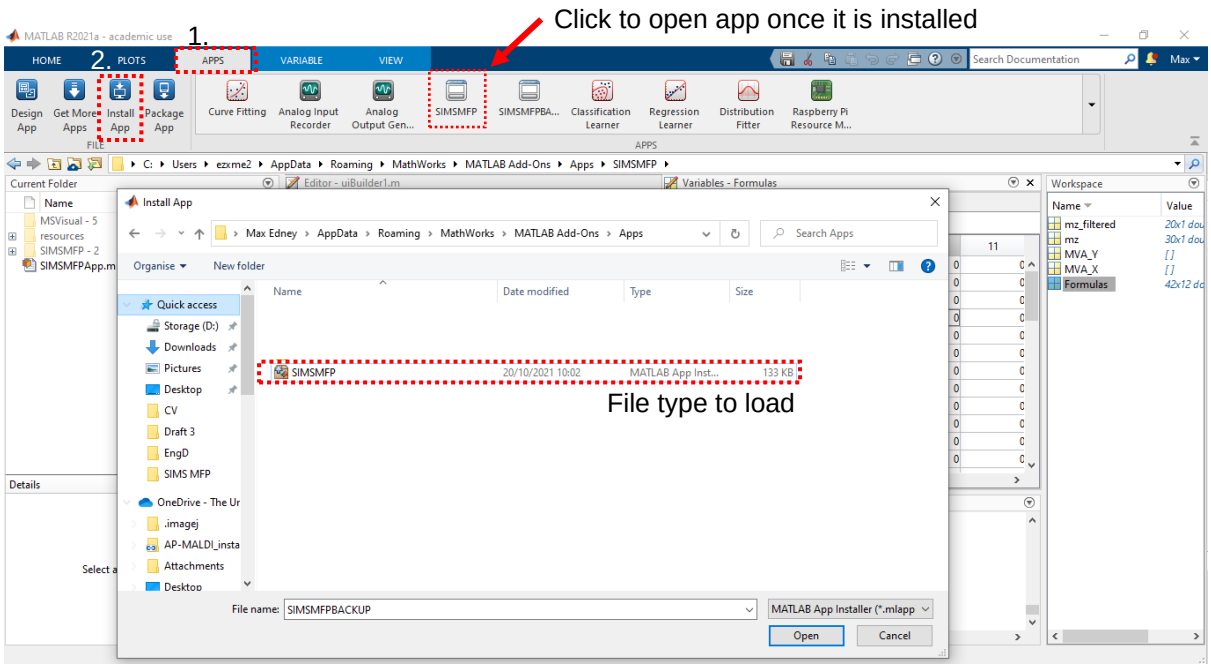
SIMSMFP app instructions

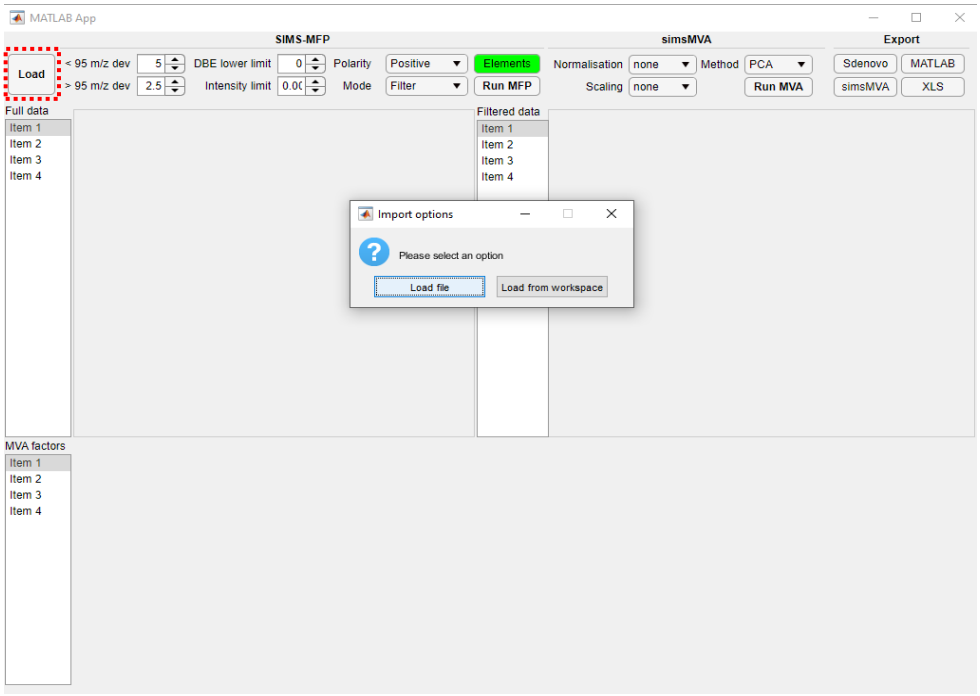
Installation

1. Open MATLAB and find the ‘install app’ button then load the MATLAB installer app file that you received (my version shows it already installed). Next time you open MATLAB you will find it in this tab to open easily.

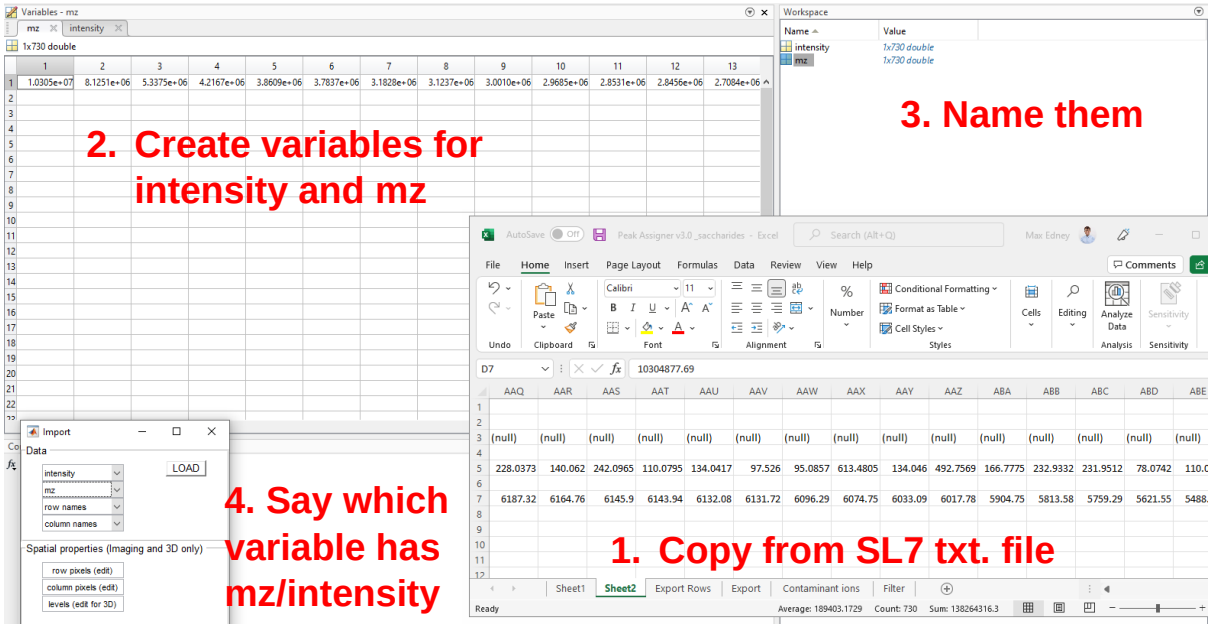


Loading data

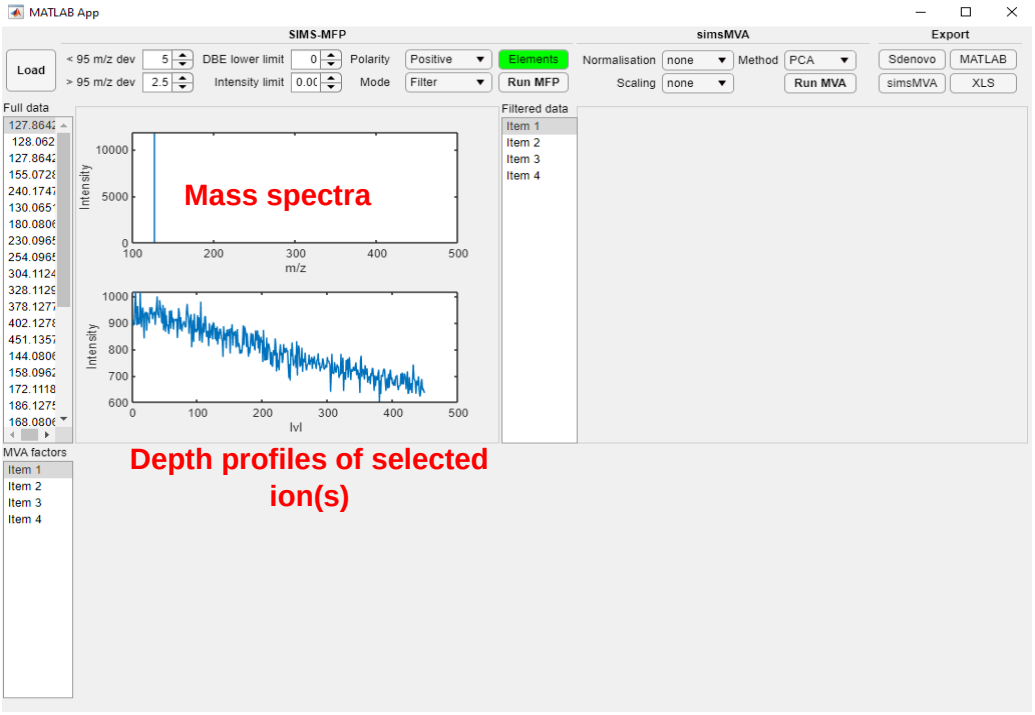
1. When you open the app you have two choices:
   a. To load a file (a **depth profile** export), this can be a txt. file from SurfaceLab or imported from the MATLAB workspace. Note when you export the data from surface lab make sure to **not** include the ‘total’ ion.



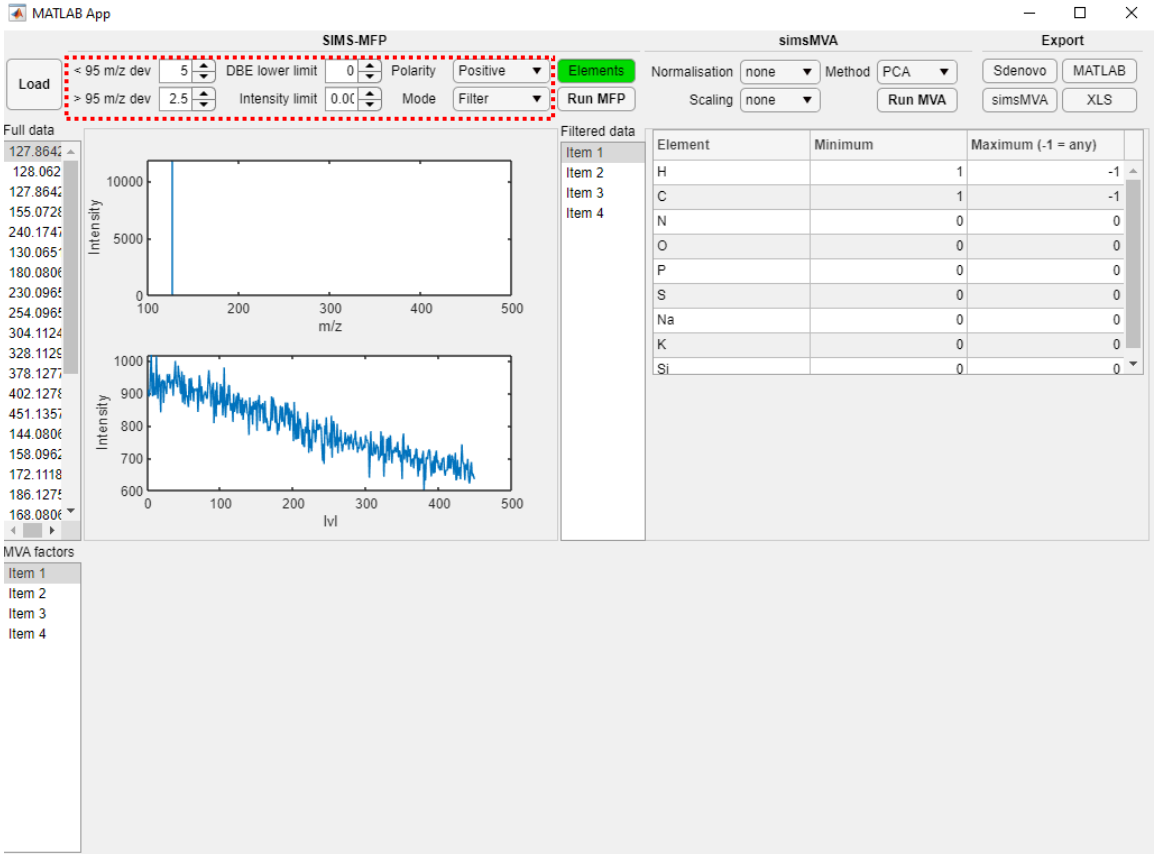
b) To load spectra – export from the peak statistics window in SL7 and copy the values into excel, then copy them into ‘variables’ in matlab put them into two variables in columns, one as mz values and other as intensity. Then click ‘load spectra’ and tell the software which variable has which from the menu.



2. Once loaded it will display the list of ions by mass on the ‘full data’ list – the depth profiles for individual and multiple ions can be also displayed. To run MFP you want it in ‘filter’ mode. Note loadings spectra will give nothing in the ‘depth profile’ window.

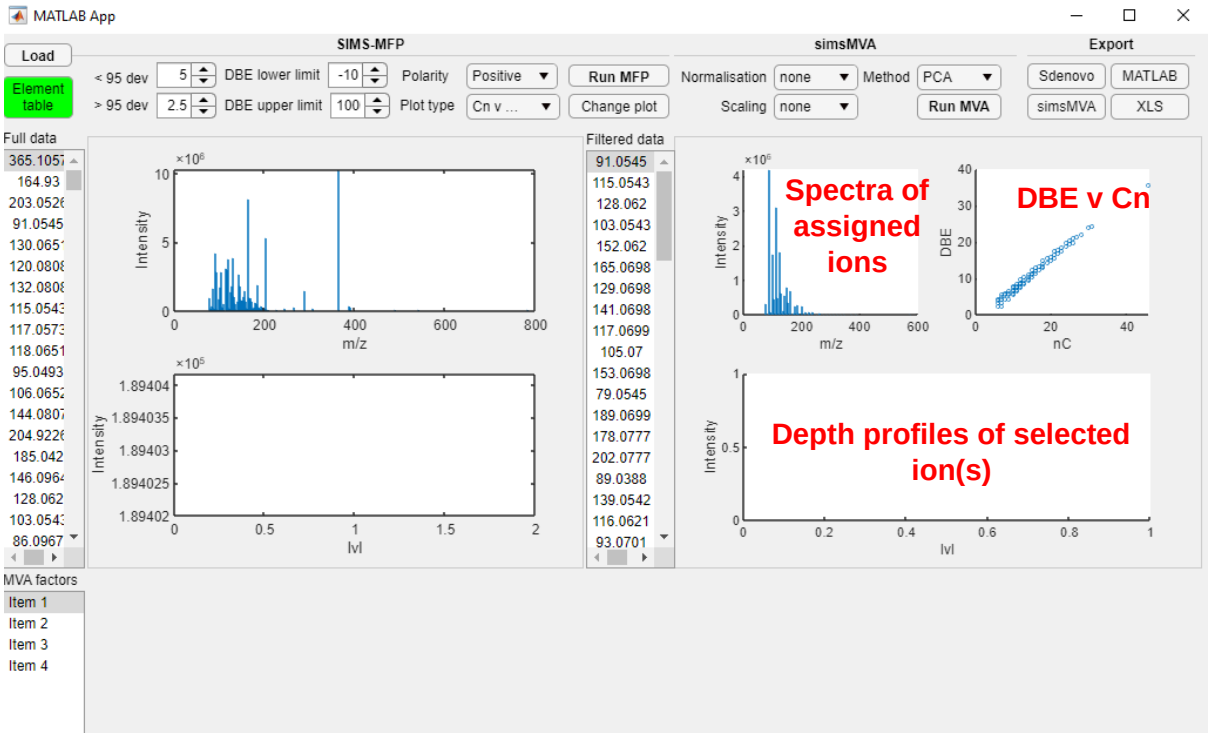


3. Next – choose the parameters including minimum and maximum DBE value, polarity of data and maximum error – we recommend a higher mass deviation for species < 95 mz. You need to click the green elements button to display the table where you can set the number and type of elements in the search. N.B. to have any number of element considered just type -1 in the ‘maximum’ box.



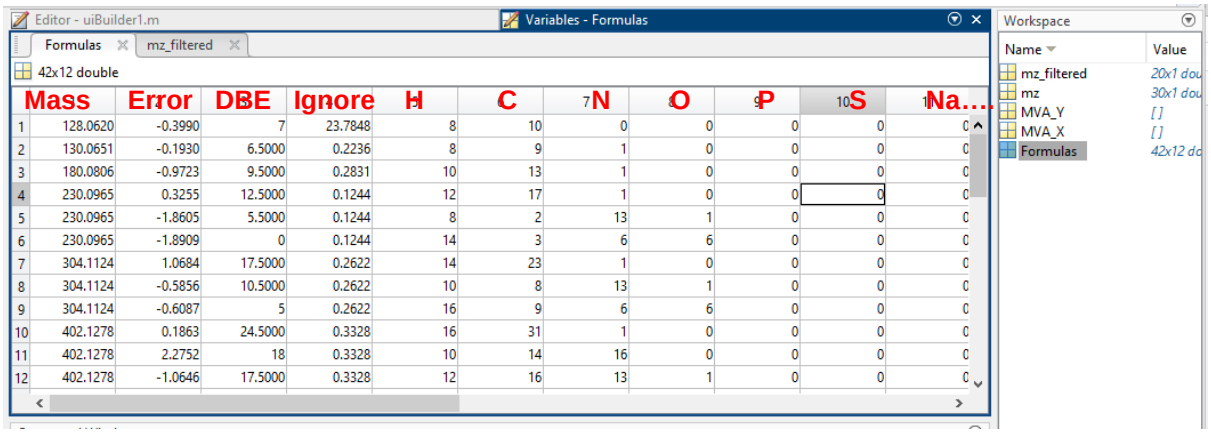
Molecular Formula Prediction (MFP)

4. Once you are all set click ‘Run MFP’. This will give the following display. Note repeated values for ions represent that multiple formula are possible in the elementla constraints. Graphs are fully interactable (e.g you can zoom and pan them by hovering over the top of the graph and selecting the options:



Initially it will plot the double bond equivalence (DBE) value v the Cn of each assignment to help visualize the data. The ‘plot type’ button can plot other elemental ratios of your data and will change this plot.

5. To export the predicted formula please select ‘MATLAB’ button in the export tab. This will create an array in the MATALB workspace called ‘formulas’ displaying the mass, error, DBE, and a column representing the number of each element in the formula. The order of elements corresponds to that in the elements table i.e. H, C, N, O, P etc.



	Mass	Error	DBE	Ignore	H	C	N	O	P	S	Na…
1	128.0620	-0.3990	7	23.7848	8	10	0	0	0	0	0
2	130.0651	-0.1930	6.5000	0.2236	8	9	1	0	0	0	0
3	180.0806	-0.9723	9.5000	0.2831	10	13	1	0	0	0	0
4	230.0965	0.3255	12.5000	0.1244	12	17	1	0	0	0	0
5	230.0965	-1.8605	5.5000	0.1244	8	2	13	1	0	0	0
6	230.0965	-1.8909	0	0.1244	14	3	6	6	0	0	0
7	304.1124	1.0684	17.5000	0.2622	14	23	1	0	0	0	0
8	304.1124	-0.5856	10.5000	0.2622	10	8	13	1	0	0	0
9	304.1124	-0.6087	5	0.2622	16	9	6	6	0	0	0
10	402.1278	0.1863	24.5000	0.3328	16	31	1	0	0	0	0
11	402.1278	2.2752	18	0.3328	10	14	16	0	0	0	0
12	402.1278	-1.0646	17.5000	0.3328	12	16	13	1	0	0	0

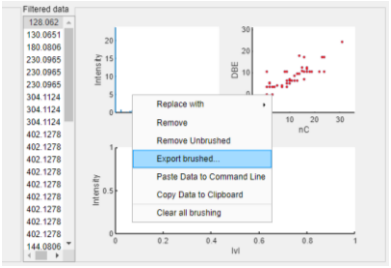
We recommend copying this table to excel to filter the data further for yourself!

It will also produce a variable (called ‘leftover variables’) which shows ions which were not assigned to species in your search. You can put these pack into the initial search using other elements if you wish.

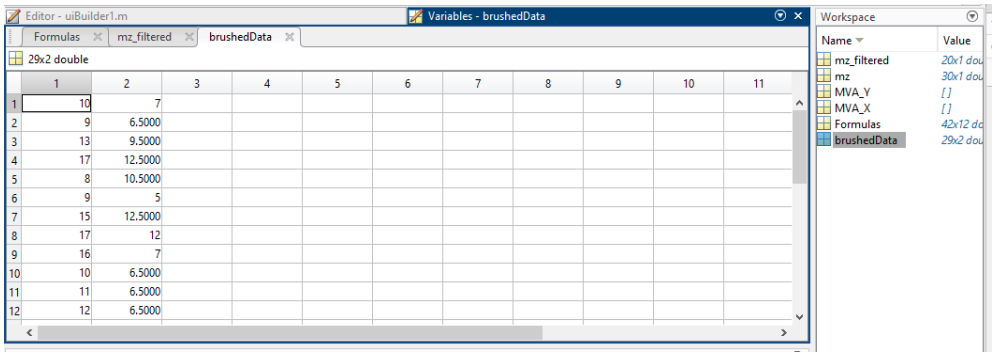
6. You can export the data from the graphs for plotting in another program in another way – by hovering over the top of a plot and clicking ‘brush/select’ data. Then right click and select ‘export brushed data’ to make an array in the workspace which you can take for further plotting. Here I brushed all the data in the DBE v Cn plot and exported this to another array.

a.

b.



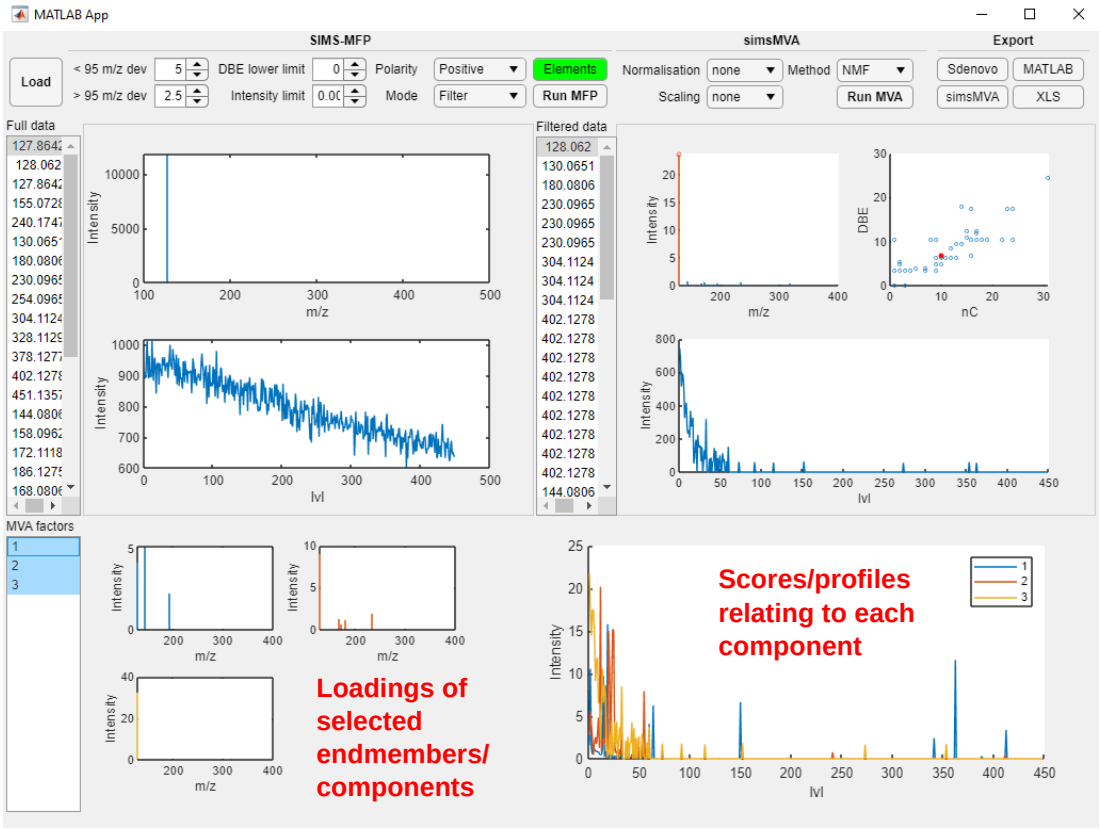
c.



	1	2
1	10	7
2	9	6.5000
3	13	9.5000
4	17	12.5000
5	8	10.5000
6	9	5
7	15	12.5000
8	17	12
9	16	7
10	10	6.5000
11	11	6.5000
12	12	6.5000

Performing MVA on your filtered data

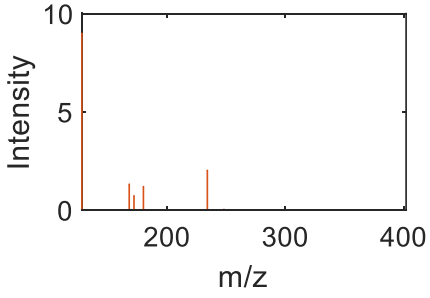
1. To perform MVA on your list of filtered data use the tab on the right. Currently we support PCA and NMF only but more will be added. As an example we show the output from NMF with no normalization with 100 iterations over 3 endmembers.



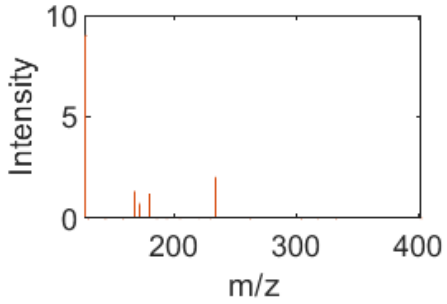
For more information on MVA please look at the SIMSMVA tutorials from Gustavo Trindade in the SIMS user group teams chat. Please contact either Gus or myself if you do not understand some of the MVA functions.

Notes

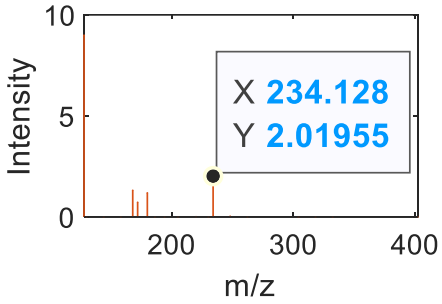
1. All plots on the matlab app can be exported to different formats e.g the endmember loadings as an svg.



Or a png.



2. All peaks on graphs are interactable – so their mass values can be displayed by clicking on them, which can also be exported.



3. A note on isotopes – particularly for Cl and Sn - you should consider other isotopes in your search, we have included the major isotopes in the software but if you need more adding then please just ask. This link takes you to a useful page showing the abundance of each isotope (https://physics.nist.gov/cgi-bin/Compositions/stand_alone.pl).

4. Please do not send the software onto anyone else – if you know someone who wants a copy please send an email to the address above.

5. If you use this app in your publications please do cite it, we have a manuscript under review so we will send an update with its citation when it comes out.

We hope you enjoy using this software! If you have any questions do send an email to Max.Edney@nottingham.ac.uk. Please also use this to report bugs and to suggest any improvements or add-ons to the app that would help in your analysis.