

Vion Unifi 1.8.2

Investigate Mode Elemental Composition

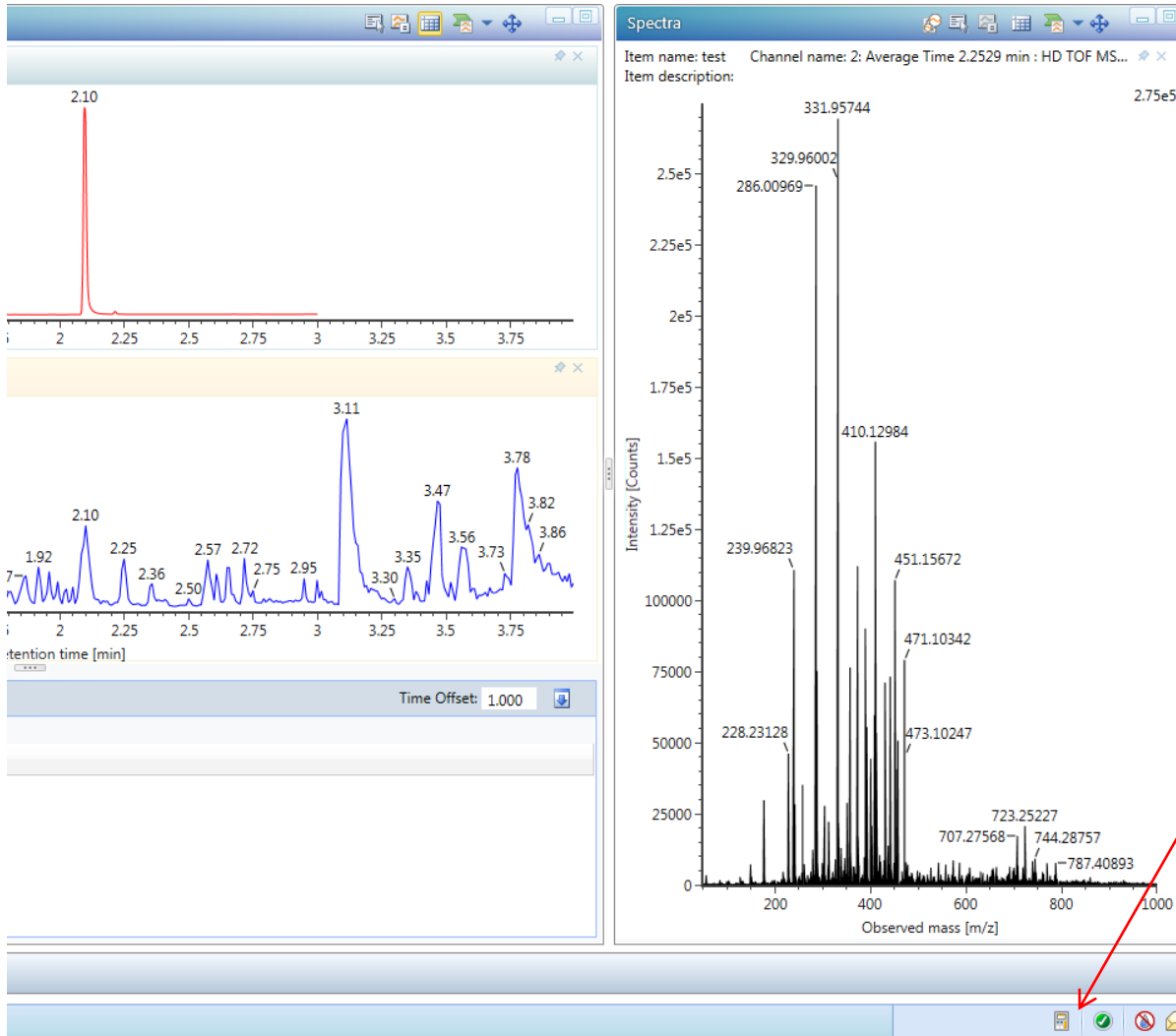
Elemental Composition from Investigate

The screenshot displays the Waters UNIFI software interface. The top navigation bar includes 'Review', 'Investigate', and 'Report' tabs. The main workspace is divided into several panels:

- Injections and Components:** Shows 'Tray 1' with a grid of injection points (A-F, 1-8) and an 'Injections' table with one entry: 'test' (Type: ?, Acquisition status: Complete).
- Chromatograms:** Two plots are shown. The top plot, 'Item name: test, Channel name: TUV 254', shows a single sharp peak at 2.10 minutes. The bottom plot, 'Item name: test, Channel name: 2: HD TOF MSe (50-1000) 6eV ESI+ (BPI)', shows a mass spectrum with multiple peaks labeled with retention times: 1.72, 1.81, 1.87, 1.92, 1.96, 2.10, 2.25, 2.36, 2.50, 2.57, 2.72, 2.75, 2.95, 3.00, 3.11, 3.21, 3.30, 3.35, 3.47, 3.56, 3.67, 3.73, 3.78, 3.82, 3.86, 3.98.
- Channel Information:** A table with columns 'Name' and 'Value' is visible, currently empty.

A red arrow points from the 2.10 peak in the top chromatogram to the 2.10 peak in the mass spectrum plot. Below the plots, a text box contains the instruction: 'Right drag across a chromatographic peak of interest to extract mass spectrum'.

Elemental Composition from Investigate



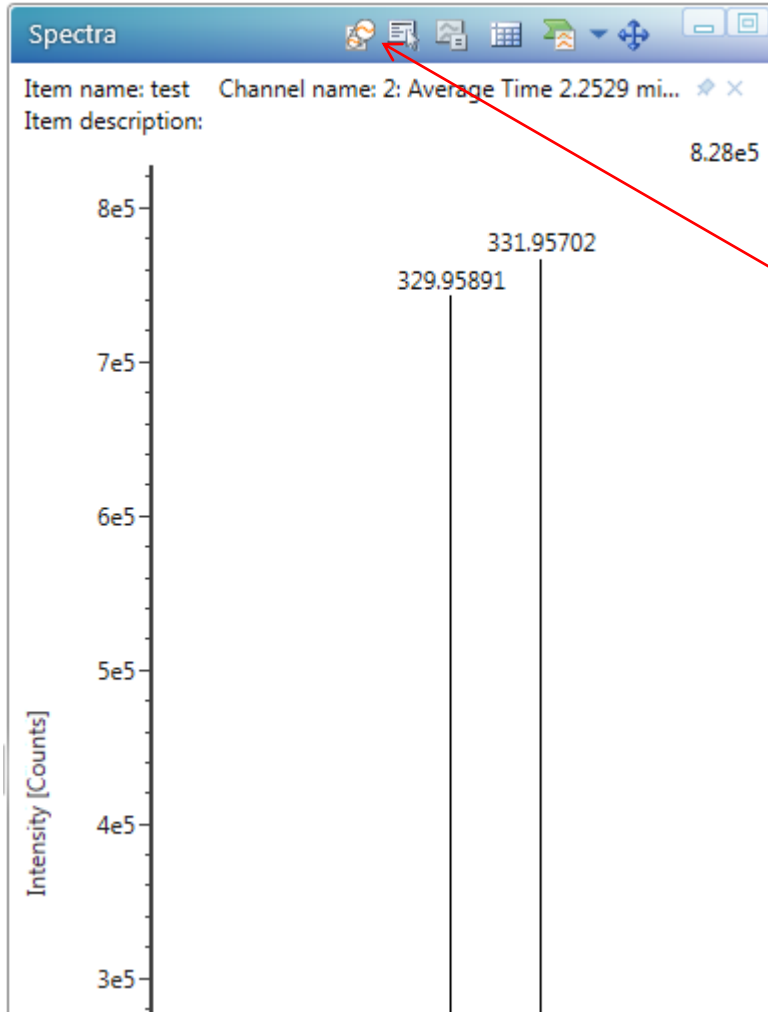
Open „Process Data“

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

Elemental Composition from Investigate

The screenshot displays the Waters Investigate software interface. On the left, a mass spectrum plot shows Intensity [Counts] on the y-axis (0 to 8e5) and Observed mass [m/z] on the x-axis (324 to 336). The base peak is at m/z 331.95702. Other significant peaks are labeled at m/z 329.95891, 330.96226, 332.95954, 333.95530, 324.25333, 325.21053, 326.37712, 327.24945, 329.19358, and 335.29767. The plot title is 'Spectra' and the item name is 'test'. Channel name: 2: Average Time 2.2529 min : HD TOF MSe (50-1000) 6eV ESI+ : Centroided : Combined. Item description: 8.28e5.

On the right, the 'Select/View Analysis' panel is open. The 'Operations' section has a dropdown menu with a red arrow pointing to it. Below it is a 'Selected data' field. The 'Results' section contains a table of elemental composition results.

	Composition	i-FIT Confidence (%)	m/z RMS (PPM)	Intensity RMS (%)	Predicted m/z	m/z error
1	C12H9BrFNO2S	28.265800	0.485489	2.527244	329.959417	-0.000000
2	C12H6Cl3N3O2	18.972386	1.423428	4.822629	329.959836	-0.000000
3	C12H11BrFNP2	12.372729	4.445155	5.062737	329.960690	-0.000000
4	C11H7BrF2N3P	8.593609	2.809144	5.601852	329.960179	-0.000000
5	C10H3BrF3N5	5.462471	1.212455	6.229747	329.959669	-0.000000
6	C15H8BrNOS	5.220636	2.943201	6.767377	329.958274	0.000000
7	C11H8BrNO6	4.628315	4.795753	6.177112	329.960776	-0.000000
8	C11H9Cl3F2NP	3.458190	5.448667	7.017792	329.957902	0.000000
9	C10H5Cl3F3N3	2.018619	7.020057	7.695701	329.957391	0.000000
10	C10H13Cl2NOS3	0.788541	3.949951	16.086219	329.960908	-0.000000
11	C9H7Cl3FN3O3	0.715214	4.195810	9.405878	329.960979	-0.000000
12	C9H10BrF2NO3S	0.689583	3.860844	9.056010	329.960560	-0.000000
13	C10H10Cl2FNO2S2	0.417822	3.259786	18.799034	329.958680	0.000000
14	C9H7BrF3NO4	0.362388	2.690226	10.760100	329.958332	0.000000
15	C7H4BrN7O4	0.347532	3.691361	10.772137	329.958091	0.000000
16	C7H12BrN3O3S2	0.299819	5.300519	10.802890	329.957622	0.000000
17	C6H5BrN9OP	0.235821	5.361724	11.787227	329.961082	-0.000000
18	C6H13BrN5PS2	0.220027	3.701045	11.759636	329.960613	-0.000000
19	C10H12Cl2FNP2S	0.207110	1.767301	22.299793	329.959953	-0.000000
20	C13H9Cl2NOS2	0.203087	6.449415	23.298264	329.957537	0.000000

From drop down you can get elemental composition

Elemental Composition from Investigate

The screenshot displays the Waters Investigate software interface. On the left, the 'Spectra' panel shows a mass spectrum with intensity in counts on the y-axis (0 to 8e5) and observed mass in m/z on the x-axis (324 to 336). A prominent peak is highlighted at m/z 329.95891. Other labeled peaks include 324.25333, 325.21053, 326.37712, 327.24945, 329.19358, 330.96226, 331.95702, 332.95954, 333.95530, and 335.29767. The 'Select/View Analysis' panel on the right is set to 'Elemental composition' and shows the selected data as 'test - 2: Average Time 2.2529 min : HD TOF MSe (50-1000) 6eV ESI+ : Centroided : Combined'. The 'Advanced' section is expanded, showing the following settings:

- Composition: Automatic elements and adduct selection
- Selected elements: C, H, N, O, P, S, F
- Selected adduct: +H
- Total adducts charge: 1
- Electron state: Even
- Minimum DBE: -1.5
- Maximum DBE: 50
- Number of isotopes before selected peak: 0
- Number of isotopes to use: 3
- Use Senior rule
- Use Carbon/Hydrogen ratio filter
- Use Carbon/Hetero-atom ratio filter
- Use multi-atom filter

A red arrow points from the 'Start' button at the bottom right of the 'Select/View Analysis' panel to the peak at m/z 329.95891 in the mass spectrum. A text overlay in the center reads: 'Select a peak of interest, set the respective parameters and start.' The status bar at the bottom left shows 'Poschner, Bernhard [Administrator]'.

Elemental Composition from Investigate

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	C10H8BrF4N5	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

Waters

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