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Vion Unifi 1.8.2
Investigate Mode Elemental Composition

Elemental Composition from Investigate

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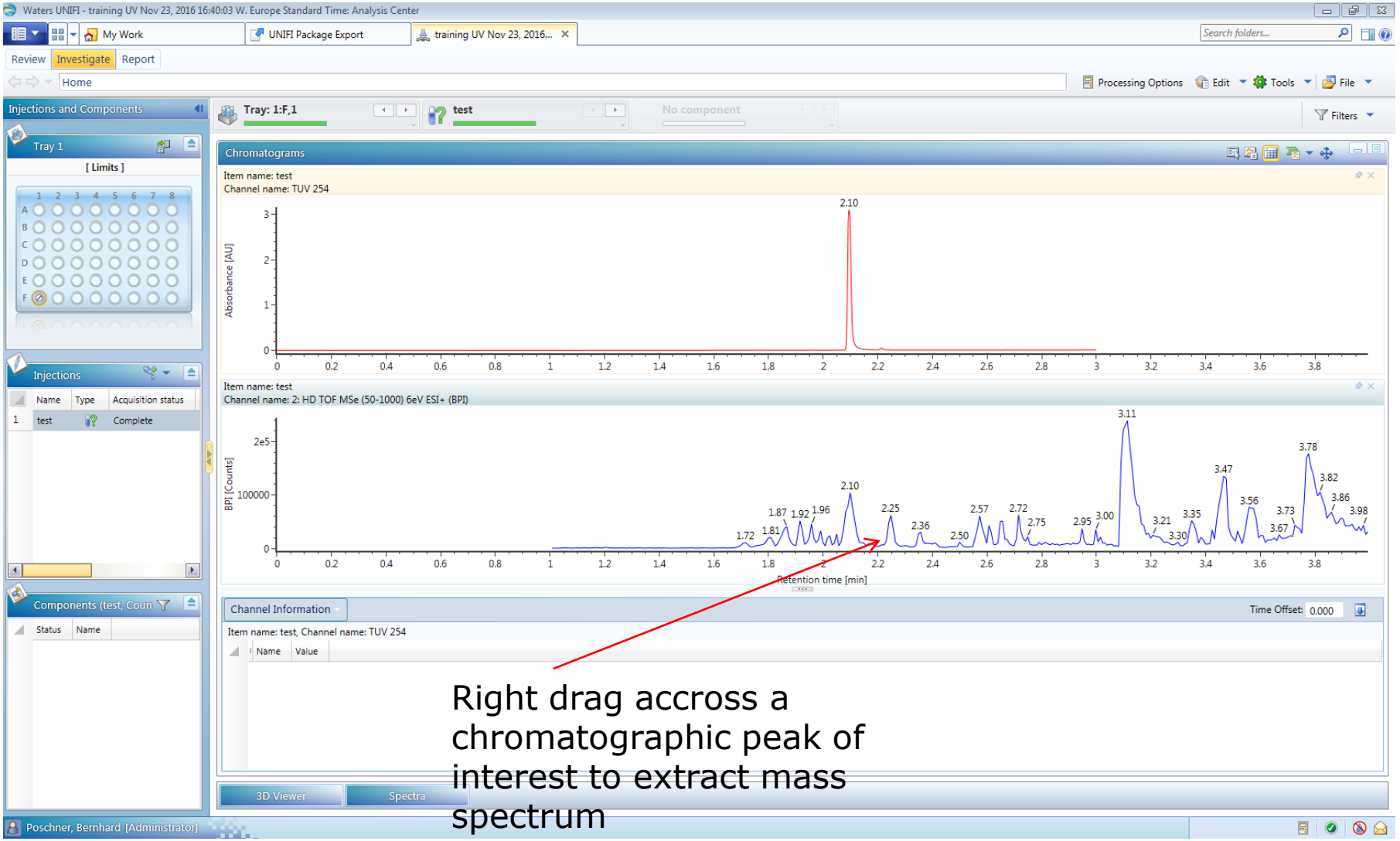
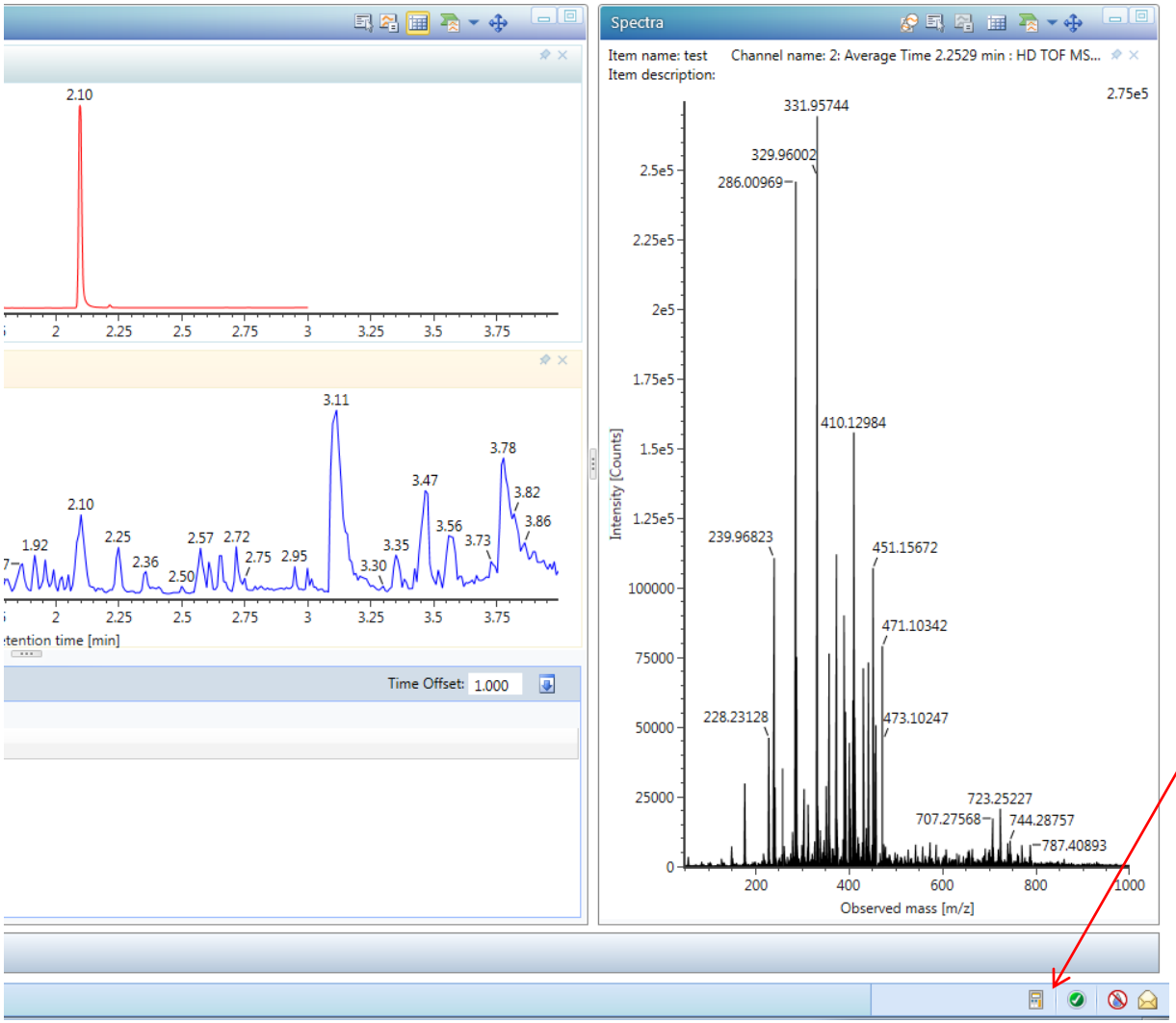


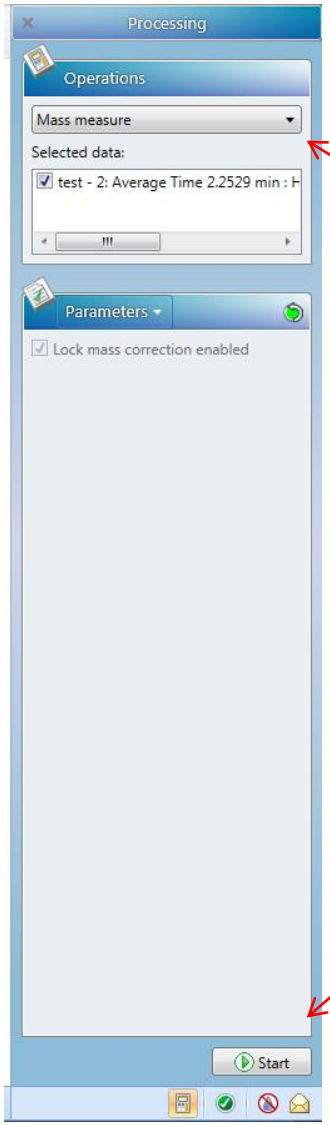
Right drag accross a chromatographic peak of interest to extract mass spectrum

Elemental Composition from Investigate



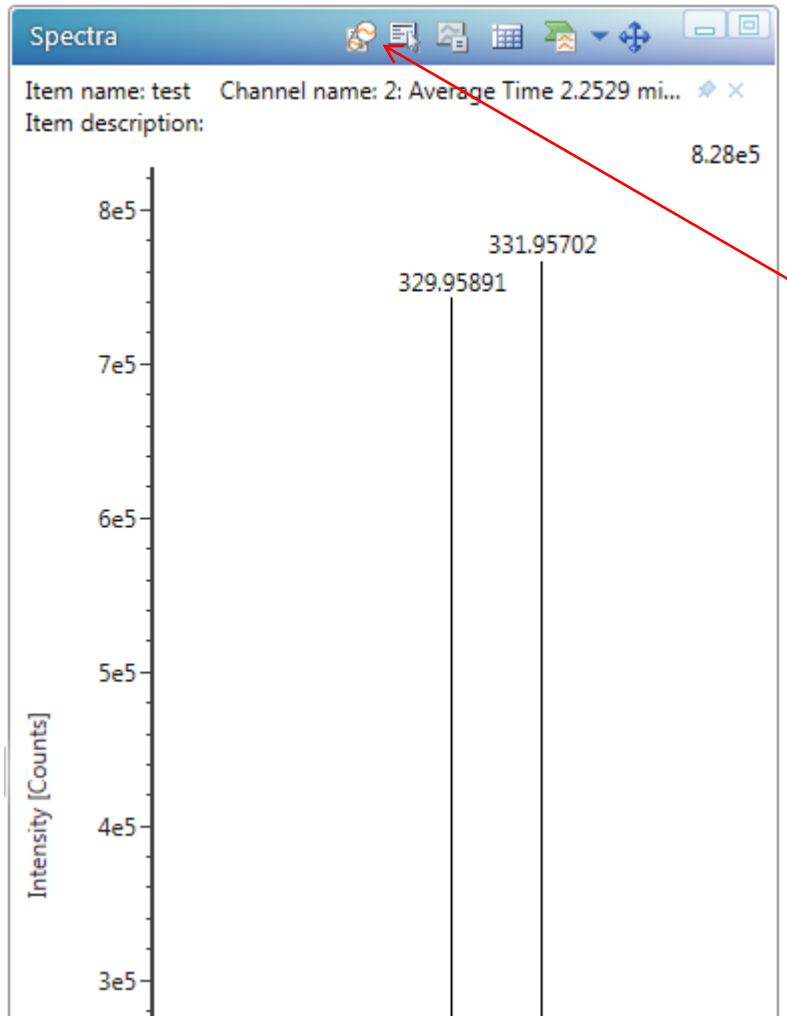
Open „Process Data“

Elemental Composition from Investigate



Select „Mass Measure" from Drop Down and hit „Start". This will center the data.

Elemental Composition from Investigate



Select „Show spectral analysis“ button

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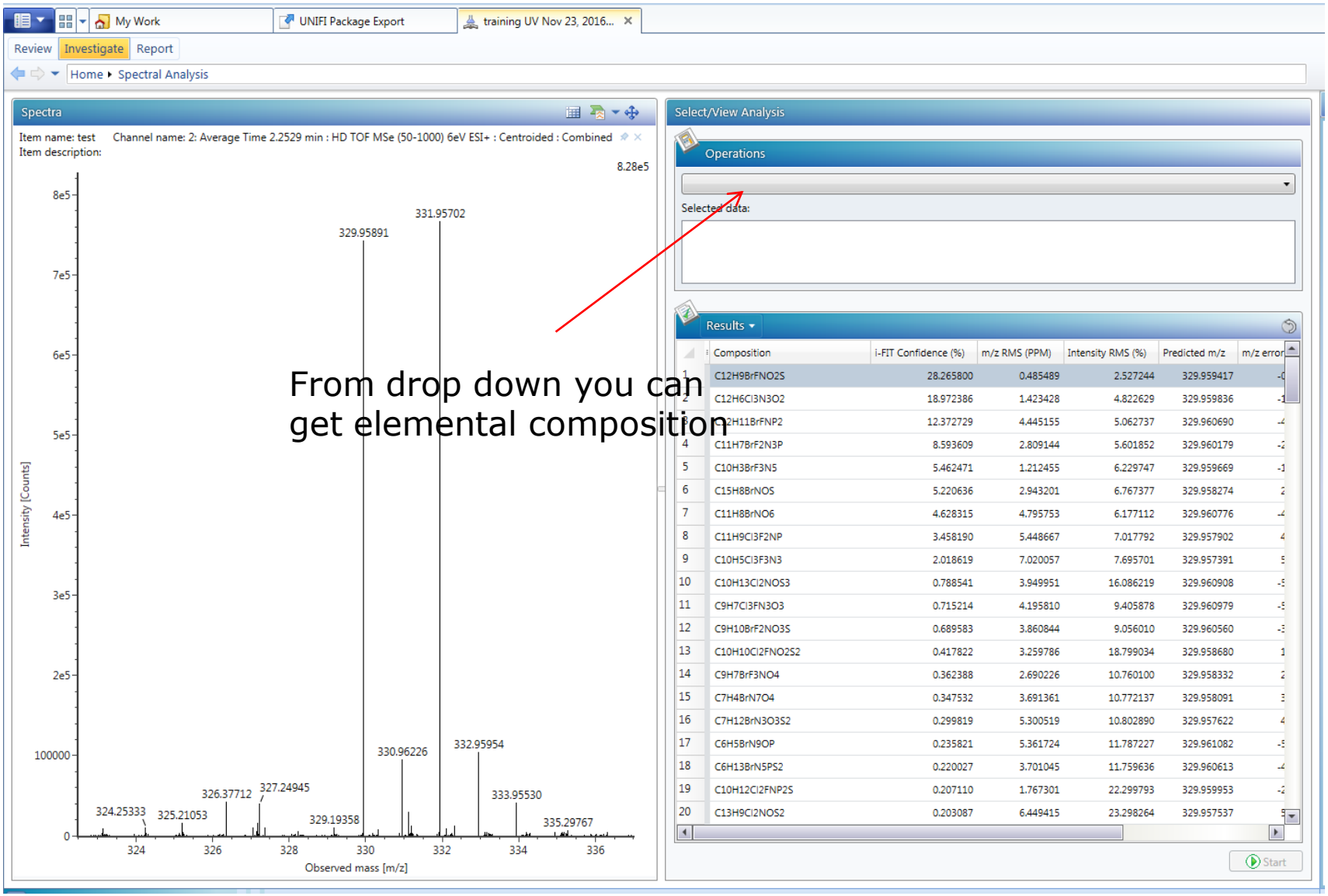

From drop down you can get elemental composition

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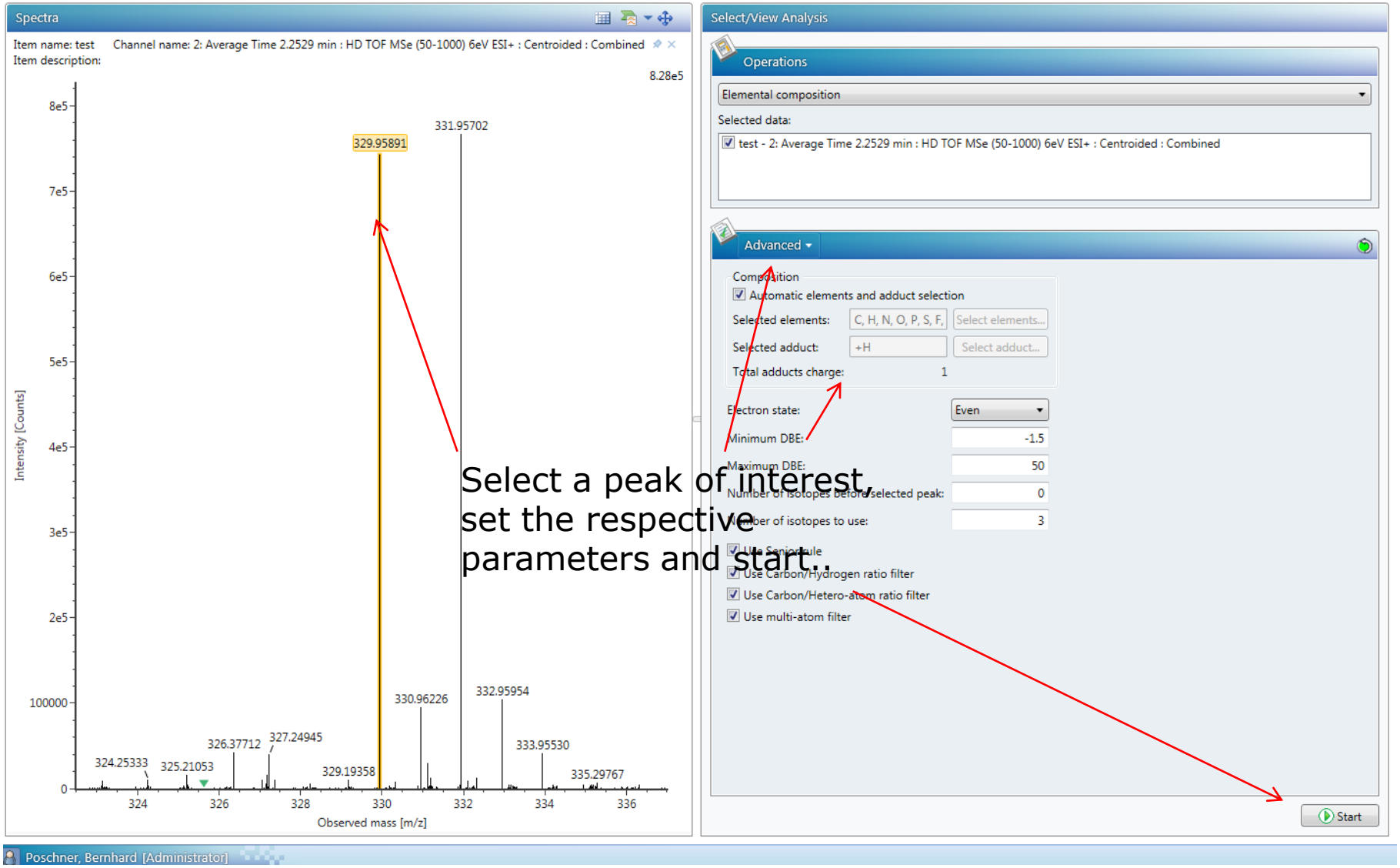

Select a peak of interest, set the respective parameters and start..

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Results

	Composition	i-FIT Confidence (%)	m/z RMS (PPM)	Intensity RMS (%)	Predicted m/z	m/z error (PPM)	m/z error (mDa
1	C9H9BrN5PS	10.369674	5.593200	0.904269	329.957242	5.070970	1.6681
2	C11H8BrNO6	10.079793	5.592455	1.911720	329.960776	-5.673626	-1.8663
3	C10H3BrF3N5	9.710929	2.081564	2.600679	329.959669	-2.307588	-0.7590
4	C11H9Cl3F2NP	8.657239	4.691561	3.169564	329.957902	3.064990	1.0082
5	C10H8BrF4NS	8.467439	6.224048	1.940497	329.956972	5.891004	1.9378
6	C11H7BrF2N3P	8.070964	3.627996	3.104649	329.960179	-3.859192	-1.2694
7	C10H5Cl3F3N3	7.485479	6.256426	3.353595	329.957391	4.616595	1.5186
8	C8H2Cl3N9	6.992738	7.240700	3.355763	329.957151	5.348165	1.7592
9	C12H6BrF2NO3	5.801215	5.291670	3.751791	329.957189	5.232326	1.7211
10	C12H11BrFNP2	5.712658	5.236848	3.919725	329.960690	-5.410796	-1.7798
11	C12H9BrFNO2S	3.975318	1.284036	4.464690	329.959417	-1.540716	-0.5068
12	C9H10BrF2NO3S	2.778192	4.682913	4.506031	329.960560	-5.014948	-1.6496
13	C12H6Cl3N3O2	2.242041	1.969456	6.278371	329.959836	-2.815126	-0.9260
14	C9H7BrF3NO4	1.048893	1.868986	6.276701	329.958332	1.758095	0.5783
15	C7H4BrN7O4	0.999904	2.979098	6.290435	329.958091	2.489665	0.8189
16	C7H12BrN3O3S2	0.652293	4.537529	6.908732	329.957622	3.915214	1.2879
17	C6H13BrN5PS2	0.372045	4.570798	7.858683	329.960613	-5.176304	-1.7027
18	C7H14BrN3OP2S	0.304366	0.799774	8.167526	329.958895	0.045134	0.0148
19	C7H4BrF4N5O	0.286651	5.465825	8.365676	329.960812	-5.781819	-1.9019
20	C5HBrFN11O	0.286612	4.763309	8.379583	329.960571	-5.050249	-1.6612

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