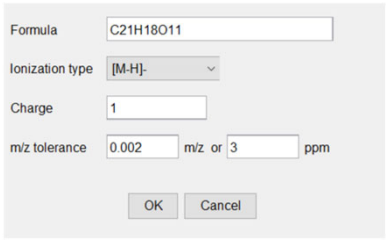
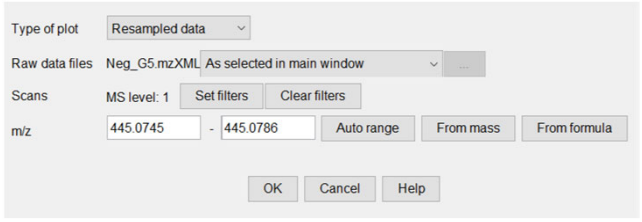
Class on 02-03-20

1

Looking at the data with a 2D view





2

Set the run time for GenGlcA

Scan number -

Base Filtering Integer

Retention time 10 - 22 min. Auto range

MS level 1

Scan definition

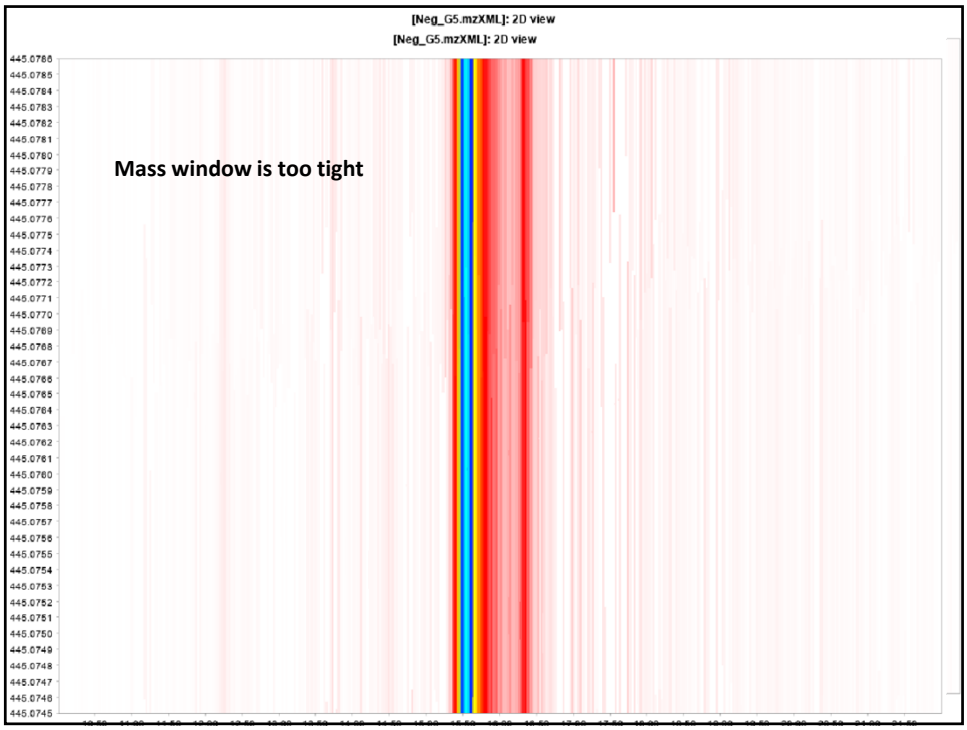
Polarity -

Spectrum type Any

Include only spectra of this type

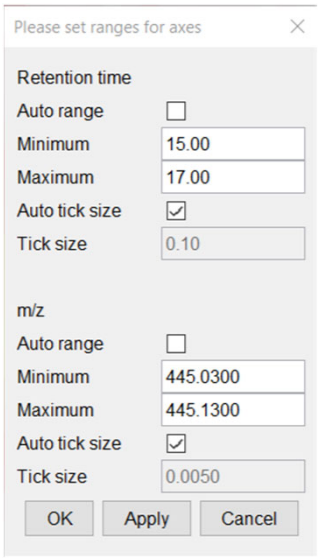
OK Cancel

3

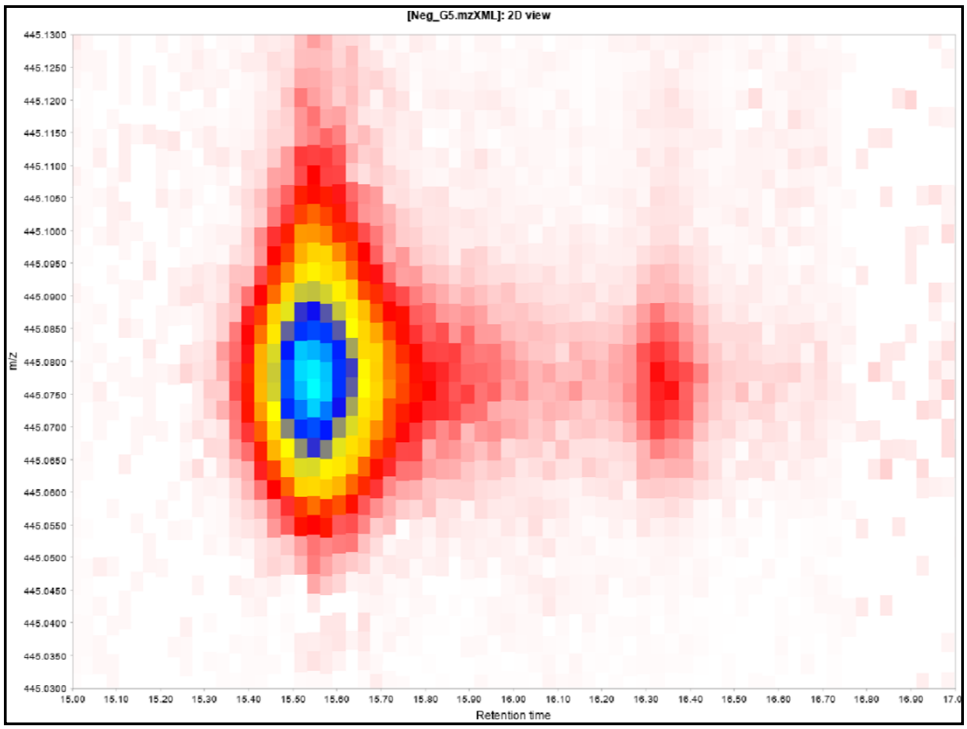


4

Reset the retention time and mass ranges

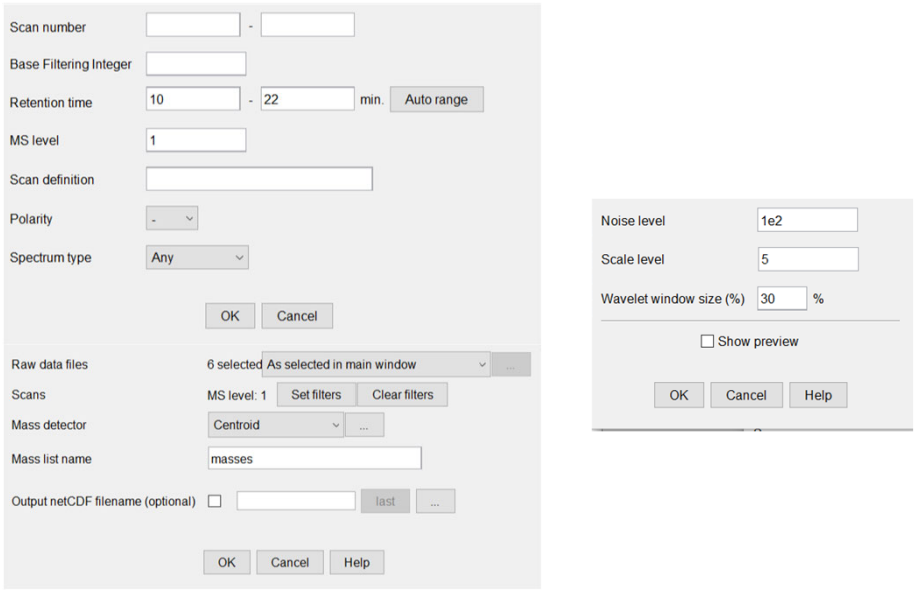


5



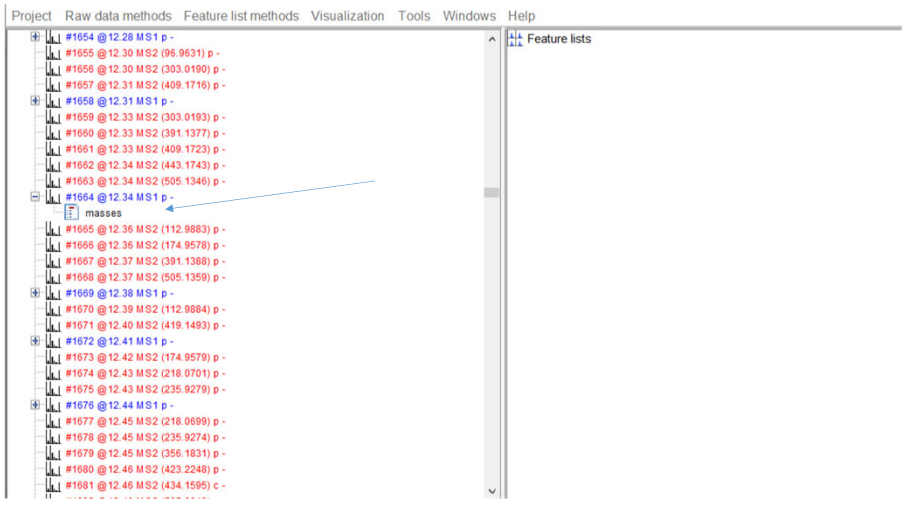
6

Select // and masses



7

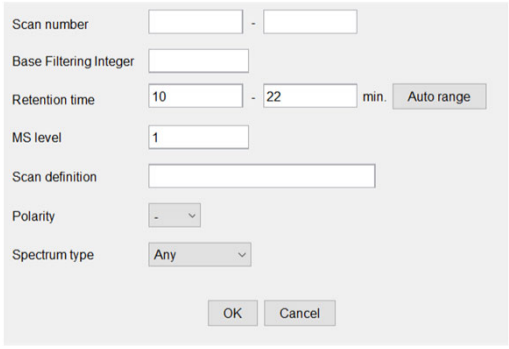
The initial raw files now have masses



8

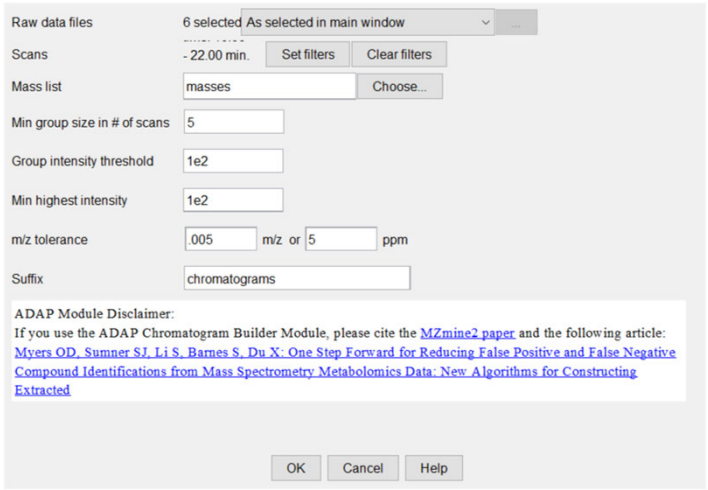
Go to // and select ADAP chromatogram builder

First set the retention time range



9

Setting the parameters



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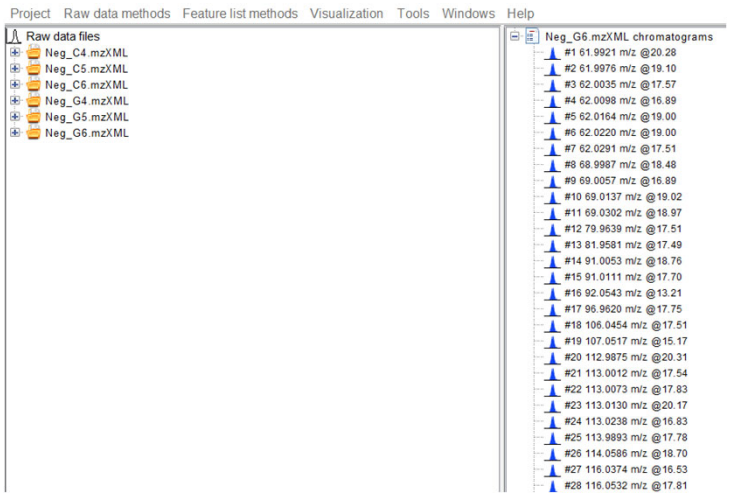
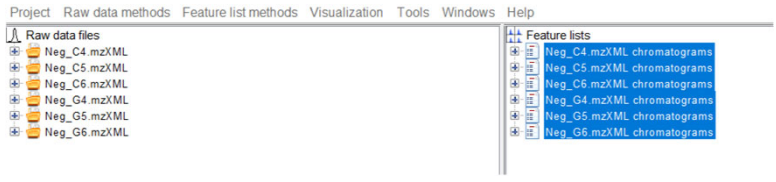
Mass chromatogram file content



11

Selecting files for chromatogram deconvolution



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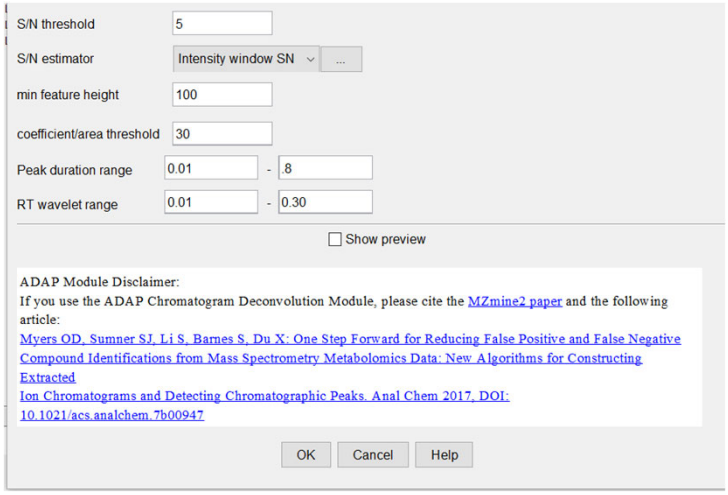
Setting parameters for deconvolution



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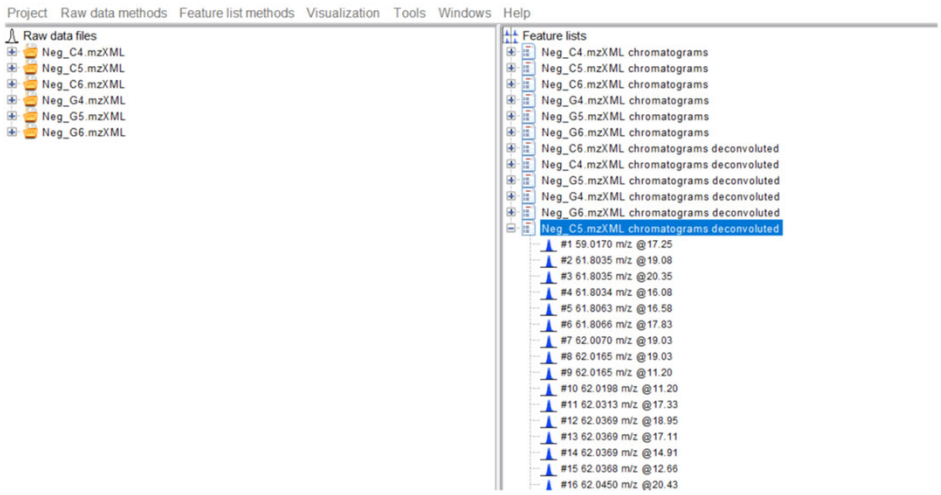
Content of the deconvoluted files



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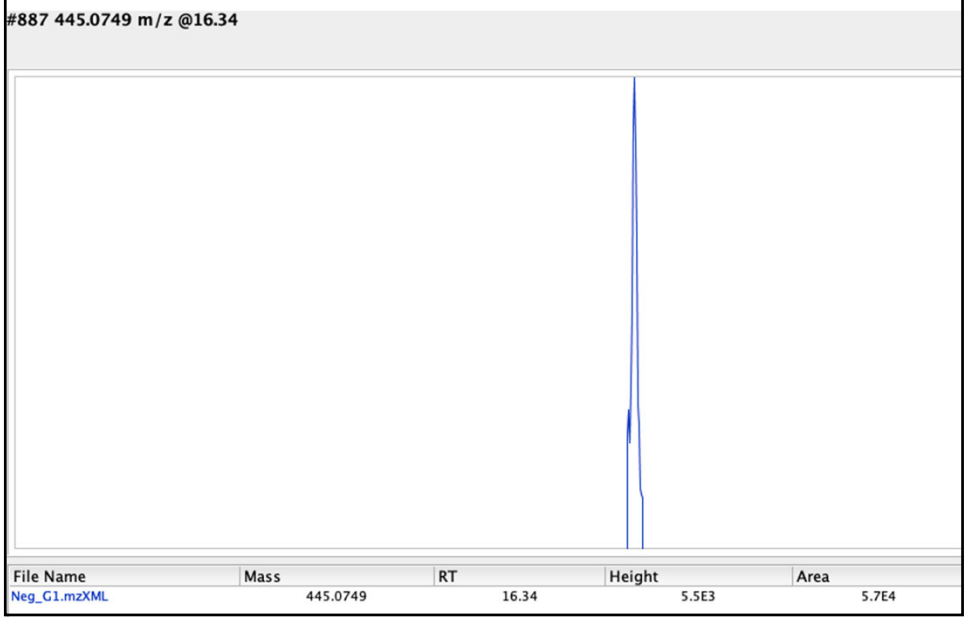
A single deconvoluted ion feature



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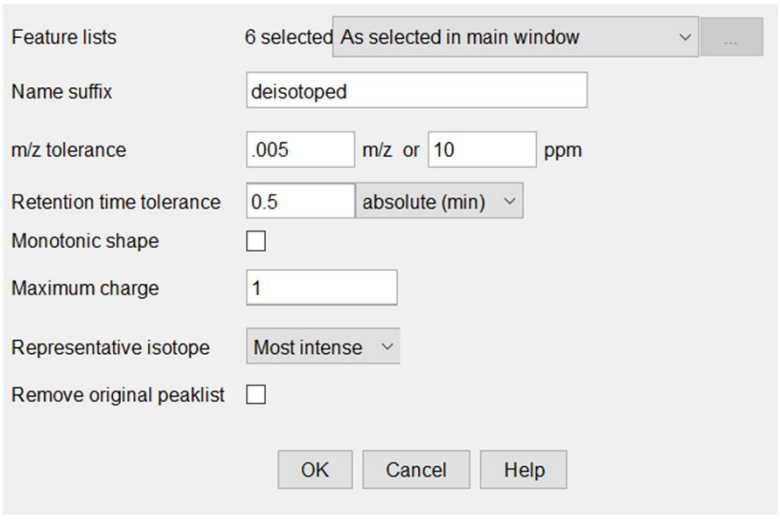
Isotope grouping



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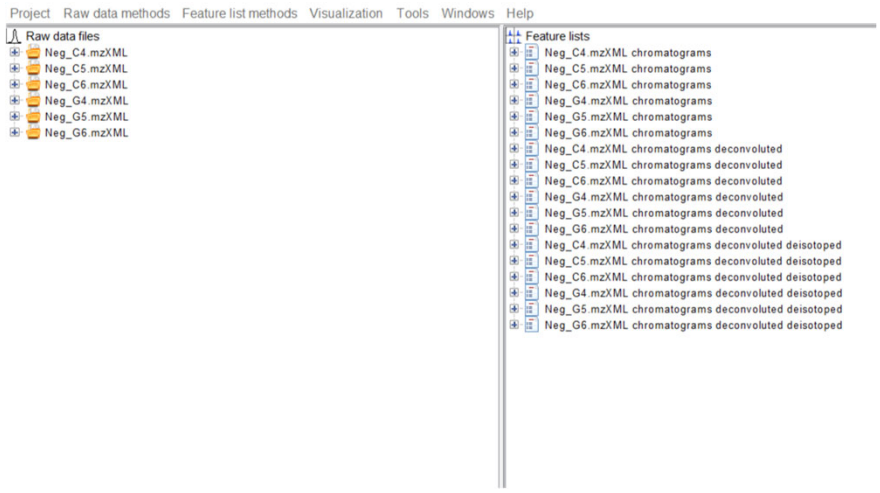
De-isotoped files



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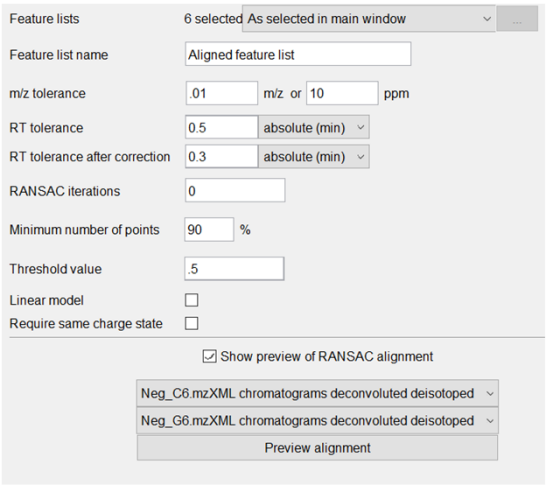
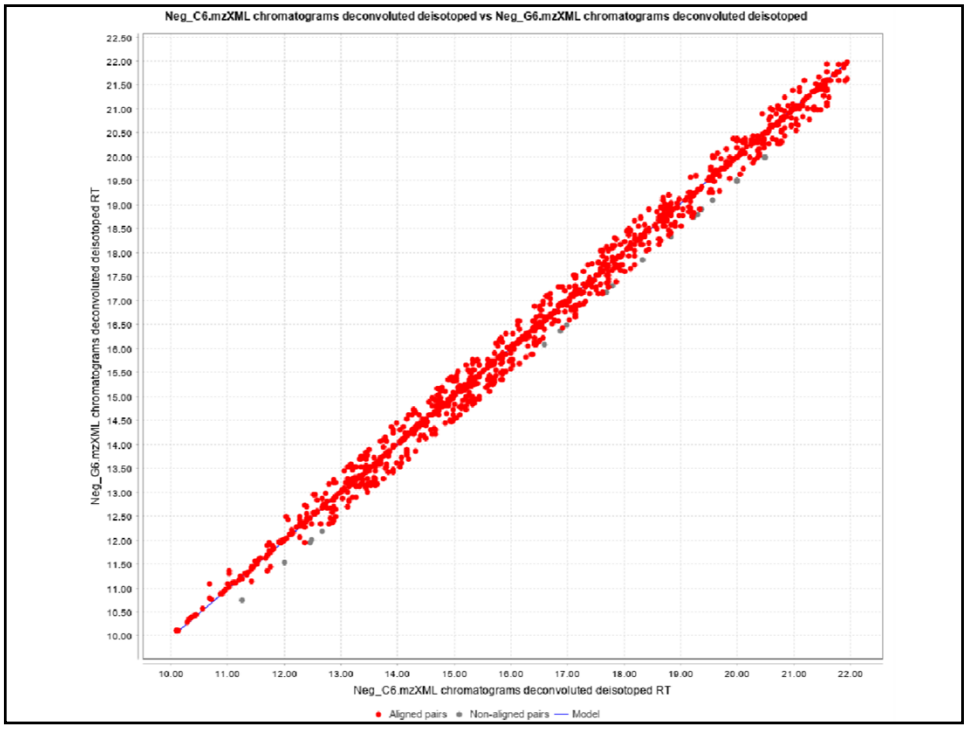
Peak and chromatogram alignment



18



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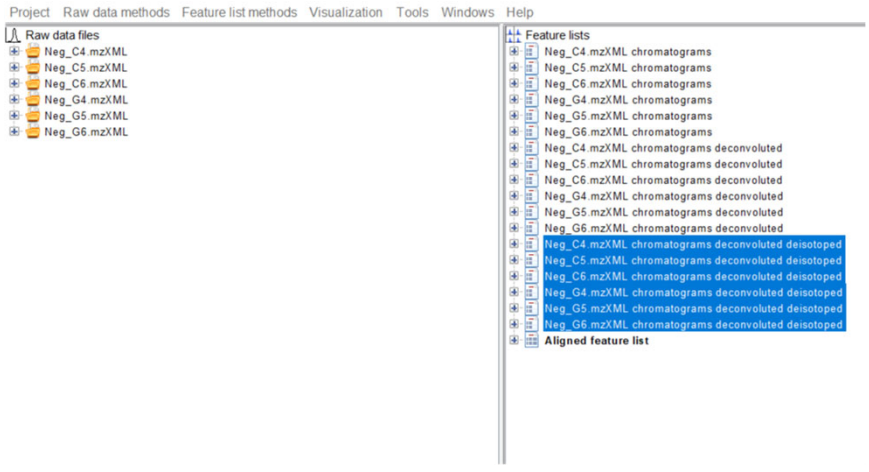
The aligned file appears



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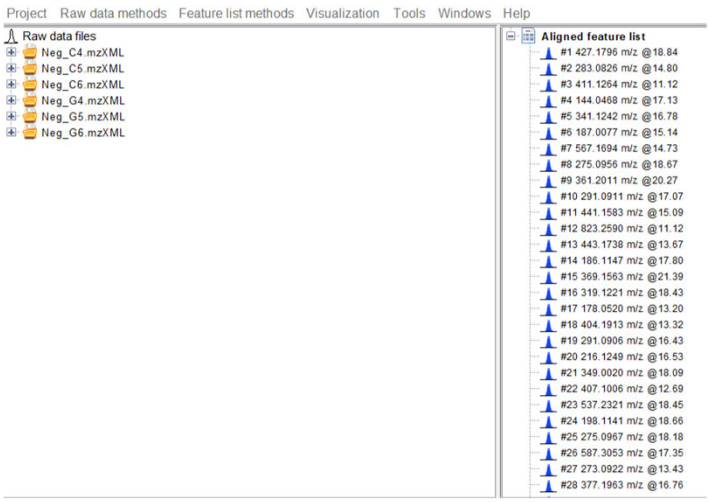
Content of the aligned file



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Initial version of the aligned table

Windows

ID: m/z: RT: Identity: Comment:

ID	Average		Identity	Comment	Peak shape	Neg_C4.mzXML			N
	m/z	RT				Status	Height	Area	Status
1	427.1796	18.84					2.4E5	2.1E6	
2	283.0826	14.80					1.6E5	1.2E6	
3	411.1264	11.12					1.3E5	8.4E5	
4	144.0468	17.13					1.3E5	1.2E6	
5	341.1242	16.78					1.2E5	9.6E5	
6	187.0077	15.14					1.1E5	1.2E6	
7	567.1694	14.73					1.1E5	5.3E5	
8	275.0956	18.67					8.4E4	6.7E5	
9	361.2011	20.27					8.3E4	7.0E5	
10	291.0911	17.07					7.5E4	6.6E5	
11	441.1583	15.09					6.7E4	4.7E5	
12	823.2590	11.12					6.5E4	3.0E5	
13	443.1738	13.67					6.5E4	5.8E5	

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Locating Gen GlcA in the table

ID	Average		Peak shape	Neg_C4.mzXML			Neg_C5.mzXML			Neg_C6.mzXML			Neg_G4.mzXML			Neg_G5.mzXML			Neg_G6.mzXML		
	m/z	RT		Status	Height	Area	Status	Height	Area	Status	Height	Area	Status	Height	Area	Status	Height	Area	Status	Height	Area
17013	445.0425	14.46															2.8E3	1.4E4			
21846	445.0456	15.94																		1.1E2	7.2E2
3240	445.0581	13.58			1.6E2	1.1E3															
4815	445.0581	13.89			1.1E2	4.2E2															
19074	445.0758	20.38															1.3E2	5.4E2			
12253	445.0766	16.33												2.8E4	2.1E5		2.1E3	1.1E4		3.6E3	2.4E4
12243	445.0772	15.58												1.1E5	1.3E6					8.7E4	9.0E5
21281	445.0786	13.76																		1.5E2	5.5E2
8000	445.1309	17.77						1.1E2	9.1E2												
6531	445.1328	10.91						2.4E2	7.8E2								9.1E2	5.6E3			
6667	445.1666	15.50						2.1E2	1.2E3												
7268	445.1668	18.26						1.5E2	7.3E2												
6685	445.1669	16.17						2.1E2	1.9E3												
20049	445.1705	14.51																		1.7E3	9.6E3
20018	445.1884	13.57																		4.0E3	2.1E4
20123	445.1884	16.09																		9.1E2	7.2E3
21267	445.1884	18.32																		1.5E2	6.1E2
20252	445.1884	17.32																		5.5E2	4.8E3
17235	445.1916	14.57															7.5E2	3.6E3		1.3E3	8.4E3
17140	445.1948	14.61															7.5E2	3.6E3			
20335	445.2064	18.05																		4.1E2	2.1E3

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Table ordered to ions found in Genistein-treated samples

ID	Average		Peak shape	Neg_C4.mzXML			Neg_C5.mzXML			Neg_C6.mzXML			Neg_G4.mzXML			Neg_G5.mzXML			Neg_G6.mzXML		
	m/z	RT		Status	Height	Area	Status	Height	Area	Status	Height	Area	Status	Height	Area	Status	Height	Area	Status	Height	Area
4	144.0468	17.13			1.3E5	1.2E6		6.6E4	7.0E5		8.3E4	8.8E5		4.9E4	4.9E5		8.7E4	7.9E5		7.5E4	7.4E5
5	341.1242	16.78			1.2E5	9.6E5		1.3E5	1.1E6		8.6E3	4.7E4		1.6E5	1.3E6		3.7E4	2.3E5		8.2E4	5.3E5
6	187.0077	15.14			1.1E5	1.2E6		3.6E4	3.4E5		8.0E4	8.7E5		3.6E4	3.5E5		8.7E4	9.1E5		5.1E4	4.9E5
9	361.2011	20.27			8.3E4	7.0E5		5.2E4	2.5E5		1.6E5	1.2E6		1.6E5	1.1E6		2.6E4	1.2E5		5.3E4	2.2E5
10	291.0911	17.07			7.5E4	6.6E5		3.2E4	2.5E5		2.6E4	2.1E5		9.8E4	7.2E5		1.8E4	1.1E5		2.9E4	2.7E5
14	186.1147	17.80			6.3E4	4.5E5		4.0E4	2.8E5		8.0E4	6.5E5		1.1E4	8.6E4		2.0E4	1.5E5		3.0E4	2.1E5
16	319.1221	18.43			5.8E4	3.6E5		5.4E4	6.4E5		2.4E4	1.6E5		6.3E4	7.6E5		1.1E4	1.5E5		2.6E4	3.1E5
17	178.0520	13.20			5.8E4	4.1E5		6.7E4	5.2E5		1.0E4	8.1E4		7.6E4	6.1E5		3.7E4	2.8E5		6.9E4	5.0E5
18	404.1913	13.32			5.7E4	3.4E5		2.7E4	1.6E5		6.6E4	2.7E5		2.7E4	1.3E5		1.1E4	6.6E4		2.1E4	1.4E5
19	291.0906	16.43			5.7E4	4.4E5		4.8E4	2.6E5		2.8E4	1.5E5		6.3E4	4.0E5		1.7E4	1.2E5		3.1E4	2.0E5
20	216.1249	16.53			5.6E4	4.0E5					9.9E4	8.7E5		2.2E4	1.5E5		2.8E4	2.1E5		2.2E4	1.6E5
23	537.2321	18.45			4.8E4	3.0E5		3.5E4	2.5E5		1.3E5	1.1E6		1.0E5	7.7E5		1.5E4	1.0E5		3.8E4	2.5E5
25	275.0967	18.18			4.3E4	3.4E5		6.1E4	4.5E5		1.0E5	9.6E5		4.7E4	3.6E5		3.0E4	1.5E5		1.4E4	8.9E4
30	242.1402	14.90			3.5E4	1.9E5		2.6E4	1.7E5		5.1E4	2.8E5		2.7E4	2.2E5		2.5E4	1.2E5		2.7E4	1.9E5
32	421.1353	13.04			3.4E4	1.9E5		3.1E4	2.2E5		2.6E4	1.8E5		3.9E4	2.7E5		2.9E4	2.1E5		3.2E4	2.1E5
34	172.0987	15.72			3.2E4	2.5E5		1.3E4	1.0E5		5.8E4	5.1E5		5.3E3	4.0E4		1.3E4	9.7E4		1.5E4	1.2E5
36	375.1304	13.03			3.1E4	2.0E5					2.4E4	1.7E5		3.6E4	2.6E5		3.1E4	2.0E5			
39	212.0033	13.36			3.0E4	3.1E5		2.1E4	1.9E5		1.6E4	1.7E5		1.9E4	1.6E5		2.8E4	2.6E5		2.5E4	2.6E5
43	204.0674	16.06			2.7E4	2.4E5		2.5E4	2.3E5		2.3E4	1.9E5		1.6E4	1.4E5		1.7E4	1.4E5		2.1E4	1.8E5
44	415.1969	19.14			2.7E4	1.1E5					3.9E4	2.4E5		1.1E4	6.1E4		6.1E3	2.1E4		1.1E4	7.4E4
46	317.1238	14.46			2.4E4	1.8E5		1.5E4	1.1E5		3.8E4	2.3E5		1.9E4	1.3E5		1.8E4	8.6E4		1.4E4	8.9E4

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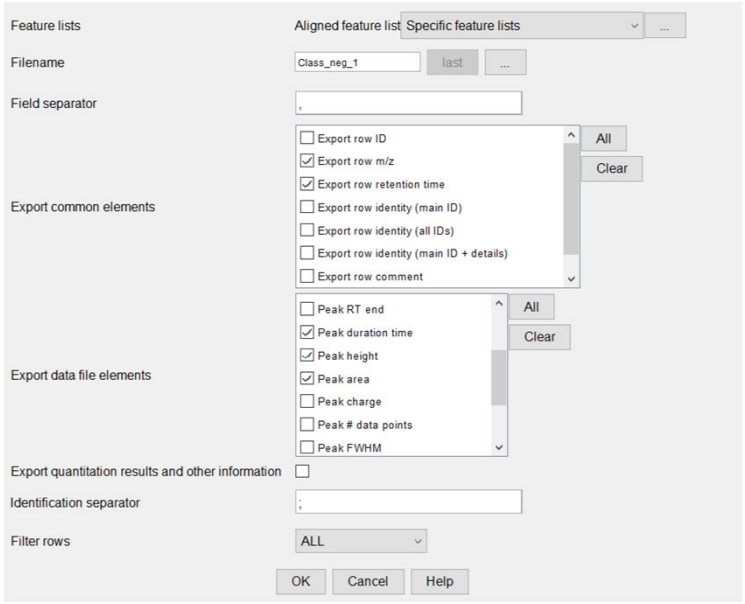
Exporting the aligned table



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Class exercise

- Load the C4-C6 and G4-G6 .mzxml files
- Locate the ions that have the ion (in negative) for p-ethylphenol glucuronide ($C_{14}H_{18}O_7$) and p-ethylphenol sulfate ($C_8H_{10}O_4S$) - what are their *m/z* values?
  - Get MSMS spectra of each one
- Identify all the *masses* in each file -– from these generate chromatograms, and then deconvolute the chromatograms
- Output the data into a .csv file (choose row ID, m/z, retention time, peak height, peak area and FWHM)
- Sort the file by retention time – identify ions that are co-eluting and are isotopes.

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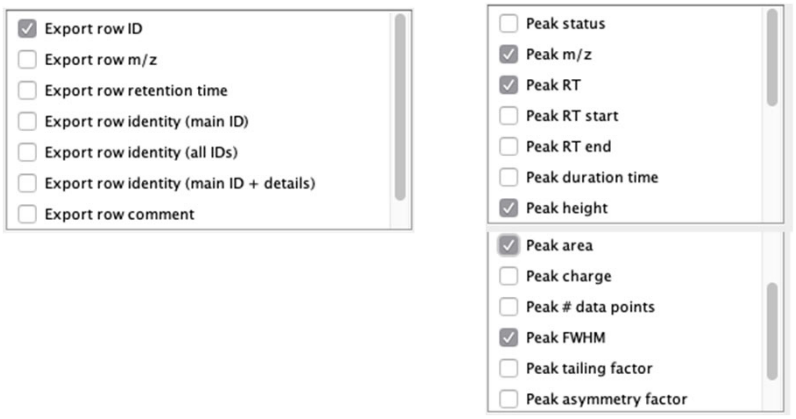
Export to .CSV file



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