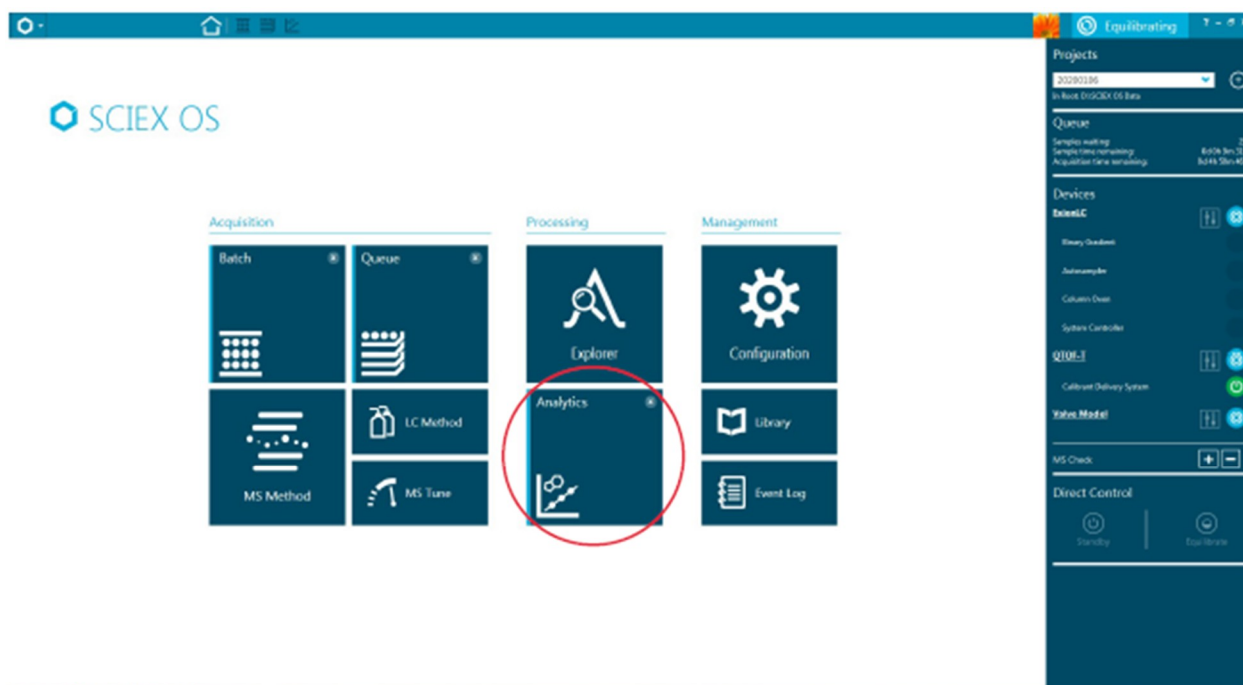
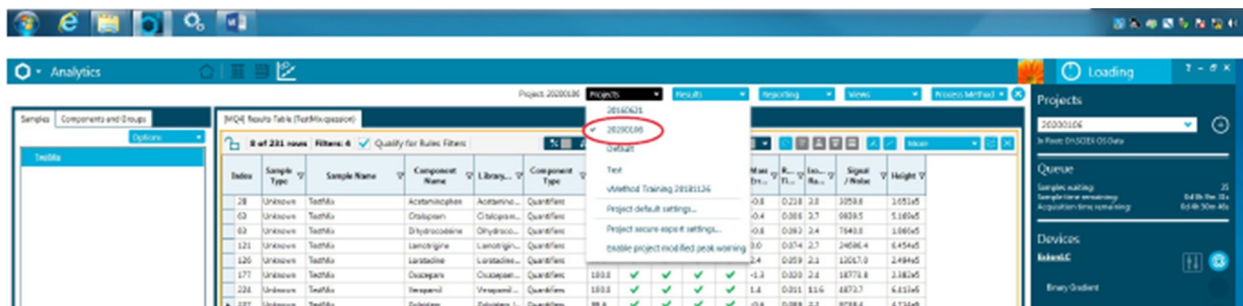


## Processing Guide – QTOF

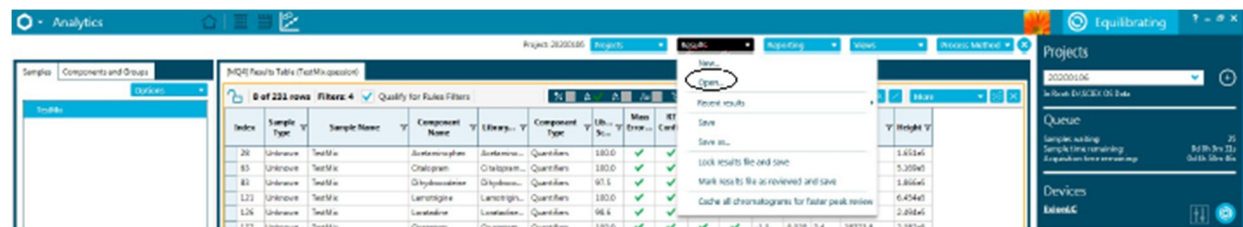
**Step 1:** Select “Analytics” from the “Home” screen.



**Step 2:** Go to the “Project” drop-down and select the date analyzed.



**Step 3:** Go to the “Results” drop-down and select “Open”



**Step 4:** Select the file to process – should be the data “2021XXXX”


**Step 5:** Go to the “More” drop-down located on the right-side of the data toolbar. Select “Recent Table Settings”. Select the INITIAL option (this will re-format the data to include only the information relevant)

The screenshot displays the QTOF software interface. The main window shows a table of results with columns for Index, Sample Name, Component Name, Library, Component Type, and various numerical values. A context menu is open over the table, showing options like 'Add custom column...', 'Remove custom column...', 'Hide selected row(s)', 'Show previously hidden row(s)', 'Add sample...', 'Remove selected sample', 'Set Used', 'Get peaks to "Not Found" for selected row(s)', 'Create Matrix Plot with new settings', and 'Create Matrix Plot with saved settings'. The 'Initial' option is selected in the menu.

**Step 7:** Process the data. Fill out the “QC Supplement Form” for the Positive Controls and the QTOF Screen List spreadsheet (Shown below)

The screenshot shows the QTOF Screen List spreadsheet. The spreadsheet has columns for QTOF, QTOF STANDARDS, Formula, m/z, 1000 (m/z), Control (m/z), and Relative 1. The data is organized into rows for various compounds and standards. The spreadsheet is titled 'QTOF Screen List' and 'Effective 3/1/2021'.

QTOF	QTOF STANDARDS	Formula	m/z	1000 (m/z)	Control (m/z)	Relative 1
1	Acetaminophen	C <sub>9</sub> H <sub>9</sub> NO <sub>2</sub>	151.05	151.05	151.05	1.00
2	Aspirin	C <sub>9</sub> H <sub>7</sub> NO <sub>4</sub>	181.02	181.02	181.02	1.00
3	Chlorzoxazone	C <sub>15</sub> H <sub>13</sub> ClN <sub>2</sub> O <sub>4</sub>	309.05	309.05	309.05	1.00
4	Diazepam	C <sub>16</sub> H <sub>13</sub> ClN <sub>2</sub>	254.04	254.04	254.04	1.00
5	Flunitrazepam	C <sub>16</sub> H <sub>12</sub> ClN <sub>2</sub>	252.04	252.04	252.04	1.00
6	Valium	C <sub>17</sub> H <sub>14</sub> ClN <sub>2</sub> O	285.05	285.05	285.05	1.00
7	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
8	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
9	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
10	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
11	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
12	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
13	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
14	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
15	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
16	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
17	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
18	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
19	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
20	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
21	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
22	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
23	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
24	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
25	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
26	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
27	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
28	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
29	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
30	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
31	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
32	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
33	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
34	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
35	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
36	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
37	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
38	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
39	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
40	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
41	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
42	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
43	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
44	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
45	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
46	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
47	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
48	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
49	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
50	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
51	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
52	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
53	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
54	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
55	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
56	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
57	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
58	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
59	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
60	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
61	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
62	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
63	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
64	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
65	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
66	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
67	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
68	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
69	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
70	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
71	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
72	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
73	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
74	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
75	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
76	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
77	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
78	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
79	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
80	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
81	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
82	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
83	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
84	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
85	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
86	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
87	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
88	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
89	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
90	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
91	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
92	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
93	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
94	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
95	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
96	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00
97	Triazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
98	Temazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>2</sub> O	270.05	270.05	270.05	1.00
99	Alprazolam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub>	279.05	279.05	279.05	1.00
100	Clonazepam	C <sub>15</sub> H <sub>10</sub> ClN <sub>4</sub> O	277.05	277.05	277.05	1.00

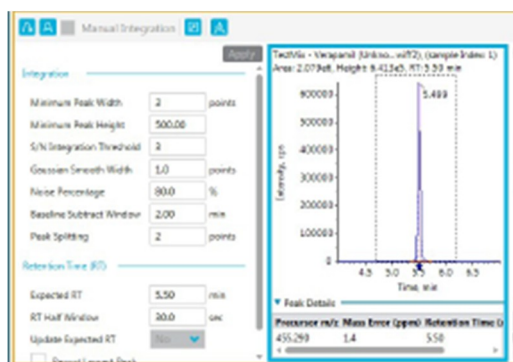
**To see the Tables:** Select the  icon on the toolbar (located next to the grayed out boxes).



**The Retention Times need to be updated for all the analytes included in the control**– Starting with the Positive QCs can assist in the rest of the data.

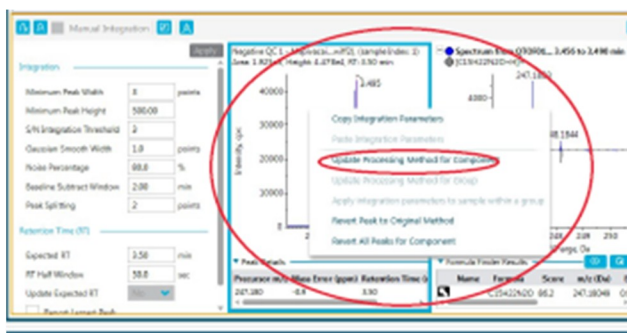
#### To update retention times:

Click and Drag in the “Peak Table” (Highlighted in a blue outline below). The Retention time will automatically update.

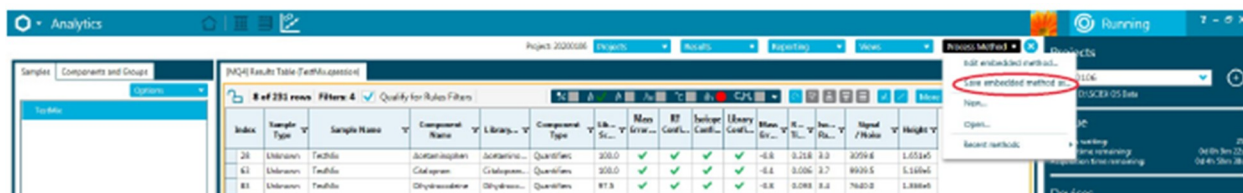


#### To save the retention times:

Right-click in the “Peak Table” and select “Update Processing Method for Component”. The new retention time will now be applied to the other case samples.



Then go to the “Process Method” drop-down, select “Save Embedded method as” and overwrite the “QSCREEN20191231” method. (Recommend doing this after both Positive QCs have been processed)

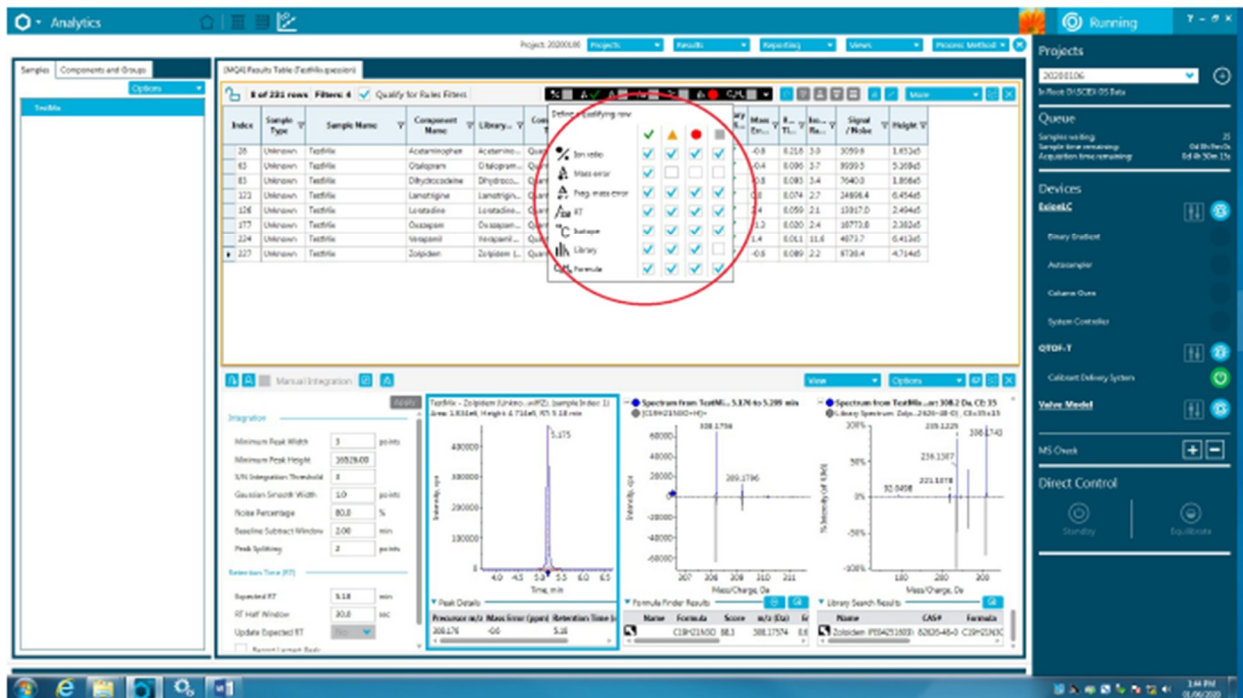


**Negative QCs:** should only have “Mepivacaine” but if anything with Four (✓) is seen, it needs to be included in the “Summary Report”.

**Positive QCs:** Reference the QTOF Screen List for what should be included in the Sample. Make sure to include the analytes that should be there on the “Summary Report”.

**Step 8:** After the Controls have been processed – process the case data.

Remove analytes without library matches first, then evaluate the below criteria– For summary page:



Mass Error: ✓ ▲

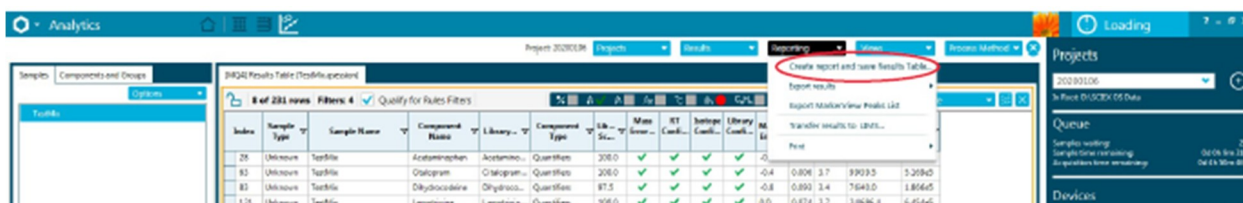
RT: ✓ ▲ ●

Isotope: ✓ ▲

Library: ✓ ▲ ● (as long as it matches to a library)

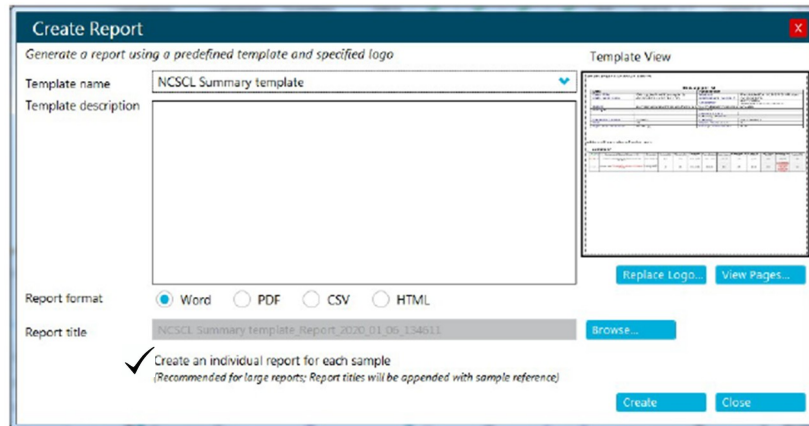
**Step 9:** To Print the “Summary Report” – select all the samples

Go to the “Reporting” drop-down and select “Create report and save Results table”

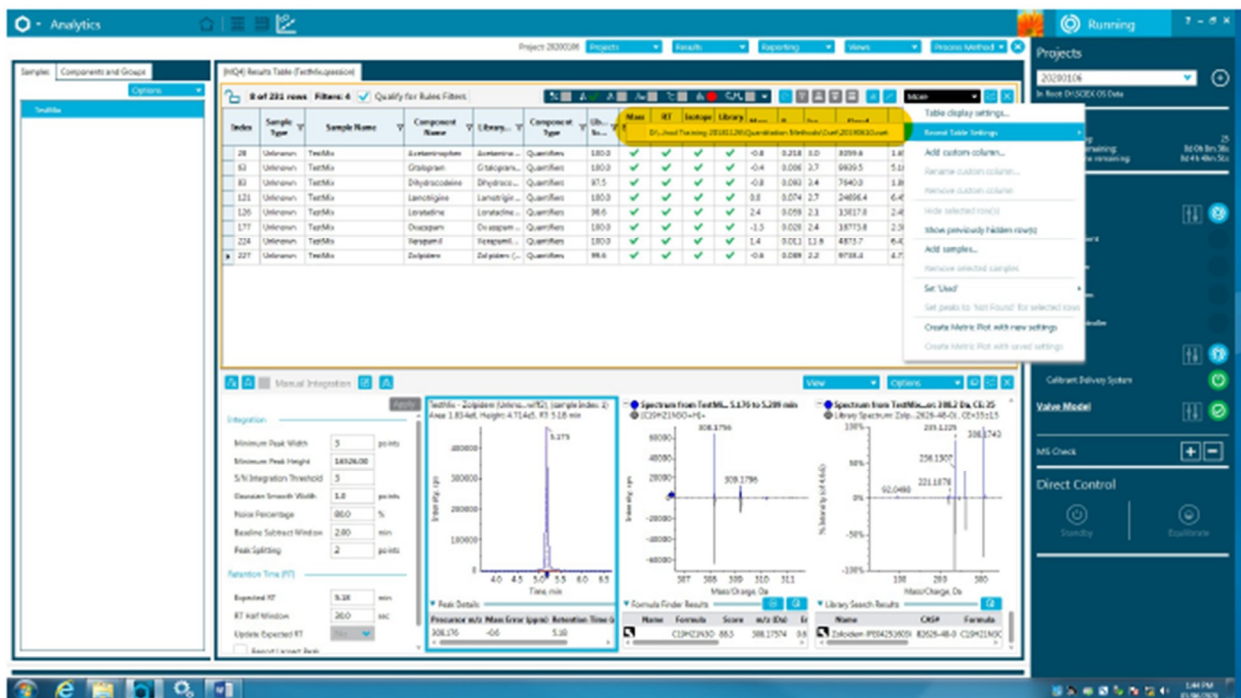




Select the “NCSCL Summary Template3” option. **CHECK the “Create an individual report”**. Click “Create”. The folder containing the reports will be under Data(D:)→ Reports (rename the folder: Date-Summary)



**Step 10:** Go to the “More” drop-down located on the right-side of the data toolbar. Select “Recent Table Settings”. Select the FINAL option (this will re-format the data to include only the information relevant)



Re-process the data. This is the “Final Report” step.

**Negative QCs:** should only include analytes with Four (✓)

**Positive QCs:** should only include analytes with Four (✓)

**Case Data:** the table will include the following criteria:

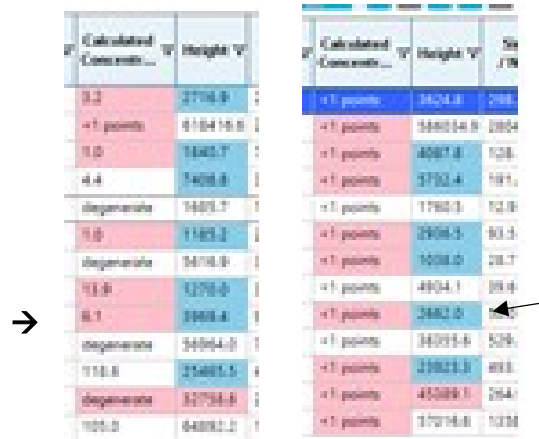
Mass Error: ✓

RT: ✓  

Isotope: ✓

Library: ✓

*Note: This is where the height/concentration criteria comes into play.*



Calculated Concentration	Height	%I
0.0	2714.8	
< 1 percent	8184.9	
0.0	1840.7	
4.4	7408.8	
diagnostic	7408.7	
0.0	1189.2	
diagnostic	1478.8	
0.0	1179.0	
6.1	2468.4	
diagnostic	2468.4	
0.0	2140.5	
diagnostic	21774.4	
0.0	6488.2	

Calculated Concentration	Height	%I
< 1 percent	1824.8	298
< 1 percent	14408.8	2804
< 1 percent	4087.8	128
< 1 percent	2702.4	187
< 1 percent	1788.8	12.8
< 1 percent	2508.5	60.5
< 1 percent	1008.0	28.7
< 1 percent	4804.1	89.8
< 1 percent	2462.0	5
< 1 percent	14091.4	528
< 1 percent	21823.3	898
< 1 percent	45088.1	264
< 1 percent	17074.8	1288

**Calculated Concentration:** These are only used for analytes contained in a **QCS** – A **red block** with a numeric value indicates it is below 90% of the cut-off for that analyte and therefore cannot be reported.

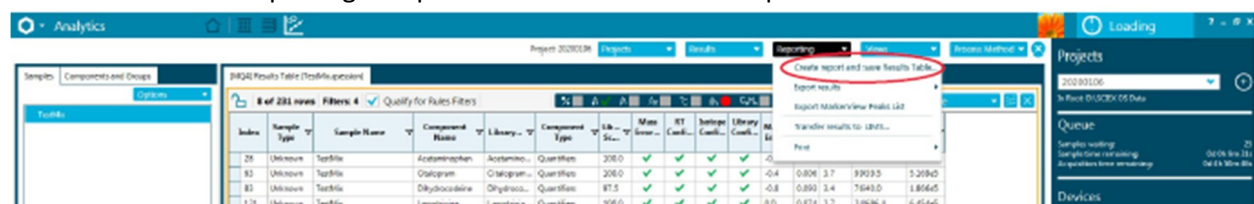
**Height:** These are only for analytes NOT contained in a **QCS** – A **blue block** indicates it is below the LLOQ for that analyte and therefore cannot be reported.

**IF** an analyte in a QCS has a **blue height block**, but **NOT** a **red concentration block**, it will be left on the **FINAL** page.

**\*\*Red height blocks** need to be noted and submitted to the QTOF coordinator

### Step 11: To print the “Final Report” – select all the samples

Go to the “Reporting” drop-down and select “Create report and save Results table”



Select the “NCSCL Final Template3” option. **CHECK the “Create an individual report”.**

Click “Create”. The folder containing the reports will be under Data(D:) → Reports (rename the folder: Date-Final)