

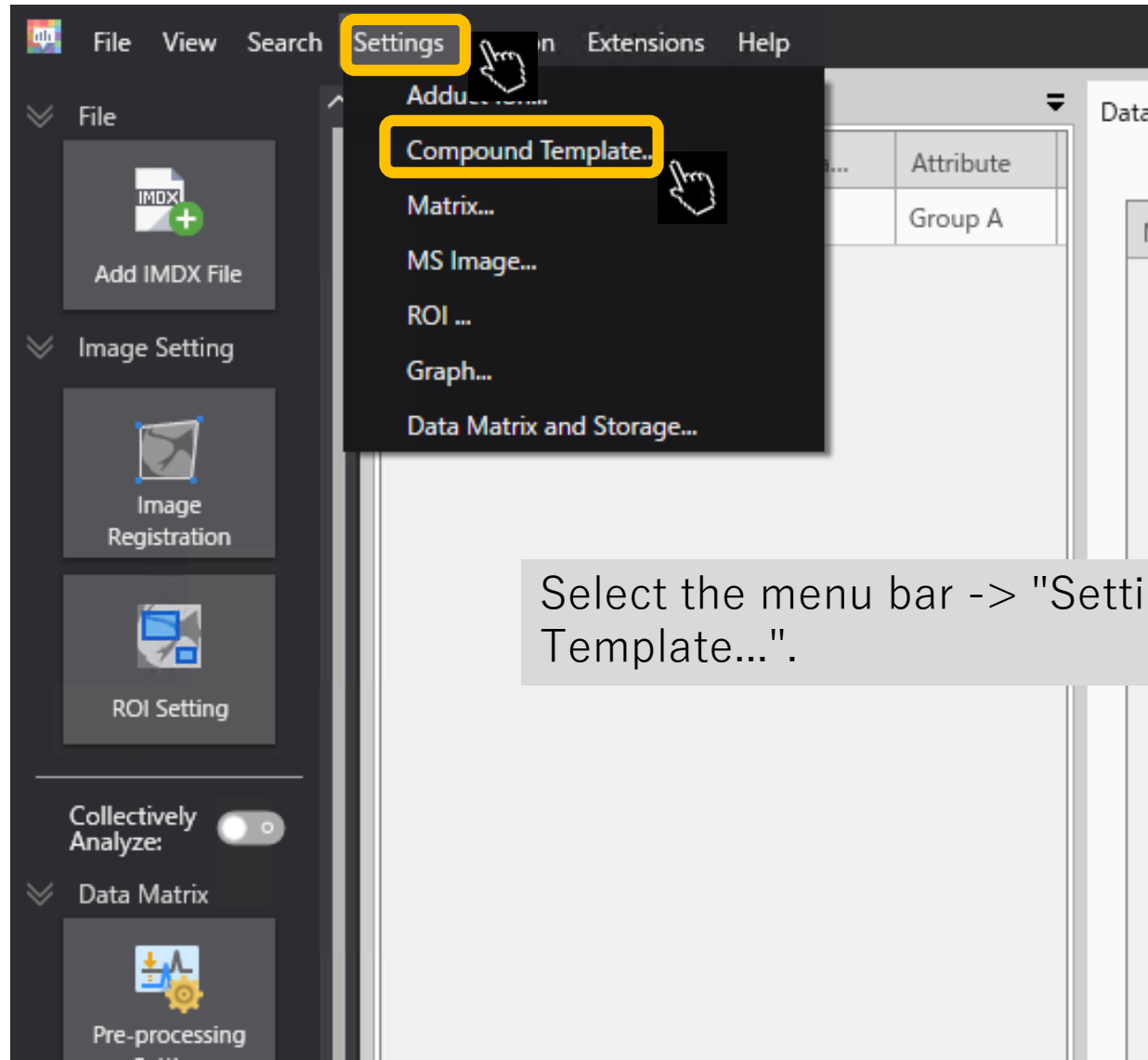
Editing the compound template

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

Compound Template Setting

Template Name

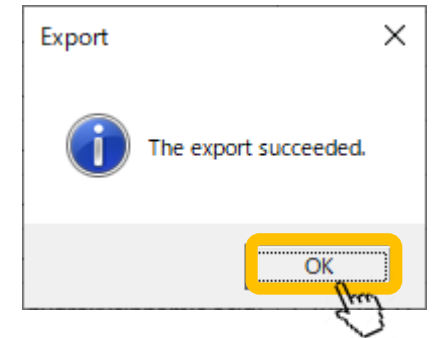
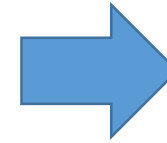
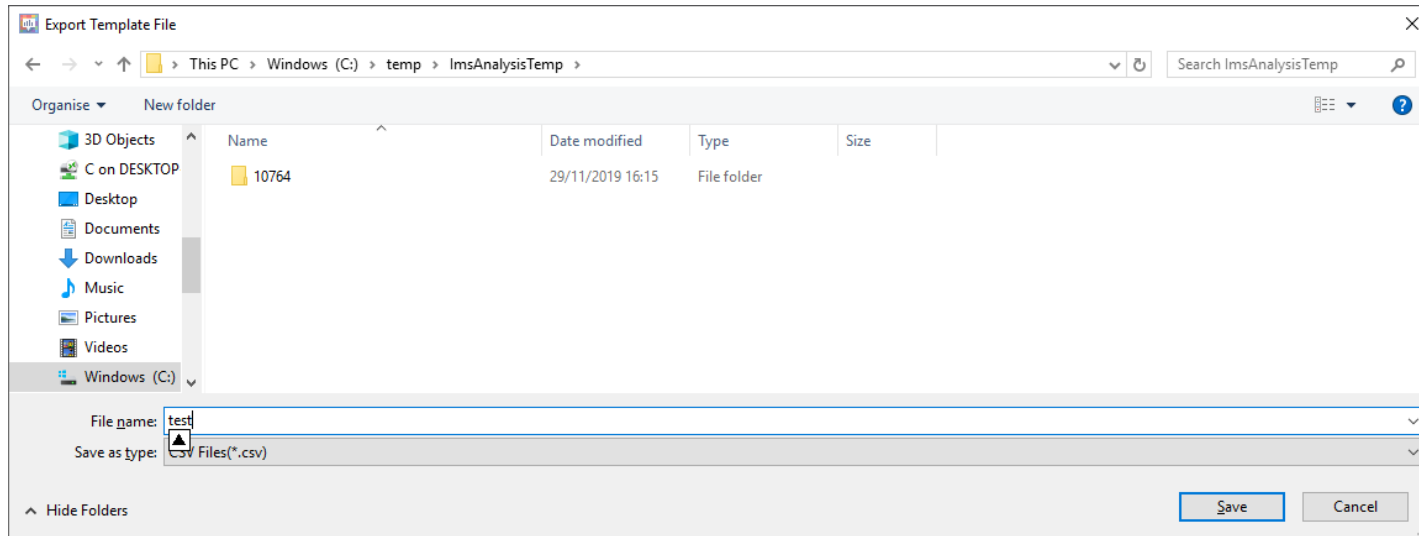
Compound

No.	m/z	Compound Name	Formula	Calcu...	Matrix	Polarity	Matrix-derived	Neutral Loss Mass	Neutral Loss Composition	Multimer	
1	194.084398300	9-AA (9-aminoacridine)	C13H10N2	<input checked="" type="checkbox"/>	9-AA	Negative	1				
2	194.084398300	9-AA (9-aminoacridine)	C13H10N2	<input checked="" type="checkbox"/>	9-AA	Negative	1	17.02654910	NH3		
3	194.084398300	9-AA (9-aminoacridine)	C13H10N2	<input checked="" type="checkbox"/>	9-AA	Negative	1			2	
4	194.084398300	9-AA (9-aminoacridine)	C13H10N2	<input checked="" type="checkbox"/>	9-AA	Negative	1	17.02654910	NH3	2	
5	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1				
6	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	18.01056468	H2O		
								43.98982924	CO2		
								26.00307400	CN		
										2	
								18.01056468	H2O	2	
11	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	43.98982924	CO2	2	
12	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	62.00039392	CO2-H2O	2	
13	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1			3	
14	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	18.01056468	H2O	3	
15	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	43.98982924	CO2	3	
16	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	26.00307400	CN	3	
17	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	87.97965848	2(CO2)	3	
18	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	62.00039392	CO2-H2O	3	
19	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1			4	
20	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	43.98982924	CO2	4	
21	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	87.97965848	2(CO2)	4	
22	154.026608700	DHB (2,5-Dihydroxy-benzoic acid)	C7H6O4	<input checked="" type="checkbox"/>	DHB	Positive	1				
23	154.026608700	DHB (2,5-Dihydroxy-benzoic acid)	C7H6O4	<input checked="" type="checkbox"/>	DHB	Positive	1	18.01056468	H2O		
24	154.026608700	DHB (2,5-Dihydroxy-benzoic acid)	C7H6O4	<input checked="" type="checkbox"/>	DHB	Positive	1			2	
25	154.026608700	DHB (2,5-Dihydroxy-benzoic acid)	C7H6O4	<input checked="" type="checkbox"/>	DHB	Positive	1	18.01056468	H2O	2	
26	154.026608700	DHB (2,5-Dihydroxy-benzoic acid)	C7H6O4	<input checked="" type="checkbox"/>	DHB	Positive	1	36.02112937	2(H2O)	2	
27	154.026608700	DHB (2,5-Dihydroxy-benzoic acid)	C7H6O4	<input checked="" type="checkbox"/>	DHB	Positive	1	18.01056468	H2O	3	

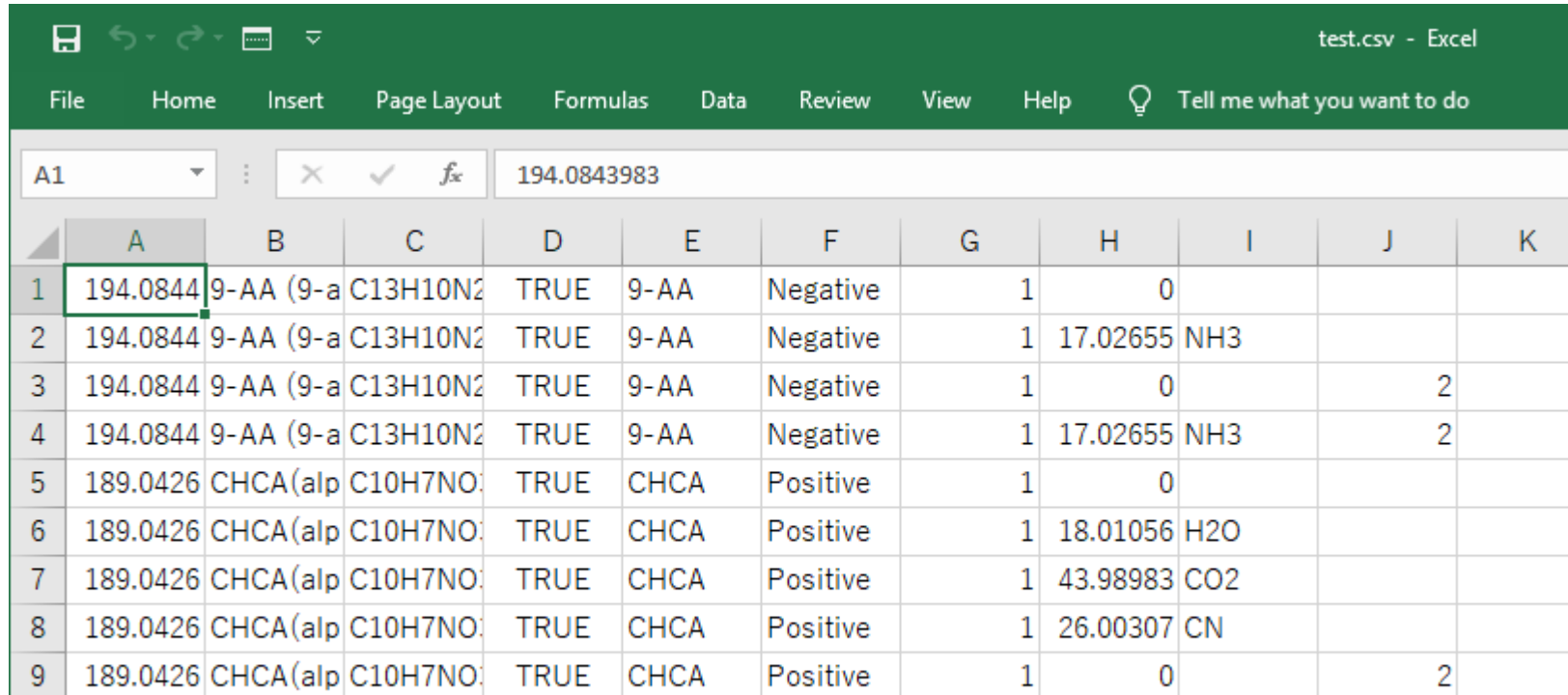
The templates that already exist will be displayed.
Let's try exporting them.

OK Cancel

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


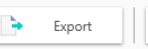



From left.

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.

Import a compound template

Compound Template Setting

Template Name  Import  Export   

Matrix Clusters

- Lipids
- Lipid Mediators
- Endogenous Metabolites
- test

Compound

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	<input checked="" type="checkbox"/>	9-AA	Negative	1				
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3	194.084398300	9-AA (9-aminoacridine)	C13H10N2	<input checked="" type="checkbox"/>	9-AA	Negative	1			2	
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7	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	43.98982924	CO2		
8	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	26.00307400	CN		
9	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1			2	
10	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	18.01056468	H2O	2	
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25	154.026608700	DHB (2,5-Dihydroxy-benzoic acid)	C7H6O4	<input checked="" type="checkbox"/>	DHB	Positive	1	18.01056468	H2O	2	
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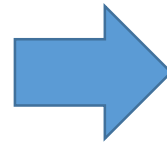
OK Cancel

Name the compound template

Template Name ✕

Input is required.

OK Cancel



Template Name ✕

OK Cancel

After importing:

The screenshot shows the 'Compound Template Setting' dialog box. On the left, a list of template categories is shown, with 'test001' selected under 'Lipid Mediators'. The 'Import' button is highlighted. In the center, a table lists the imported compounds:

No.	m/z	Compound Name	Formula	Calcul...	Matrix	Polarity	Matrix-derived	Neutral Loss Mass	Neutral Loss Composition	Multimer
1	100.00000000	test1	H2O	<input checked="" type="checkbox"/>	AAA	Negative	1			
2	111.11100000	test2	CO2	<input checked="" type="checkbox"/>	BBB	Negative	1	17.02654910	NH3	
3	222.22200000	test3	C6H12O6	<input checked="" type="checkbox"/>	CCC	Negative	1			2

An 'Import' dialog box is overlaid on the table, displaying the message 'The import succeeded.' with an information icon and an 'OK' button. A hand cursor is pointing at the 'OK' button. At the bottom of the main dialog, there are 'OK' and 'Cancel' buttons.

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