

How to change the adduct ion in use

From the menu bar, select “Settings” -> “Adduct Ion”

Create a target compound list

Data Matrix Setting

Analysis Method **Target** Non-target Threshold Value 0.000 %

Create List

Compound Template Excluded Compound Template

Matrix Clusters
Lipids
Lipid Mediators
Endogenous Metabolites

Matrix Clusters
Lipids
Lipid Mediators
Endogenous Metabolites

Tolerance 0.0100 Da

Used Adduct Ions

+H, +Na, +K
-H

Matrix 9-AA

Polarity Negative

A compound list that combines the selected compound template and the adduct ions displayed in Used Adduct Ions will be created.
From the compounds included in the compound template, the adduct ion combinations with only the compounds whose Calculate Adduct Ion checkbox is selected are added to the compound list.

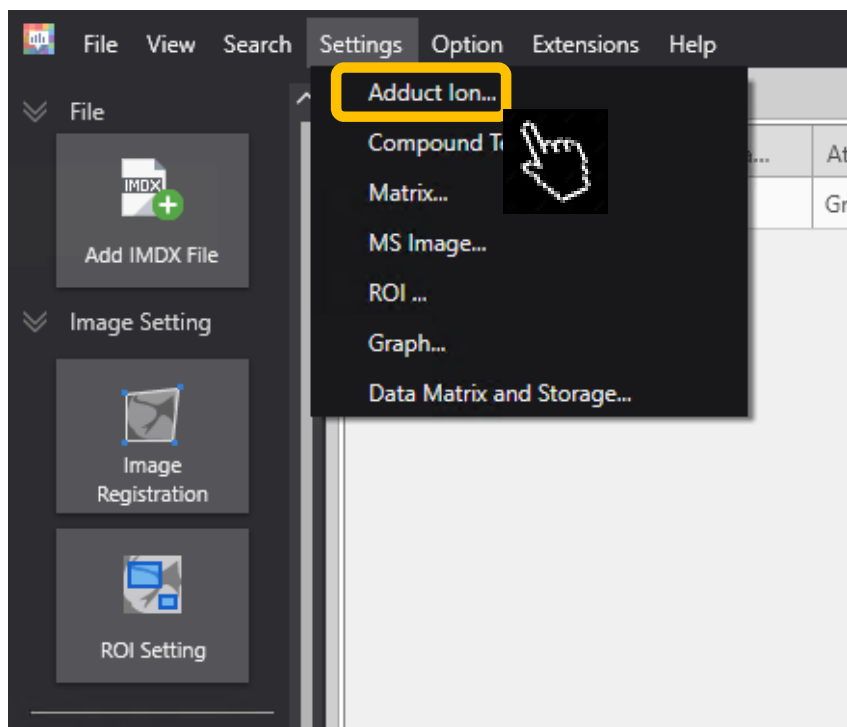
Create Cancel

Tolerance 0.0100 Da

OK Cancel

- A compound list is generated from the combination of the “Compound Template” and “Used Adduct Ions” list. (Refer to “Creating a data matrix” for the steps involved.)

Steps to change the type of adduct ion



- From the menu bar, select “Settings” -> “Adduct Ion”

Adduct ion settings screen

Adduct Ion Setting

Positive Adduct Ion

Adduct Ion	Monoisotopic Mass	Use	Matrix	Addition to Matrix Cluster
+H	1.00727600	<input checked="" type="checkbox"/>	▼	▼
+Na	22.98922000	<input type="checkbox"/>	▼	▼
+K	38.96371000	<input type="checkbox"/>	▼	▼
-e	-0.00054858	<input type="checkbox"/>	▼	▼
-H+2Na	44.97116000	<input type="checkbox"/>	▼	▼
-H+2K	76.91904000	<input type="checkbox"/>	▼	▼
-H+K+Na	60.94510000	<input type="checkbox"/>	▼	▼
-2H+3Na	66.95311000	<input type="checkbox"/>	▼	▼
-2H+3K	114.87490000	<input type="checkbox"/>	▼	▼
+DHB-H ₂ O+H	137.02330000	<input type="checkbox"/>	DHB ▼	0 ▼
+DHB-H ₂ O+Na	159.00530000	<input type="checkbox"/>	DHB ▼	0 ▼
+DHB-H ₂ O+K	174.97920000	<input type="checkbox"/>	DHB ▼	0 ▼
+2DHB-2(H ₂ O)+H	273.03940000	<input type="checkbox"/>	DHB ▼	0 ▼
+2DHB-2(H ₂ O)+Na	295.02130000	<input type="checkbox"/>	DHB ▼	0 ▼
+2DHB-2(H ₂ O)+K	310.99520000	<input type="checkbox"/>	DHB ▼	0 ▼
+3DHB-3(H ₂ O)+H	409.05540000	<input type="checkbox"/>	DHB ▼	0 ▼

Negative Adduct Ion

Adduct Ion	Monoisotopic Mass	Use	Matrix	Addition to Matrix Cluster
-H	-1.00727600	<input checked="" type="checkbox"/>	▼	▼
+Cl	34.96940000	<input type="checkbox"/>	▼	▼
+e	0.00054858	<input type="checkbox"/>	▼	▼
-2H+Na	20.97467000	<input type="checkbox"/>	▼	▼
-3H+2Na	42.95661000	<input type="checkbox"/>	▼	▼
-2H+K	36.94860000	<input type="checkbox"/>	▼	▼
-3H+2K	74.90449000	<input type="checkbox"/>	▼	▼
-3H+Na+K	58.93055000	<input type="checkbox"/>	▼	▼
-3H-2e	-3.02402400	<input type="checkbox"/>	9-AA ▼	1 ▼
+9-AA-H	193.07710000	<input type="checkbox"/>	9-AA ▼	0 ▼

Select the correct adduct ion and click "OK"

OK Cancel

The ions listed under “Used Adduct Ions” will change

Create List

Compound Template ?

Matrix Clusters
Lipids
Lipid Mediators
Endogenous Metabolites

Excluded Compound Template ?

Matrix Clusters
Lipids
Lipid Mediators
Endogenous Metabolites

Tolerance 0.0100 Da

Used Adduct Ions ?

+H
-H

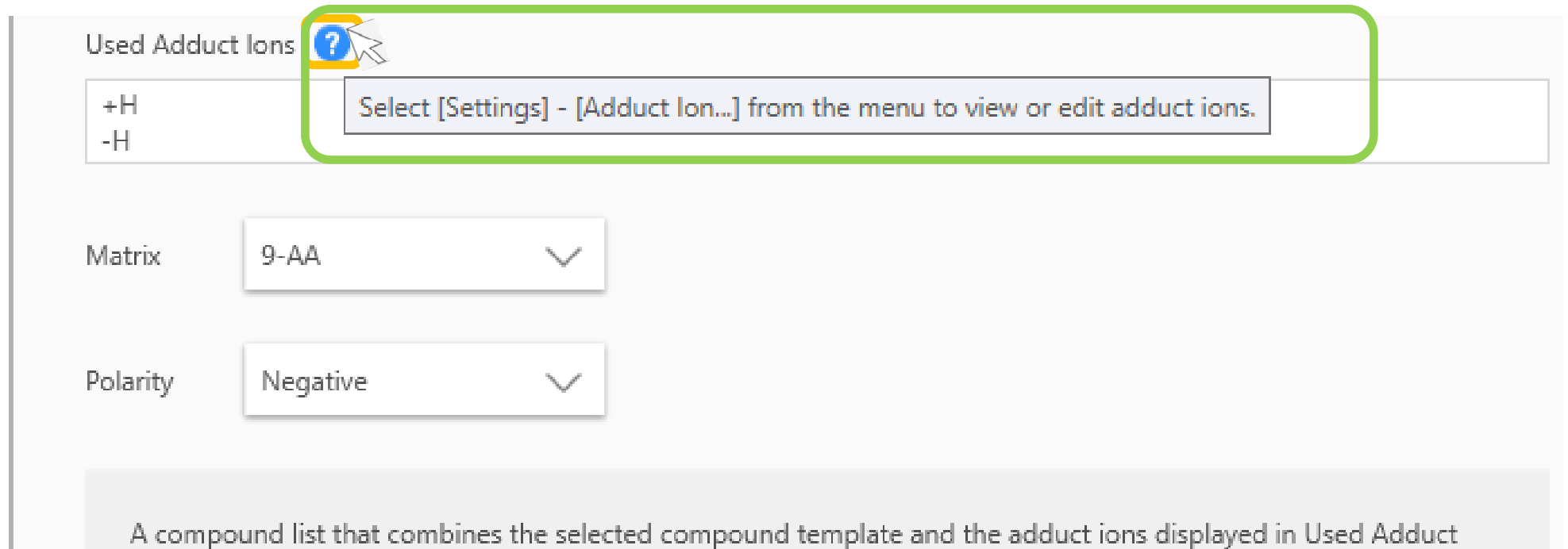
Matrix 9-AA ▾

Polarity Negative ▾


A compound list that combines the selected compound template and the adduct ions displayed in Used Adduct ions will be created.
From the compounds included in the compound template, the adduct ion combinations with only the compounds whose Calculate Adduct Ion checkbox is selected are added to the compound list.

Create Cancel

Hovering the cursor over the blue question mark icon will display a hint





The screenshot shows a software interface with a 'Used Adduct Ions' section. A blue question mark icon is highlighted with a green rounded rectangle, and a tooltip is displayed next to it. The tooltip contains the text: 'Select [Settings] - [Adduct Ion...] from the menu to view or edit adduct ions.' Below this section, there are two dropdown menus: 'Matrix' with the value '9-AA' and 'Polarity' with the value 'Negative'. At the bottom of the interface, there is a grey bar with the text: 'A compound list that combines the selected compound template and the adduct ions displayed in Used Adduct'.

Used Adduct Ions 

+H
-H

Select [Settings] - [Adduct Ion...] from the menu to view or edit adduct ions.

Matrix 9-AA 

Polarity Negative 

A compound list that combines the selected compound template and the adduct ions displayed in Used Adduct