

Editing the compound template

If the target compounds are known

What is a compound template?

- In IMAGEREVEAL MS “data matrix” are computed.
- If the target compounds are known, the m/z, compound names etc. are listed in the “compound template”, and it is used in the settings for computation of the “data matrix”.
- The compound template is in csv format (text divided up with commas “,”).

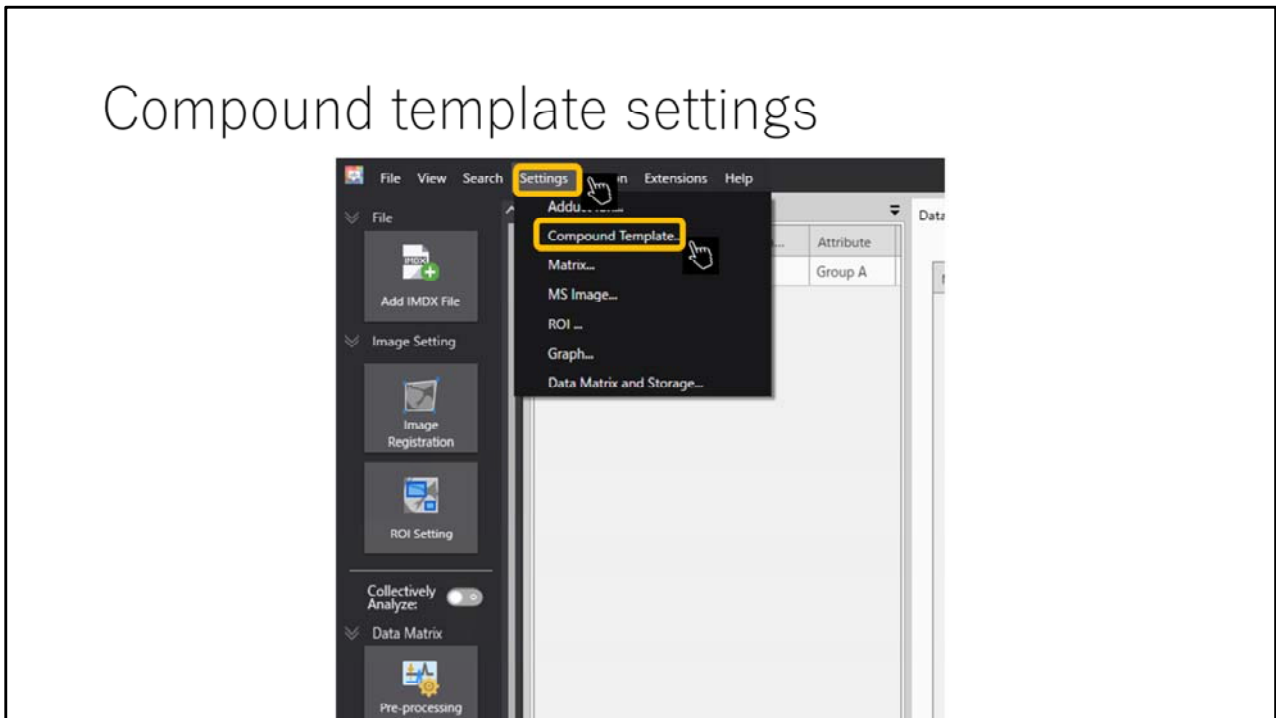
Before processing data with IMAGEREVEAL MS, the necessary information must first be isolated from the data file.

The reason for this is that MS imaging files are large and directly processing the original file would take a long time.

The data is isolated according to the “data matrix settings”.

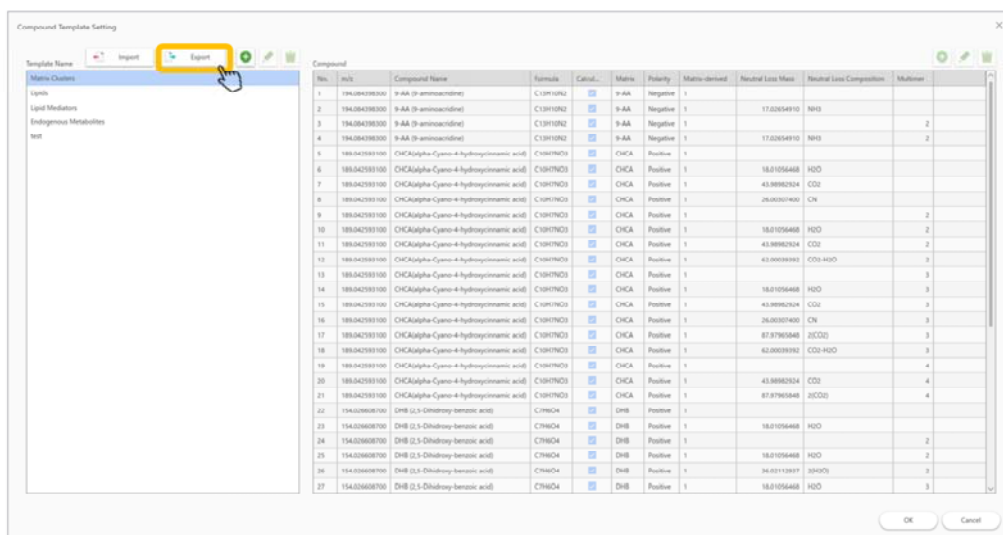
We recommend saving the data matrices to an SSD, because it much faster than saving them to an HDD.

Compound template settings



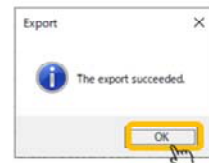
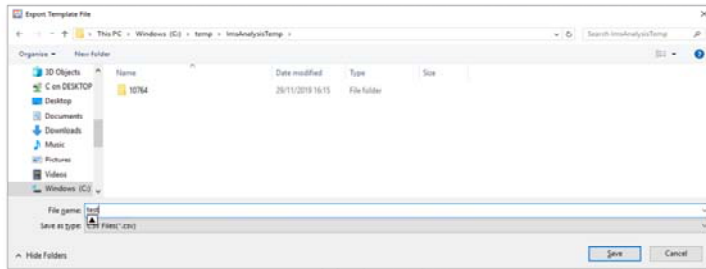
Go to Menu bar -> Settings -> Compound template

Exporting compound templates

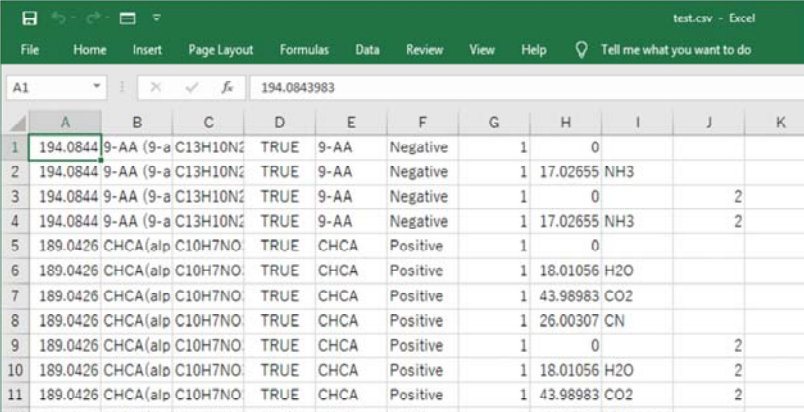


Previously-existing templates are displayed.
We will export these templates.

Save with an appropriate name



Open in Excel



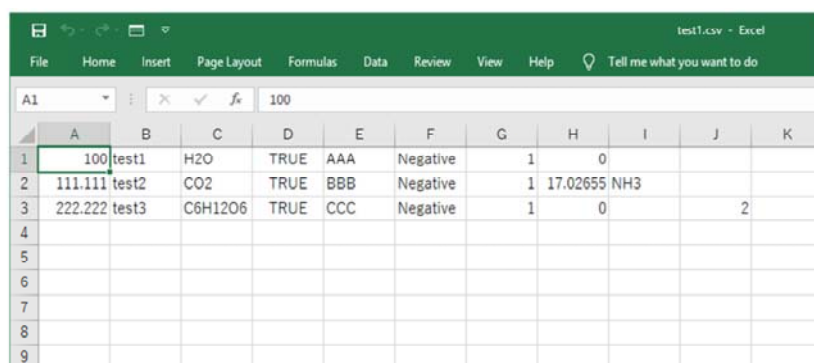
	A	B	C	D	E	F	G	H	I	J	K
1	194.0844	9-AA (9-a C13H10N2	TRUE	9-AA	Negative	1	0				
2	194.0844	9-AA (9-a C13H10N2	TRUE	9-AA	Negative	1	17.02655	NH3			
3	194.0844	9-AA (9-a C13H10N2	TRUE	9-AA	Negative	1	0			2	
4	194.0844	9-AA (9-a C13H10N2	TRUE	9-AA	Negative	1	17.02655	NH3		2	
5	189.0426	CHCA(alp C10H7NO	TRUE	CHCA	Positive	1	0				
6	189.0426	CHCA(alp C10H7NO	TRUE	CHCA	Positive	1	18.01056	H2O			
7	189.0426	CHCA(alp C10H7NO	TRUE	CHCA	Positive	1	43.98983	CO2			
8	189.0426	CHCA(alp C10H7NO	TRUE	CHCA	Positive	1	26.00307	CN			
9	189.0426	CHCA(alp C10H7NO	TRUE	CHCA	Positive	1	0			2	
10	189.0426	CHCA(alp C10H7NO	TRUE	CHCA	Positive	1	18.01056	H2O		2	
11	189.0426	CHCA(alp C10H7NO	TRUE	CHCA	Positive	1	43.98983	CO2		2	

m/z; compound name; chemical formula; whether adduct ions are computed; matrix; polarity; matrix derived; neutral loss mass; multimers.

Open up the saved template (csv template), one compound is displayed per row.

From left: m/z ; compound name; chemical formula; whether adduct ions are computed; matrix; polarity; matrix derived; neutral loss mass; multimers. For details, please refer to the manual or the help function. The user can describe their own compounds in this format.

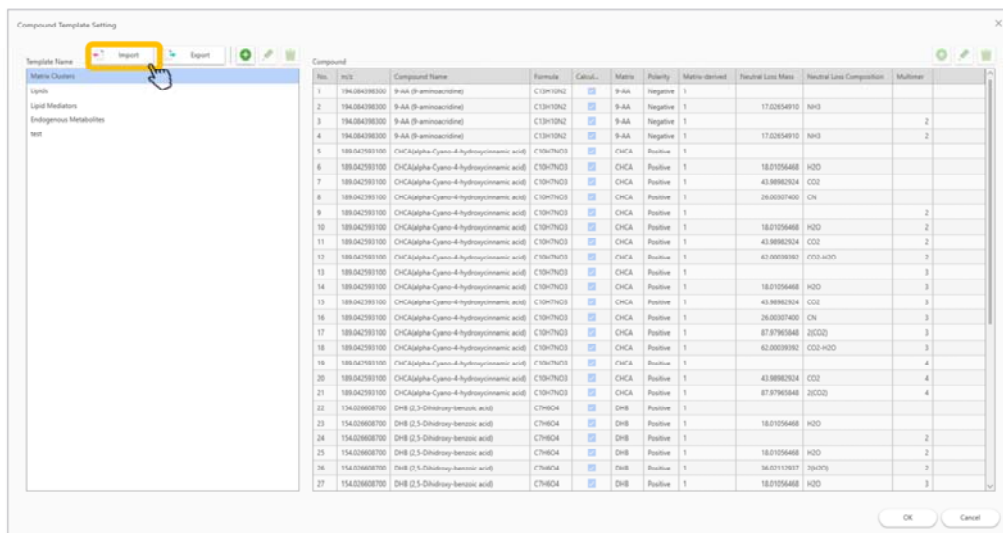
Enter information for new compounds and save



	A	B	C	D	E	F	G	H	I	J	K
1	100	test1	H2O	TRUE	AAA	Negative	1	0			
2	111.111	test2	CO2	TRUE	BBB	Negative	1	17.02655	NH3		
3	222.222	test3	C6H12O6	TRUE	CCC	Negative	1	0		2	
4											
5											
6											
7											
8											
9											

Enter information for new compounds and save the file in csv format.

Import a compound template



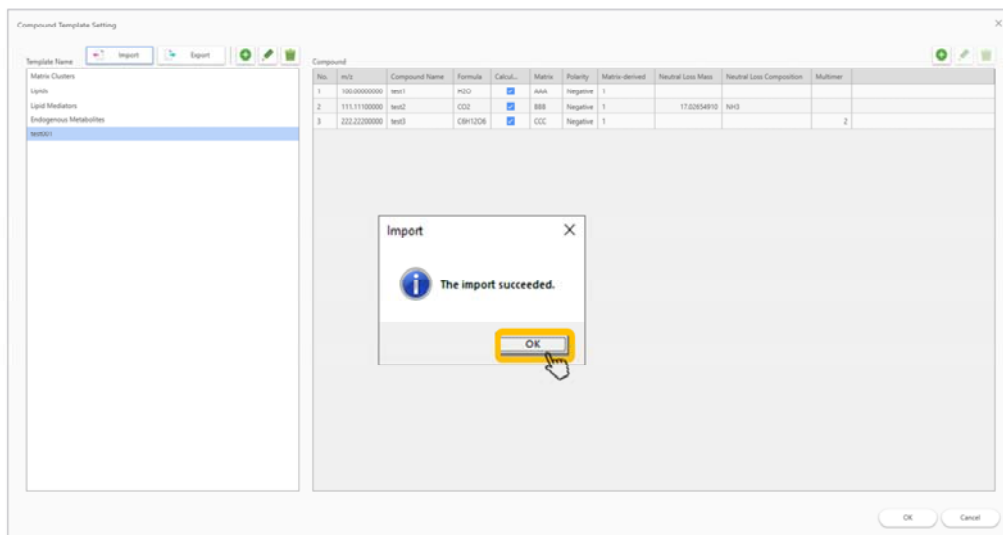
Select "Import" from the compound template settings screen, then select the edited csv file.

Name the compound template



Any name is okay.

After importing:



If the import is successful, a message window and the imported template are displayed.

If the import process fails:

- Usually the reason is that the number of commas (“,”) is incorrect.
- In Excel commas are not displayed, so it is recommended to open the file in a text viewer e.g. Notepad