

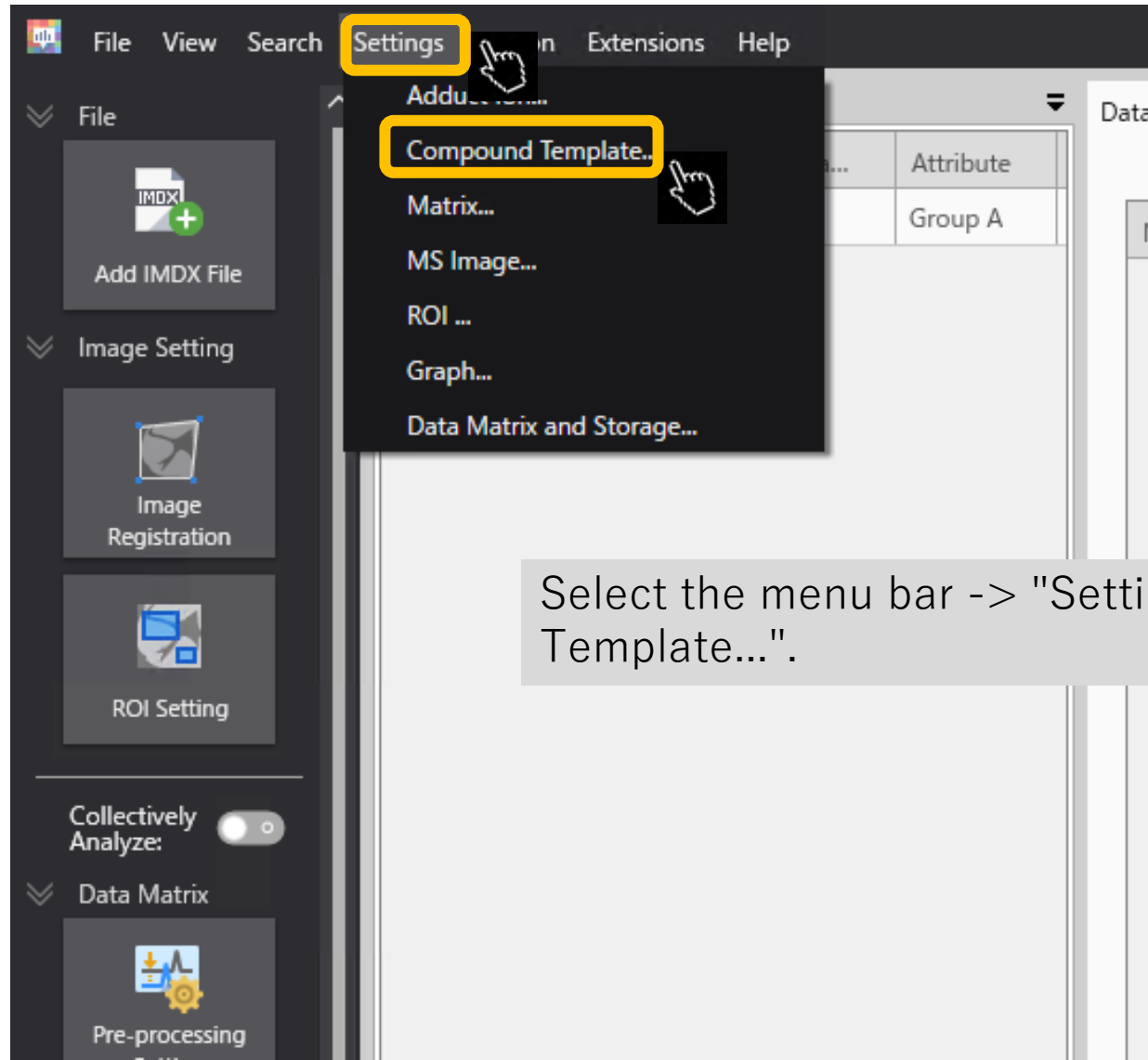
Editing the compound template

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  Import  Export   

Compound

Matrix Clusters

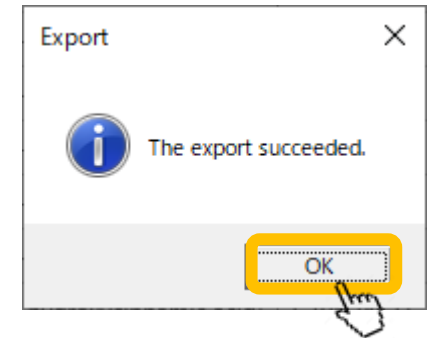
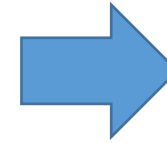
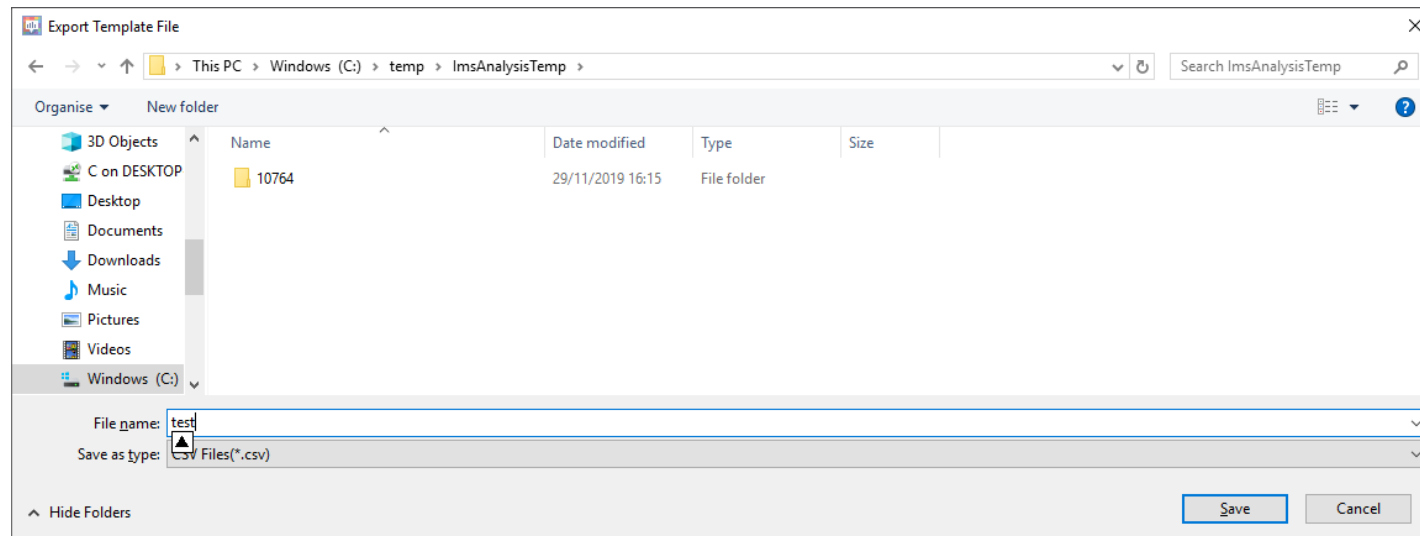
- Lipids
- Lipid Mediators
- Endogenous Metabolites
- test

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

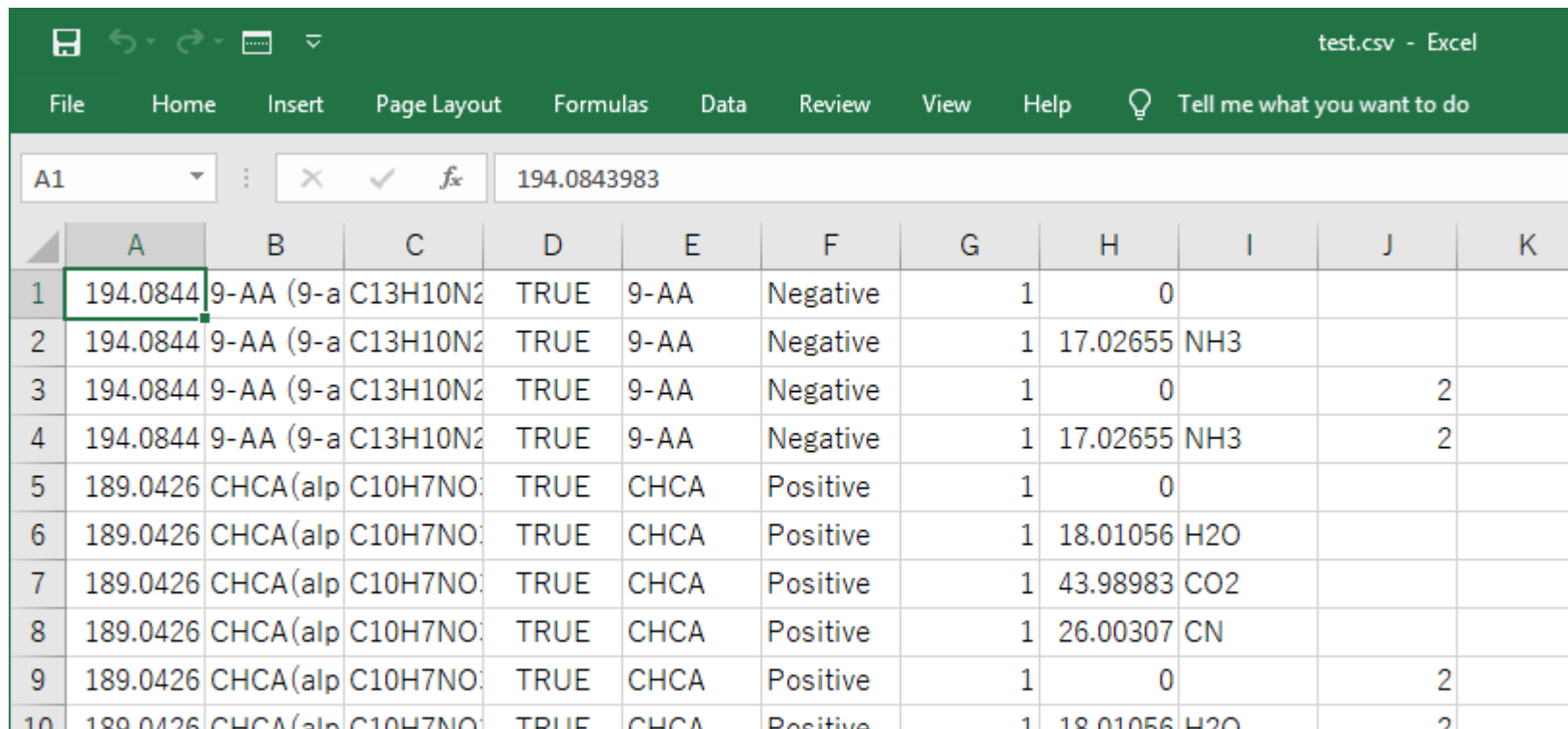
No.	m/z	Compound Name	Formula	Calcu...	Matrix	Polarity	Matrix-derived	Neutral Loss Mass	Neutral Loss Composition	Multimer
1	194.084398300	9-AA (9-aminoacridine)	C13H10N2	<input checked="" type="checkbox"/>	9-AA	Negative	1			
2	194.084398300	9-AA (9-aminoacridine)	C13H10N2	<input checked="" type="checkbox"/>	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
								43.98982924	CO2	2
								62.00039392	CO2-H2O	2
										3
								18.01056468	H2O	3
								43.98982924	CO2	3
								26.00307400	CN	3
								87.97965848	2(CO2)	3
								62.00039392	CO2-H2O	3
										4
								43.98982924	CO2	4
								87.97965848	2(CO2)	4
11	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1			
12	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1			
13	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1			
14	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	18.01056468	H2O	
15	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	43.98982924	CO2	
16	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	26.00307400	CN	
17	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	87.97965848	2(CO2)	
18	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	62.00039392	CO2-H2O	
19	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1			
20	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	43.98982924	CO2	
21	189.042593100	CHCA(alpha-Cyano-4-hydroxycinnamic acid)	C10H7NO3	<input checked="" type="checkbox"/>	CHCA	Positive	1	87.97965848	2(CO2)	
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

OK Cancel

Save with an appropriate name



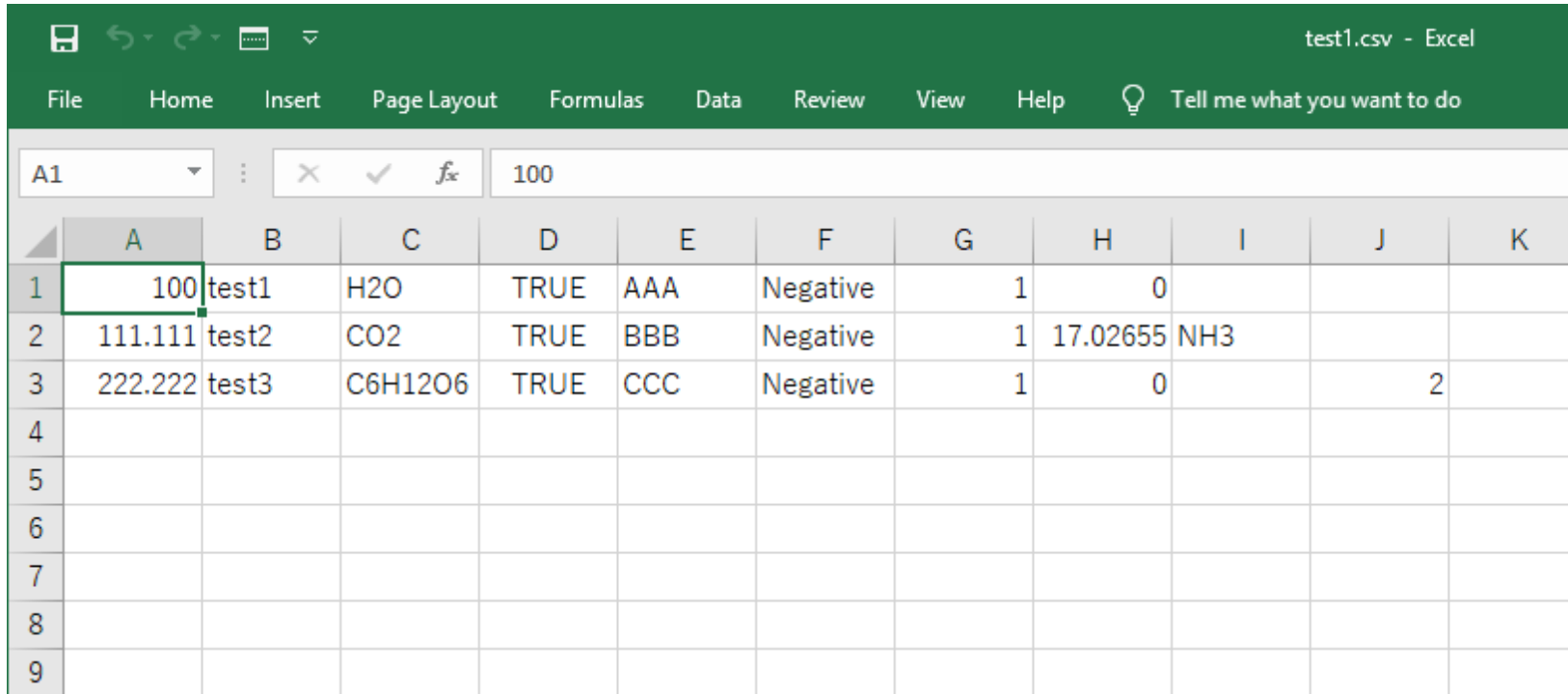
Open in Excel



	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	
10	189.0426	CHCA(alp	C10H7NO	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”








The screenshot shows an Excel spreadsheet with the following data:

	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

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				
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				
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	
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	

OK Cancel

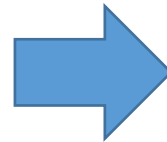
Select "Import" from the compound template settings screen, then select the edited csv file.

Name the compound template

Template Name ×

Input is required.

OK Cancel



Template Name ×

OK Cancel

After importing:

Compound Template Setting

Template Name

Matrix Clusters

Lipids

Lipid Mediators

Metabolites

test001

Compound

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	

Import

The import succeeded.

OK

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

OK Cancel

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