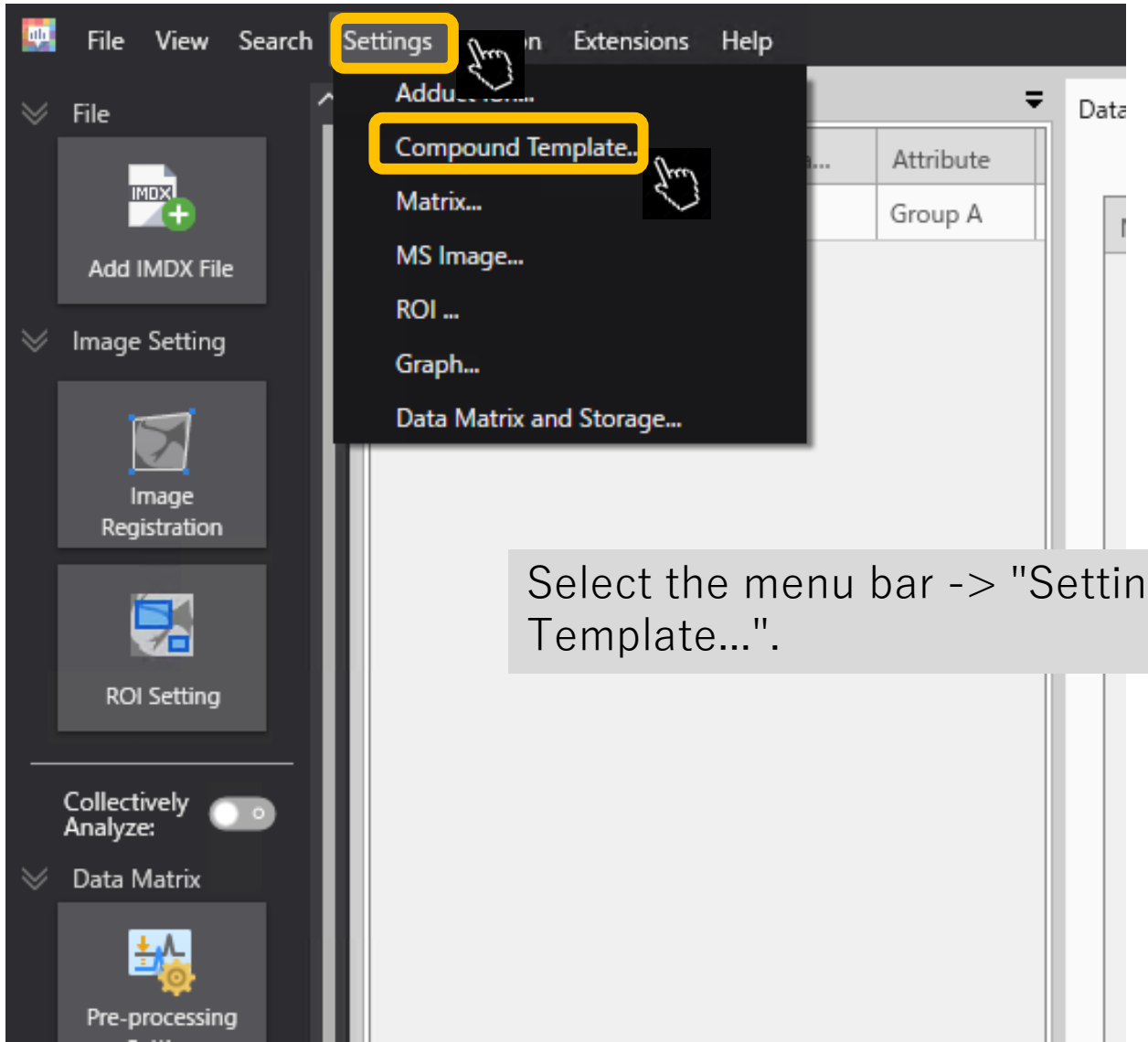
Editing the compound template

If the target compounds are known

What is a compound template?

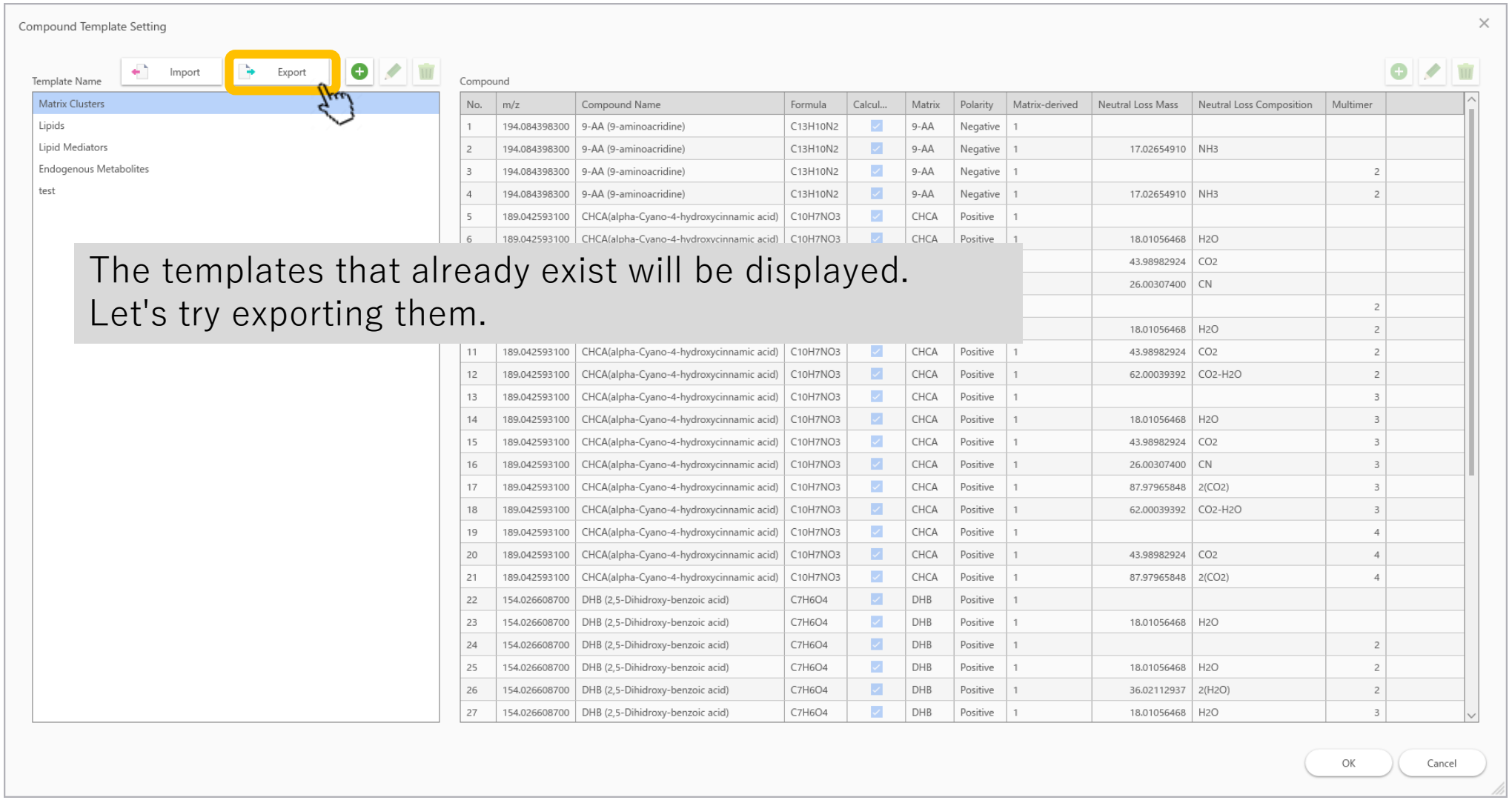
- In IMAGEREVEAL MS “data matrix” are computed.
- If the target compounds are known, the m/z, compound names etc. are listed in the “compound template”, and it is used in the settings for computation of the “data matrix”.
- The compound template is in csv format (text divided up with commas “,”).

Compound template settings



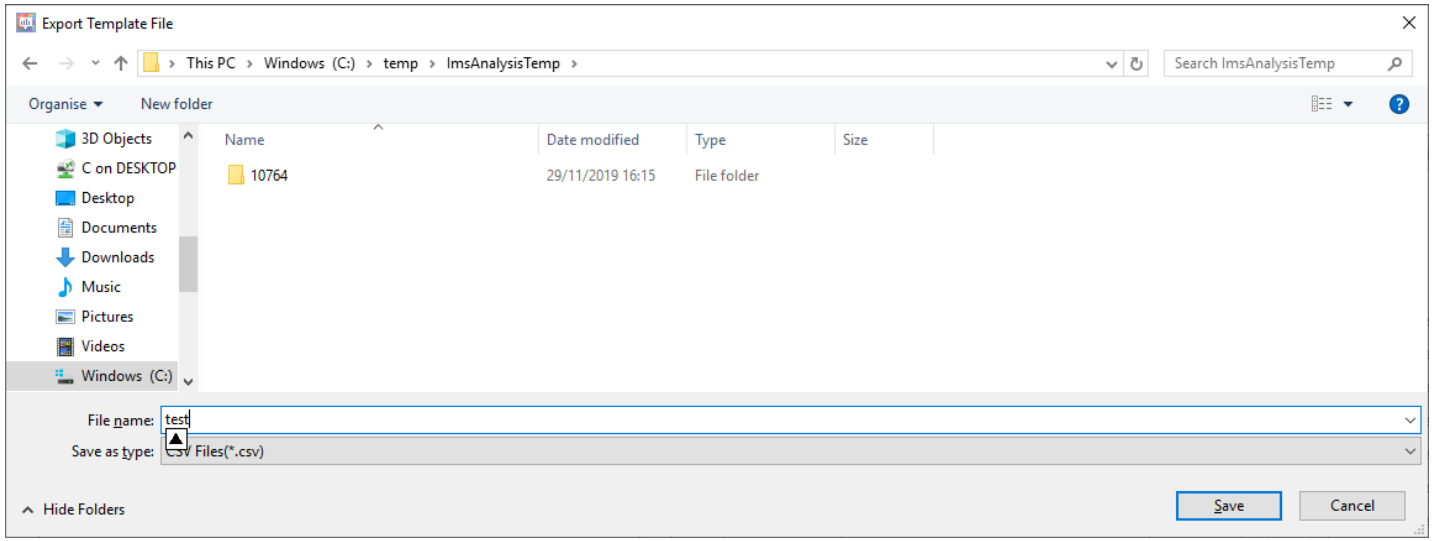
Select the menu bar -> "Settings" -> "Compound Template...".

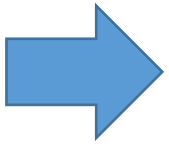
Exporting compound templates

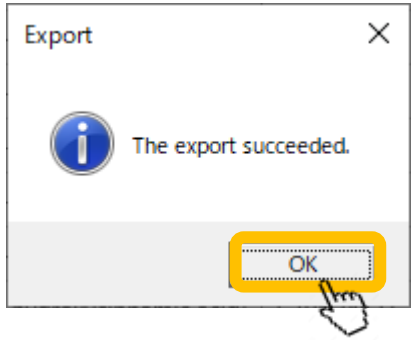


The templates that already exist will be displayed.
Let's try exporting them.

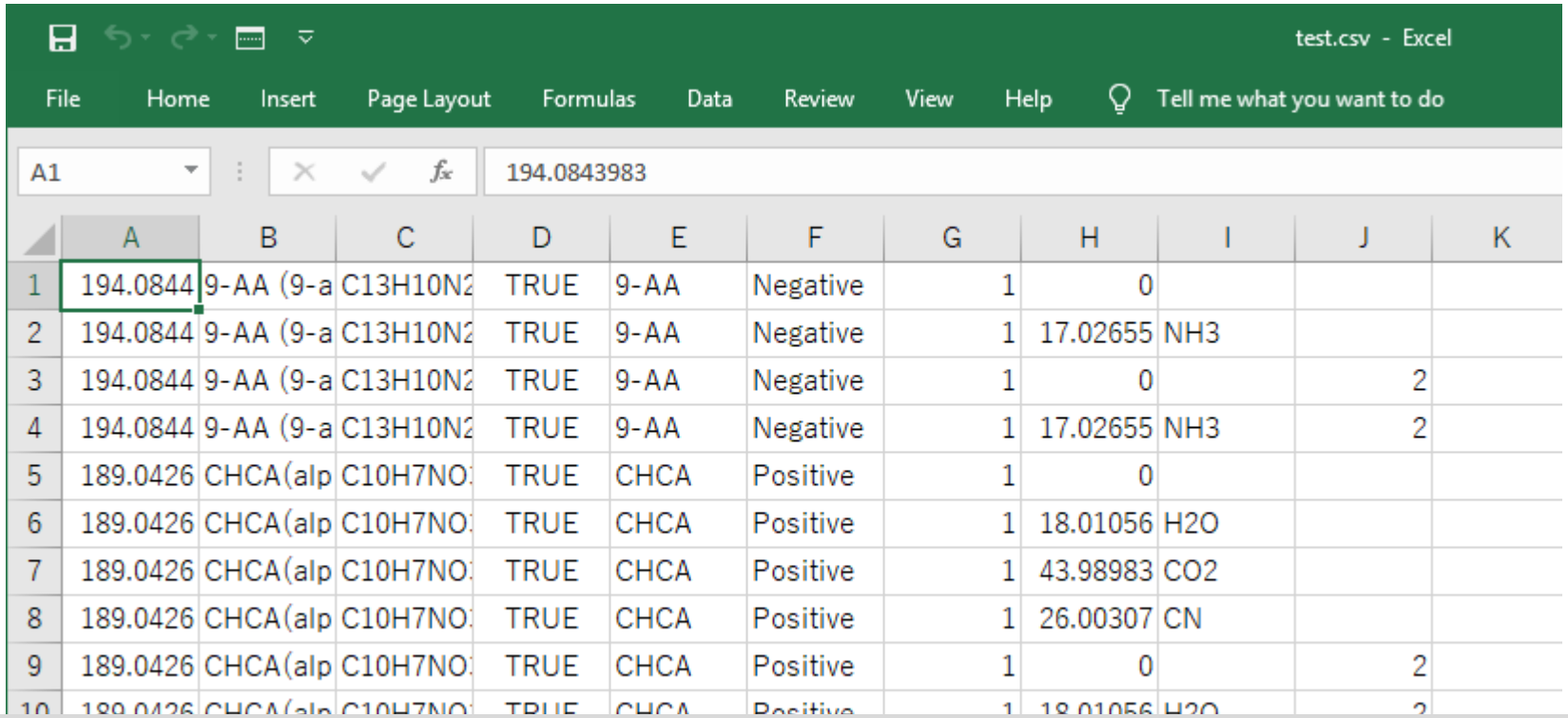
Save with an appropriate name







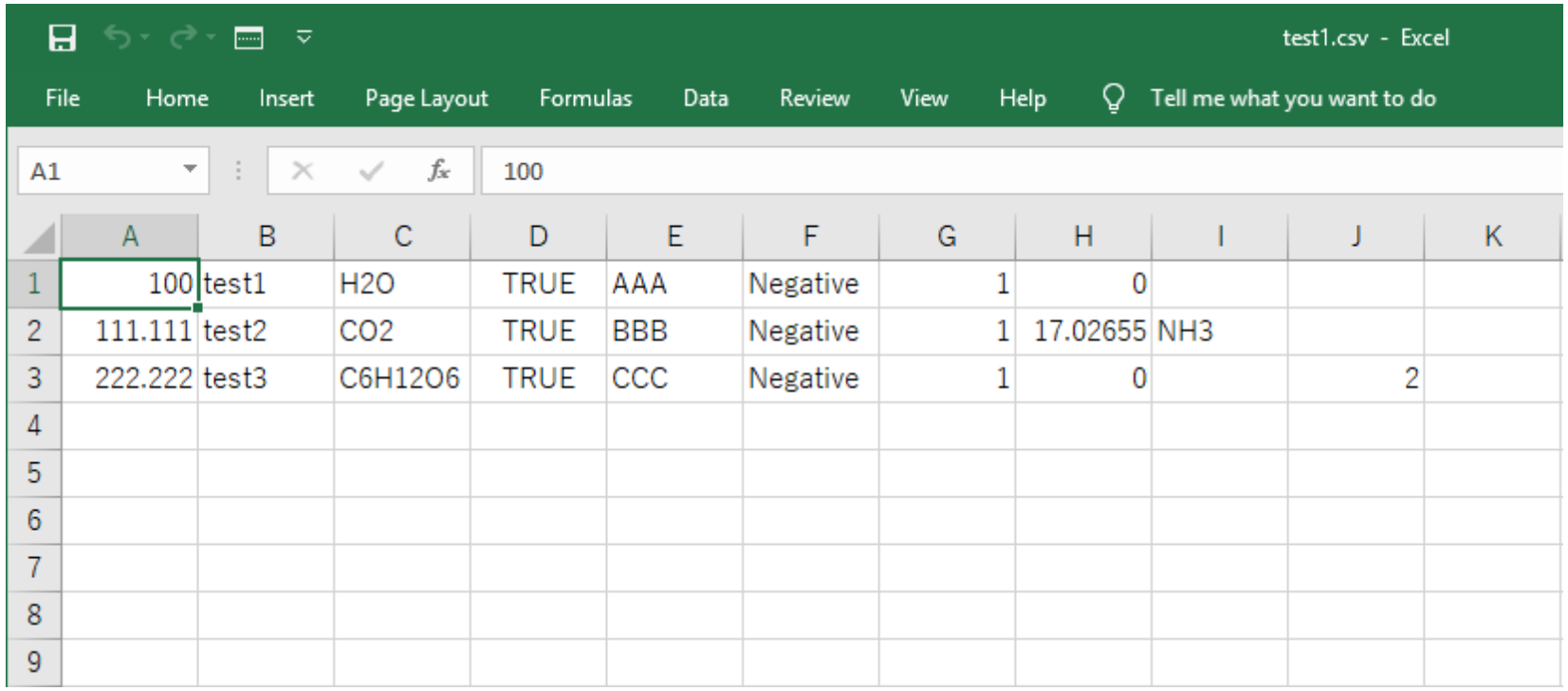
Open in Excel



	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	C10H7NO3	TRUE	CHCA	Positive	1	0			
6	189.0426	CHCA(alp	C10H7NO3	TRUE	CHCA	Positive	1	18.01056	H2O		
7	189.0426	CHCA(alp	C10H7NO3	TRUE	CHCA	Positive	1	43.98983	CO2		
8	189.0426	CHCA(alp	C10H7NO3	TRUE	CHCA	Positive	1	26.00307	CN		
9	189.0426	CHCA(alp	C10H7NO3	TRUE	CHCA	Positive	1	0		2	
10	189.0426	CHCA(alp	C10H7NO3	TRUE	CHCA	Positive	1	18.01056	H2O	2	

From left column,
m/z, compound name, formula, whether adduct ions are computed, matrix, polarity, matrix derived, neutral loss mass, neutral loss compositional formula, multimer
For more information, see the manual or help.

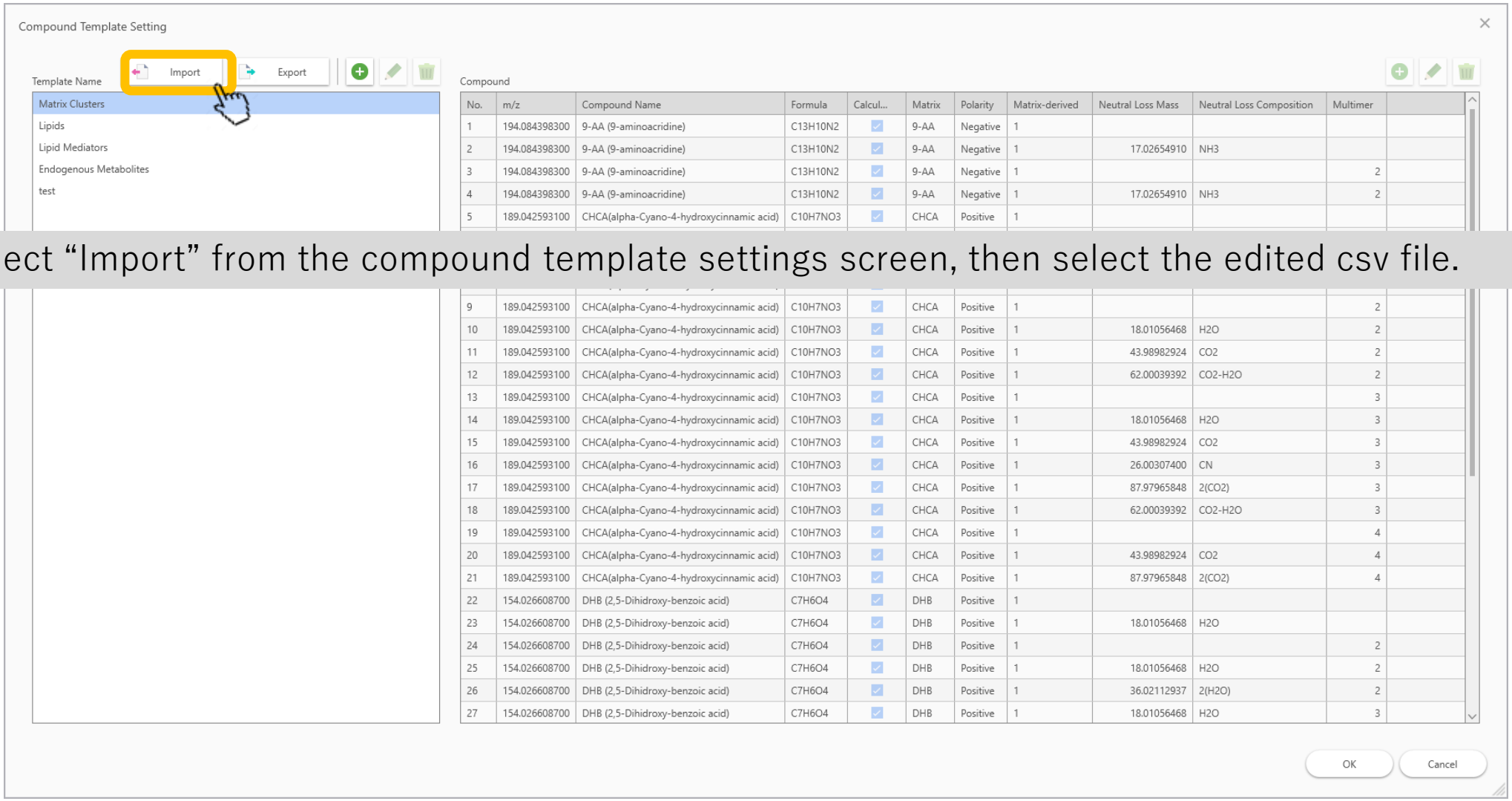
Enter information for new compounds and save as “.csv”



	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.

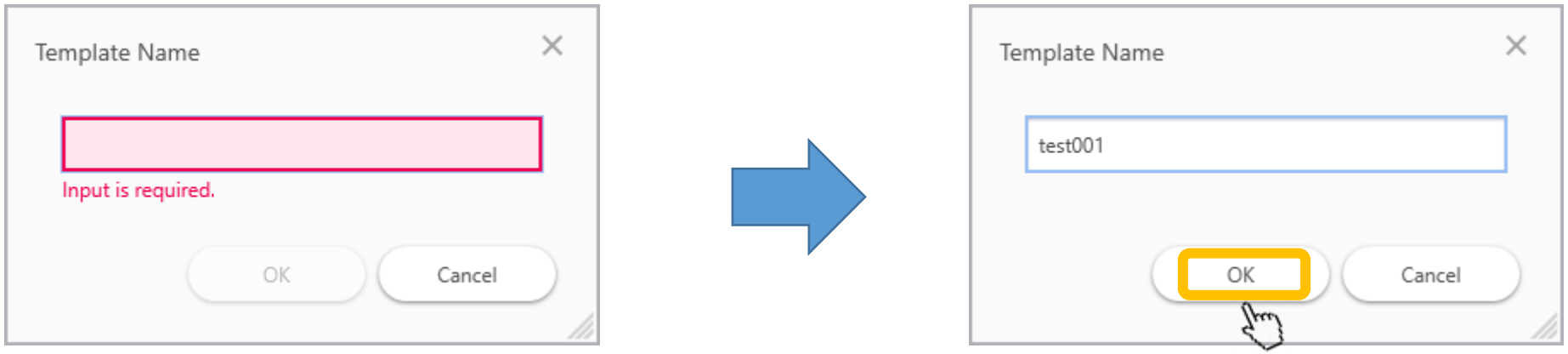
Import a compound template



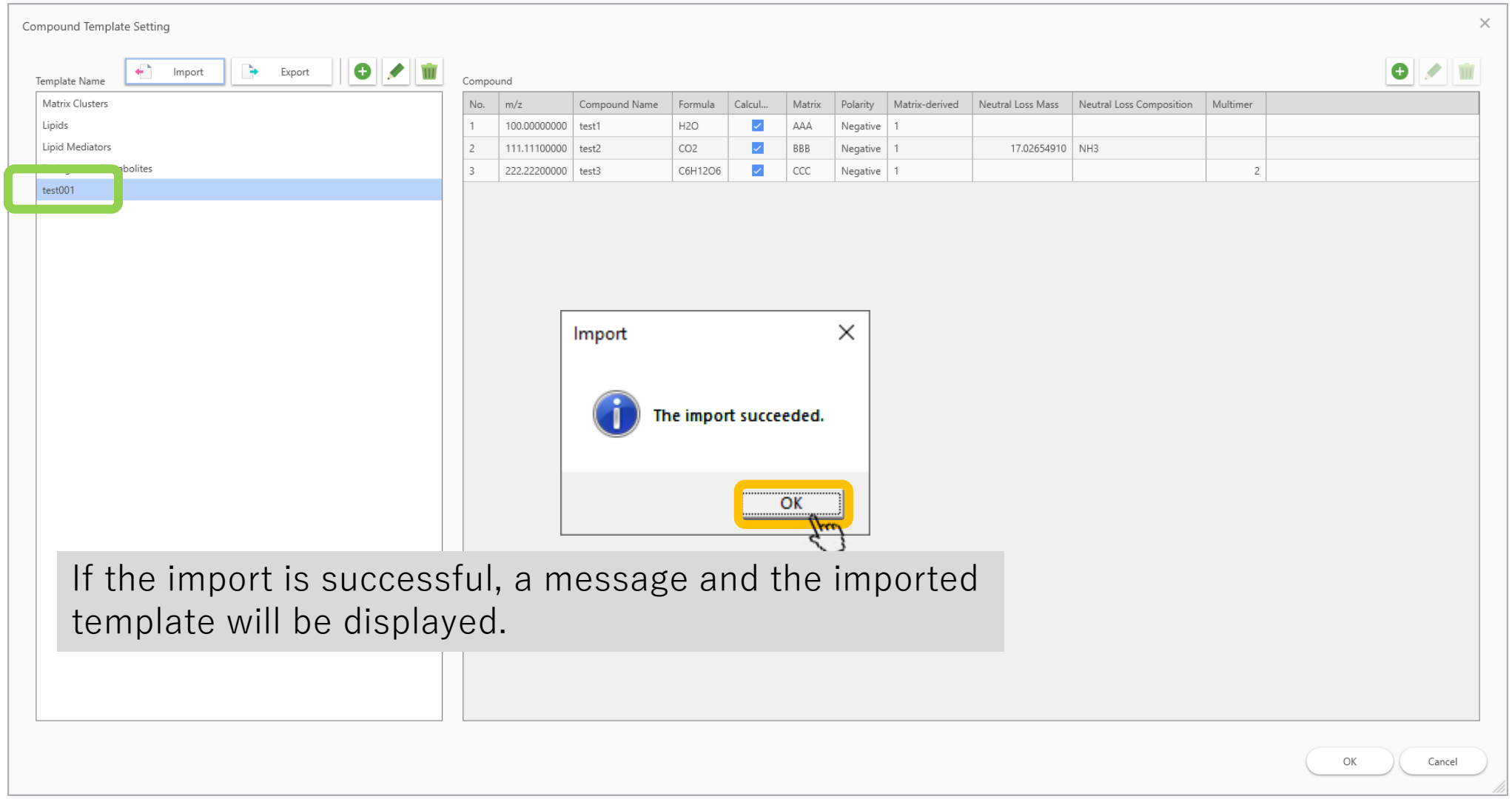
No.	m/z	Compound Name	Formula	Calcul...	Matrix	Polarity	Matrix-derived	Neutral Loss Mass	Neutral Loss Composition	Multimer
1	194.084398300	9-AA (9-aminoacridine)	C13H10N2	☑	9-AA	Negative	1			
2	194.084398300	9-AA (9-aminoacridine)	C13H10N2	☑	9-AA	Negative	1	17.02654910	NH3	
3	194.084398300	9-AA (9-aminoacridine)	C13H10N2	☑	9-AA	Negative	1			2
4	194.084398300	9-AA (9-aminoacridine)	C13H10N2	☑	9-AA	Negative	1	17.02654910	NH3	2
5	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	☑	CHCA	Positive	1			
9	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	☑	CHCA	Positive	1			2
10	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	☑	CHCA	Positive	1	18.01056468	H2O	2
11	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	☑	CHCA	Positive	1	43.98982924	CO2	2
12	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	☑	CHCA	Positive	1	62.00039392	CO2-H2O	2
13	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	☑	CHCA	Positive	1			3
14	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	☑	CHCA	Positive	1	18.01056468	H2O	3
15	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	☑	CHCA	Positive	1	43.98982924	CO2	3
16	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	☑	CHCA	Positive	1	26.00307400	CN	3
17	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	☑	CHCA	Positive	1	87.97965848	2(CO2)	3
18	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	☑	CHCA	Positive	1	62.00039392	CO2-H2O	3
19	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	☑	CHCA	Positive	1			4
20	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	☑	CHCA	Positive	1	43.98982924	CO2	4
21	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	☑	CHCA	Positive	1	87.97965848	2(CO2)	4
22	154.026608700	DHB (2,5-Dihidroxy-benzoic acid)	C7H6O4	☑	DHB	Positive	1			
23	154.026608700	DHB (2,5-Dihidroxy-benzoic acid)	C7H6O4	☑	DHB	Positive	1	18.01056468	H2O	
24	154.026608700	DHB (2,5-Dihidroxy-benzoic acid)	C7H6O4	☑	DHB	Positive	1			2
25	154.026608700	DHB (2,5-Dihidroxy-benzoic acid)	C7H6O4	☑	DHB	Positive	1	18.01056468	H2O	2
26	154.026608700	DHB (2,5-Dihidroxy-benzoic acid)	C7H6O4	☑	DHB	Positive	1	36.02112937	2(H2O)	2
27	154.026608700	DHB (2,5-Dihidroxy-benzoic acid)	C7H6O4	☑	DHB	Positive	1	18.01056468	H2O	3

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

Name the compound template



After importing:



If the import is successful, a message and the imported template will be 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