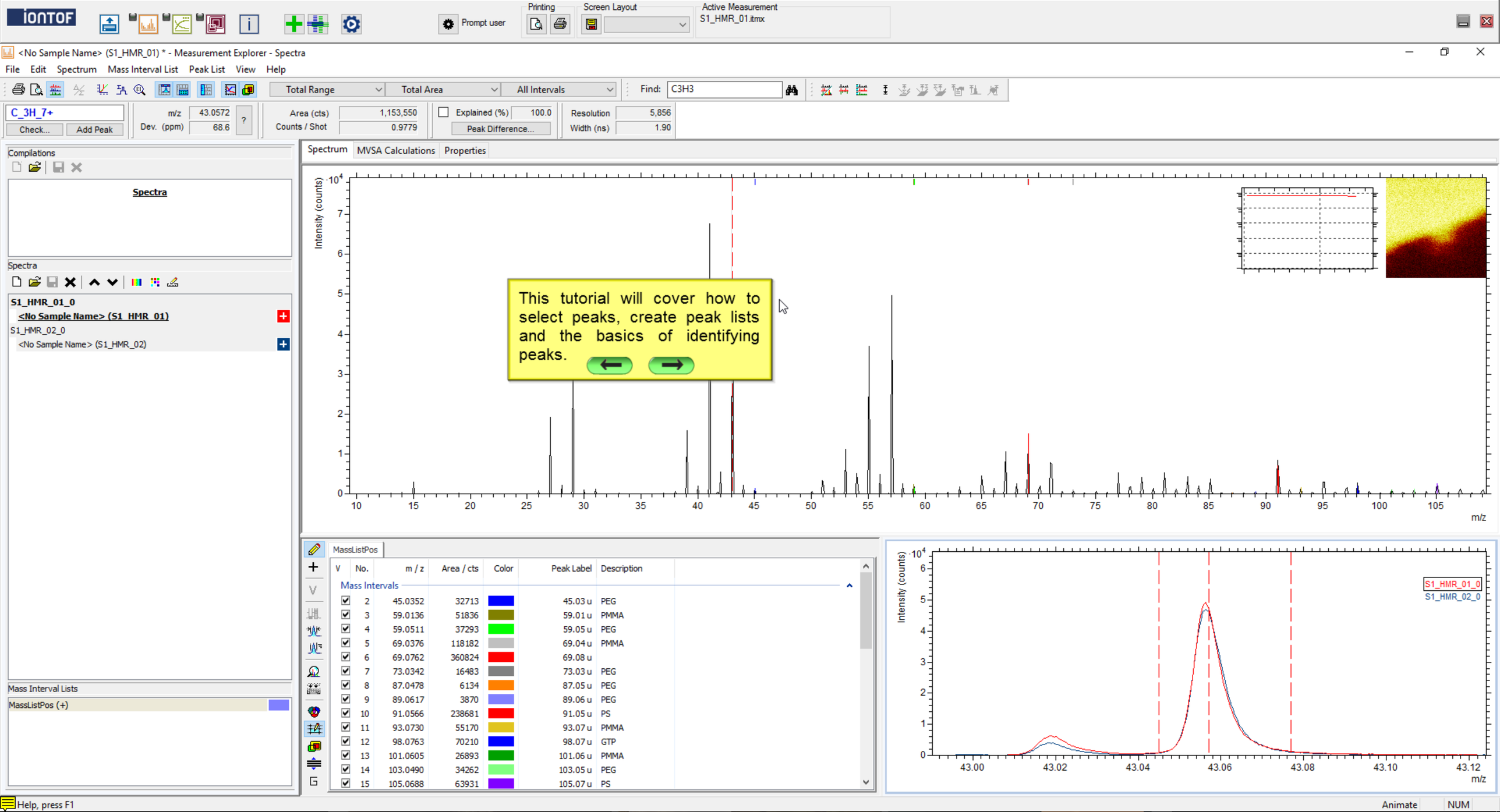
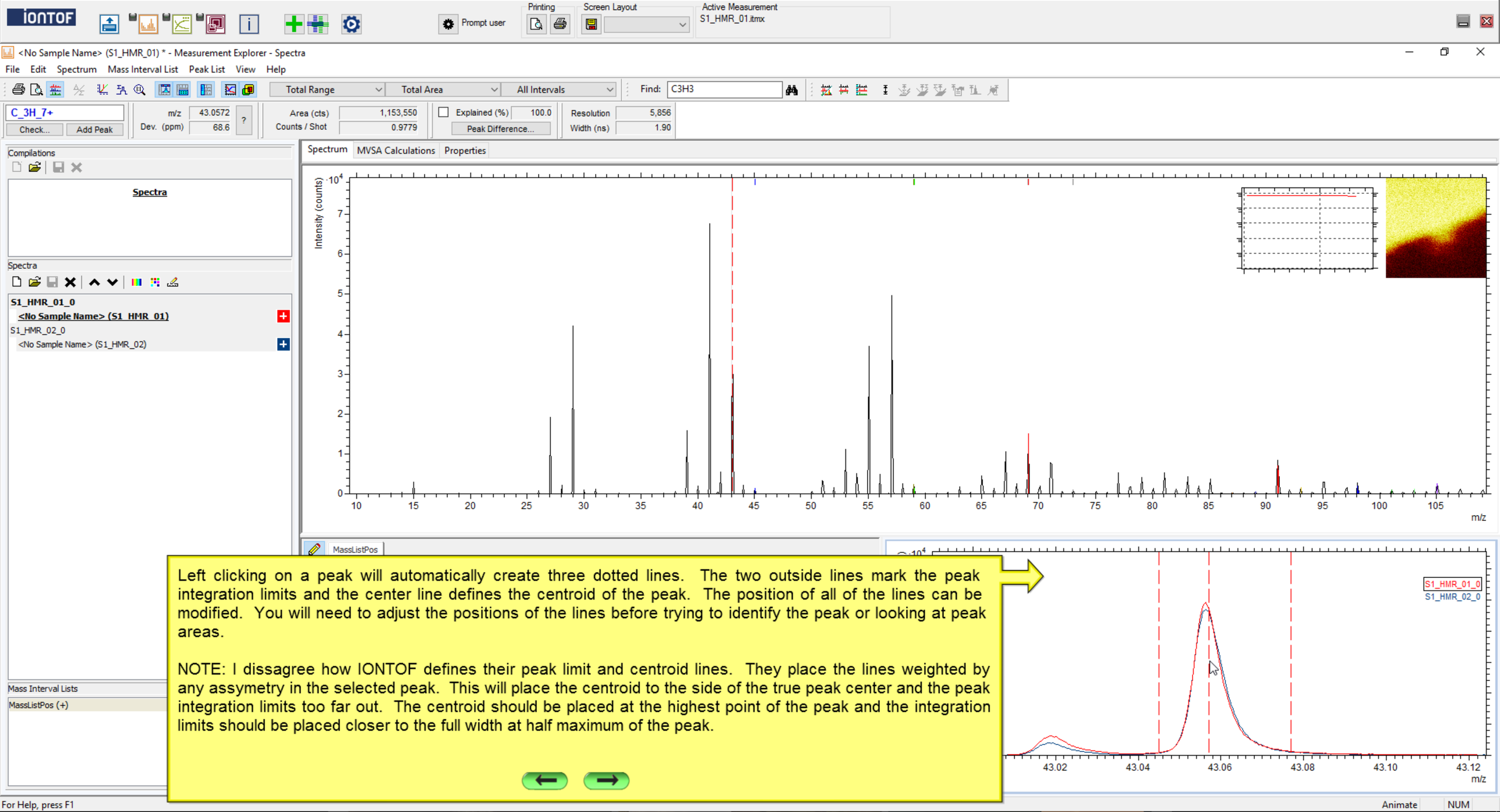
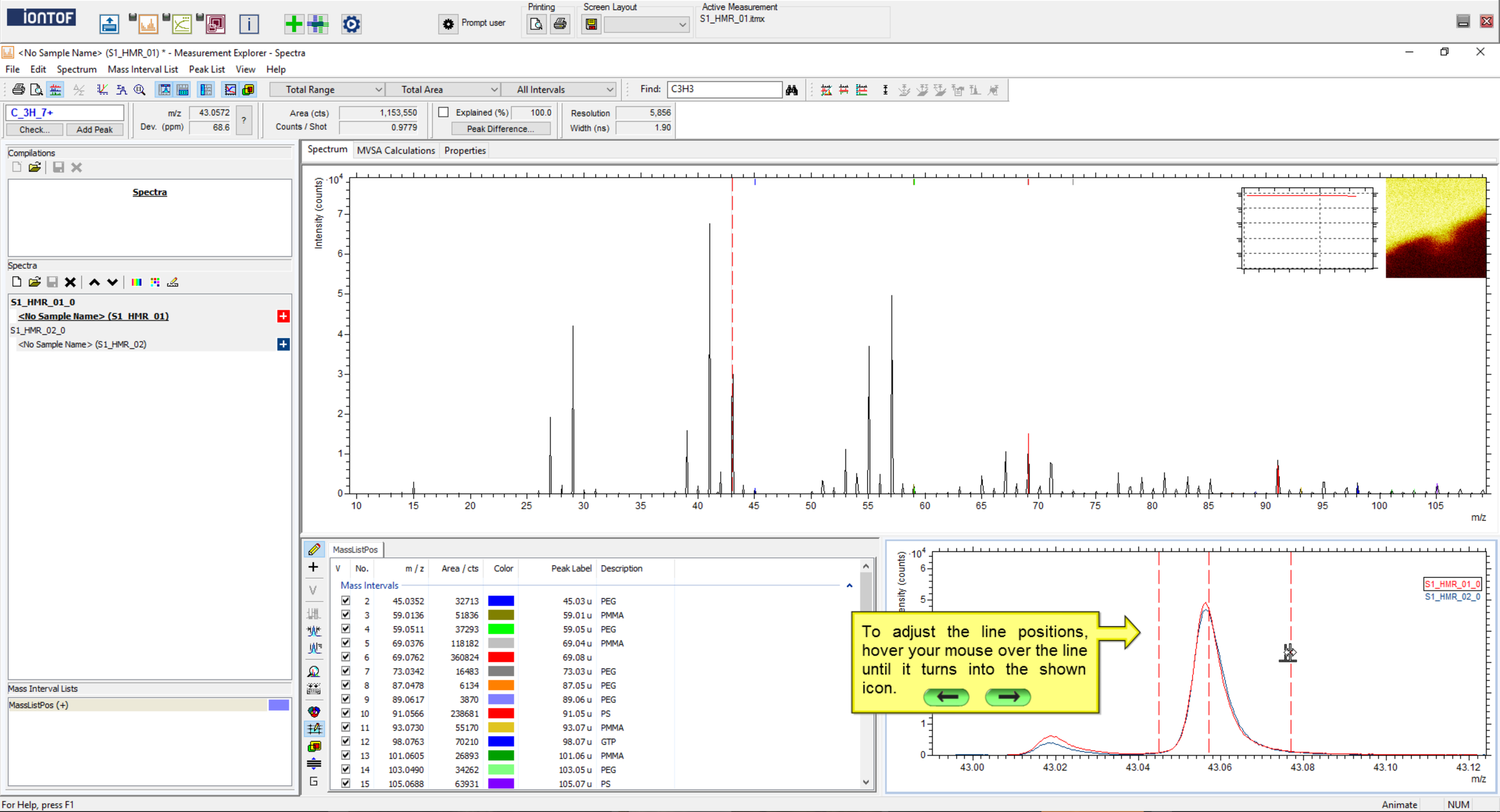
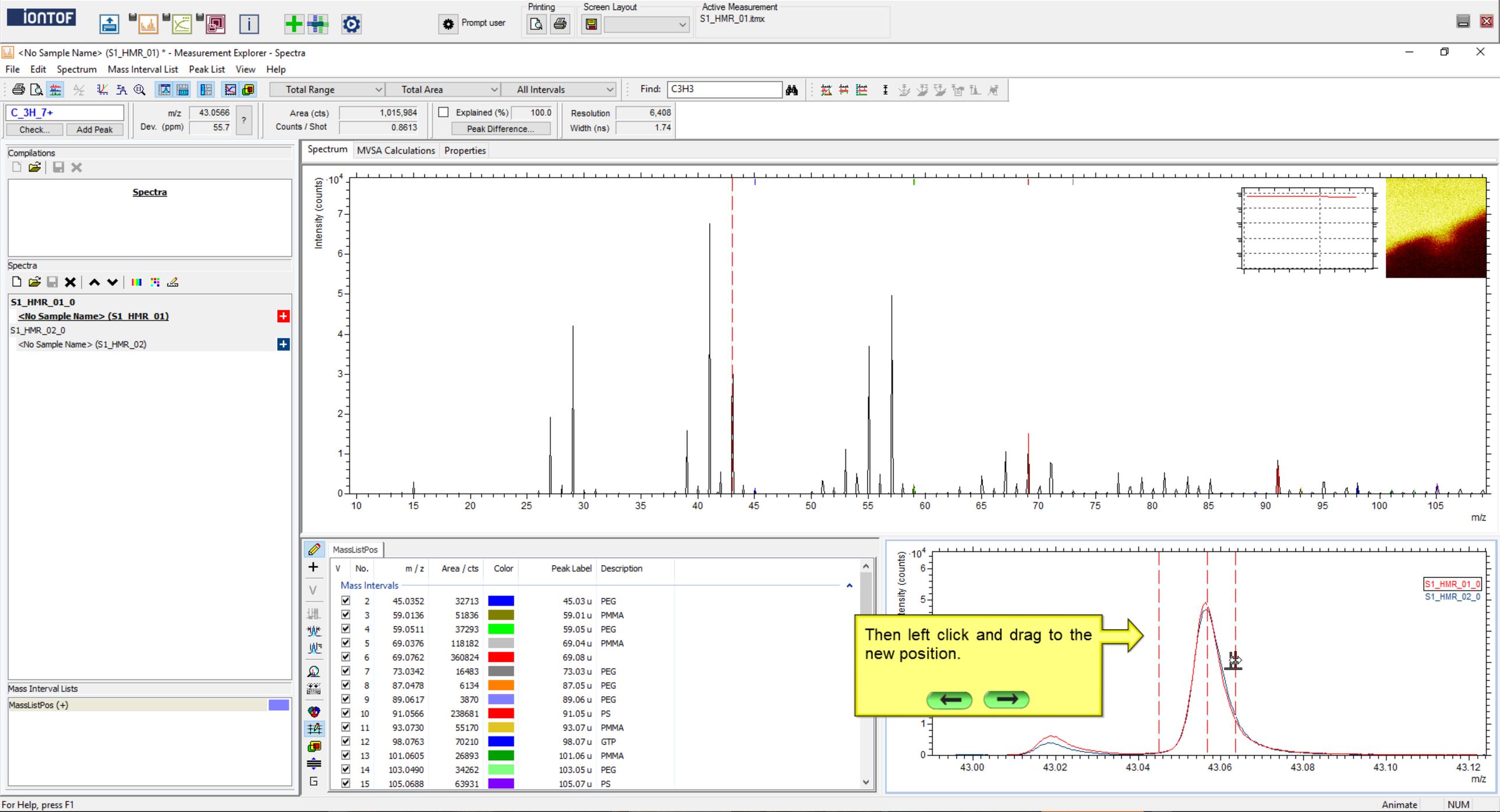
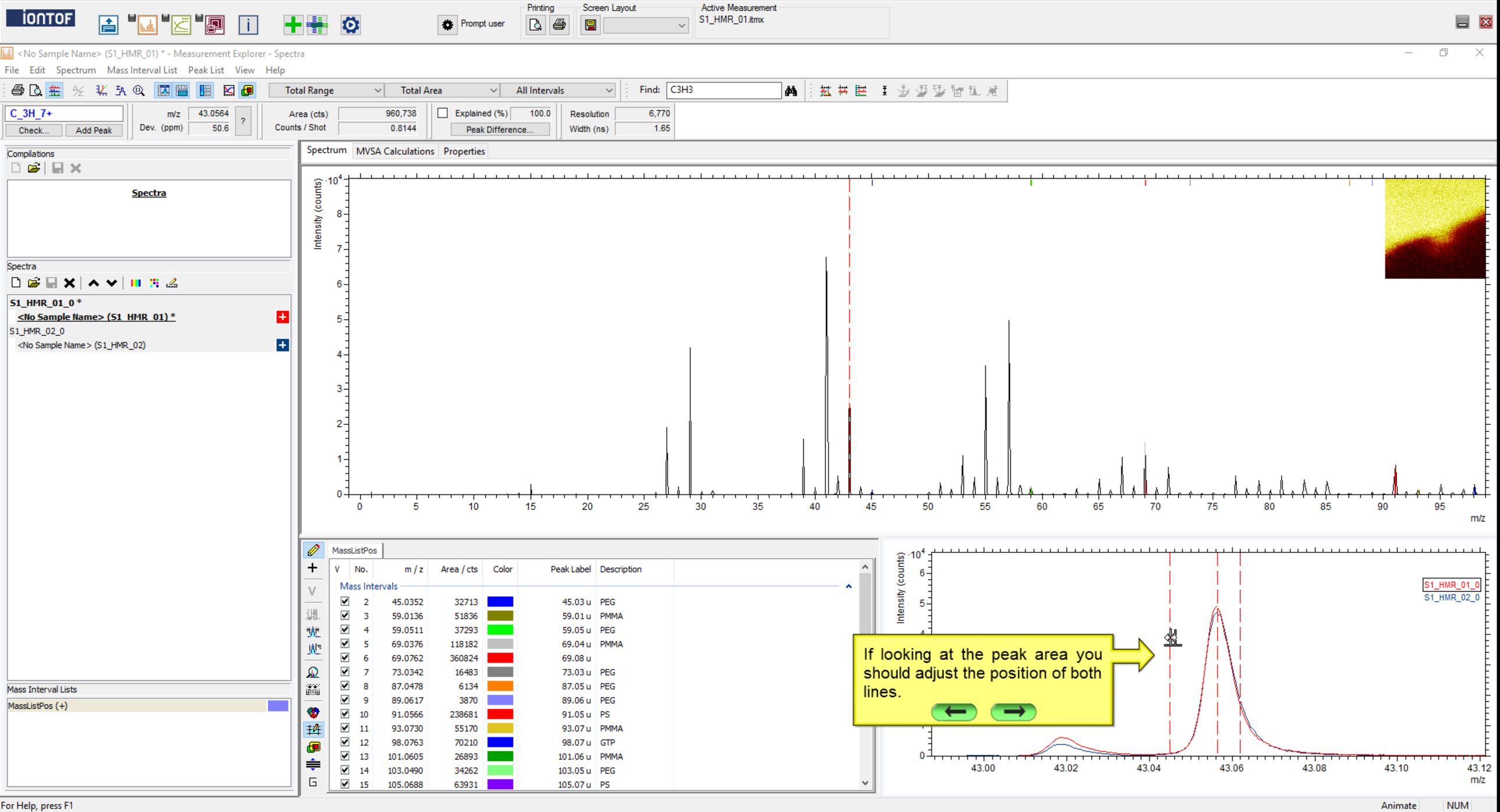
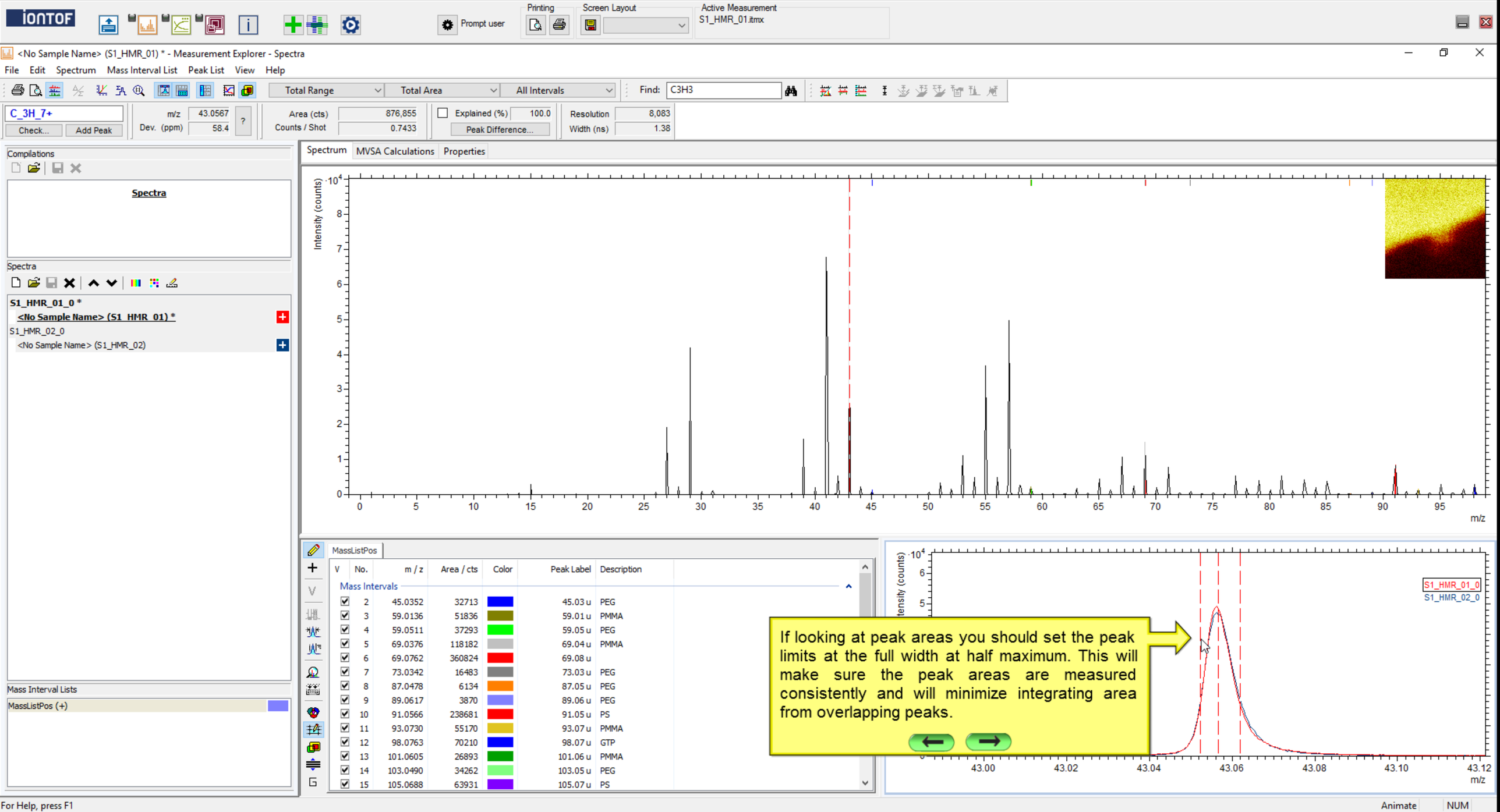

Prompt user
Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
C_3H_7+
Check...
Add Peak
m/z 43.0572
Dev. (ppm) 68.6
Area (cts) 1,153,550
Counts / Shot 0.9779
Explained (%) 100.0
Peak Difference...
Resolution 5,856
Width (ns) 1.90
Compilations
Spectra
Spectra
S1_HMR_01_0
<No Sample Name> (S1_HMR_01)
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
Spectrum
MVSA Calculations
Properties
Intensity (counts)
m/z
This tutorial will cover how to select peaks, create peak lists and the basics of identifying peaks.
MassListPos
V No. m / z Area / cts Color Peak Label Description
Mass Intervals
2 45.0352 32713 45.03 u PEG
3 59.0136 51836 59.01 u PMMA
4 59.0511 37293 59.05 u PEG
5 69.0376 118182 69.04 u PMMA
6 69.0762 360824 69.08 u
7 73.0342 16483 73.03 u PEG
8 87.0478 6134 87.05 u PEG
9 89.0617 3870 89.06 u PEG
10 91.0566 238681 91.05 u PS
11 93.0730 55170 93.07 u PMMA
12 98.0763 70210 98.07 u GTP
13 101.0605 26893 101.06 u PMMA
14 103.0490 34262 103.05 u PEG
15 105.0688 63931 105.07 u PS
S1_HMR_01_0
S1_HMR_02_0
Help, press F1
Animate
NUM

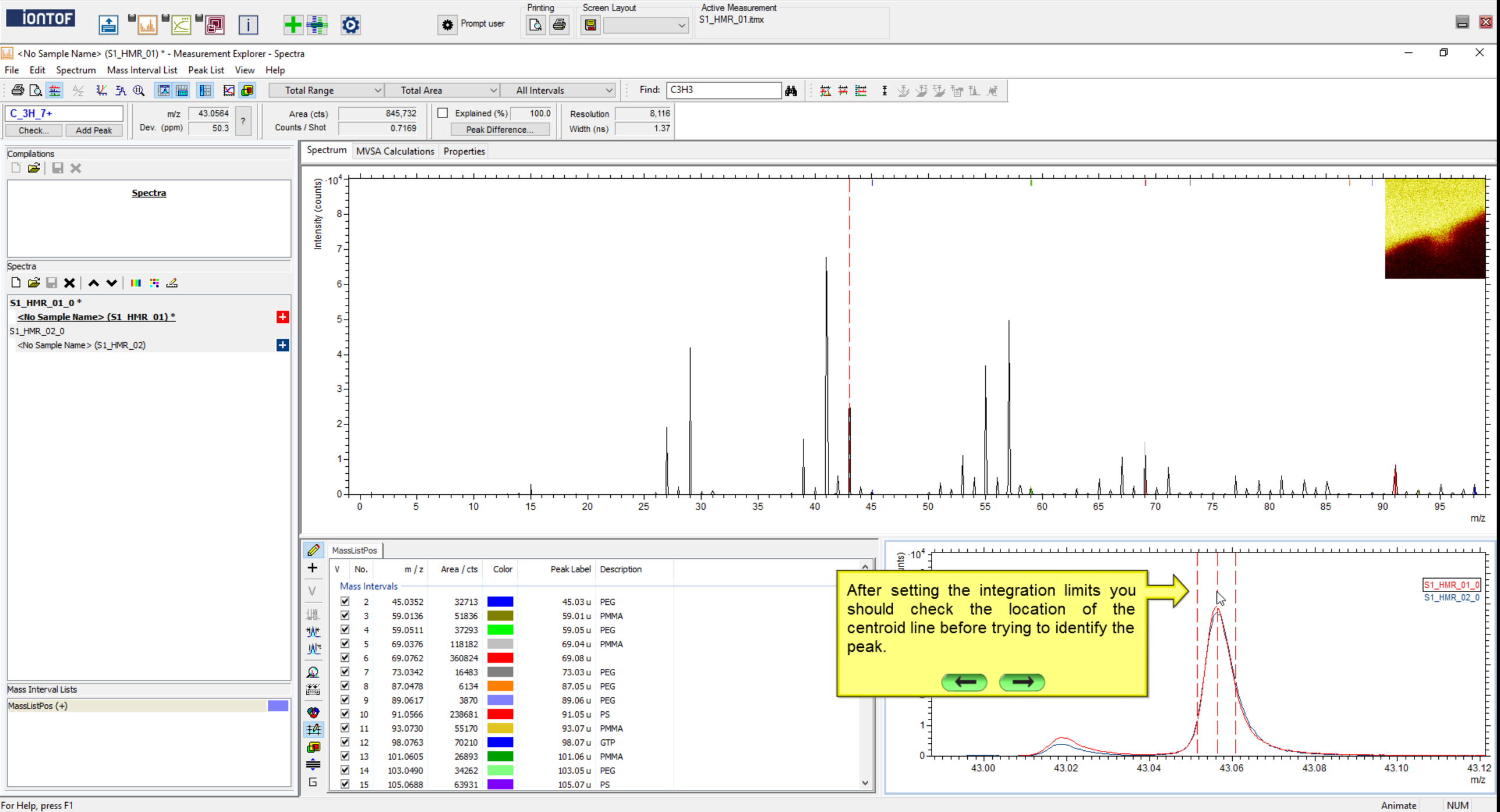

Prompt user
Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
C_3H_7+
Check... Add Peak
m/z 43.0572
Dev. (ppm) 68.6
Area (cts) 1,153,550
Counts / Shot 0.9779
Explained (%) 100.0
Peak Difference...
Resolution 5,856
Width (ns) 1.90
Compilations
Spectra
Spectra
S1_HMR_01_0
<No Sample Name> (S1_HMR_01)
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
Spectrum MVSA Calculations Properties
Intensity (counts)
m/z
MassListPos
S1_HMR_01_0
S1_HMR_02_0
Left clicking on a peak will automatically create three dotted lines. The two outside lines mark the peak integration limits and the center line defines the centroid of the peak. The position of all of the lines can be modified. You will need to adjust the positions of the lines before trying to identify the peak or looking at peak areas.
NOTE: I dissagree how IONTOF defines their peak limit and centroid lines. They place the lines weighted by any assymetry in the selected peak. This will place the centroid to the side of the true peak center and the peak integration limits too far out. The centroid should be placed at the highest point of the peak and the integration limits should be placed closer to the full width at half maximum of the peak.
For Help, press F1
Animate
NUM

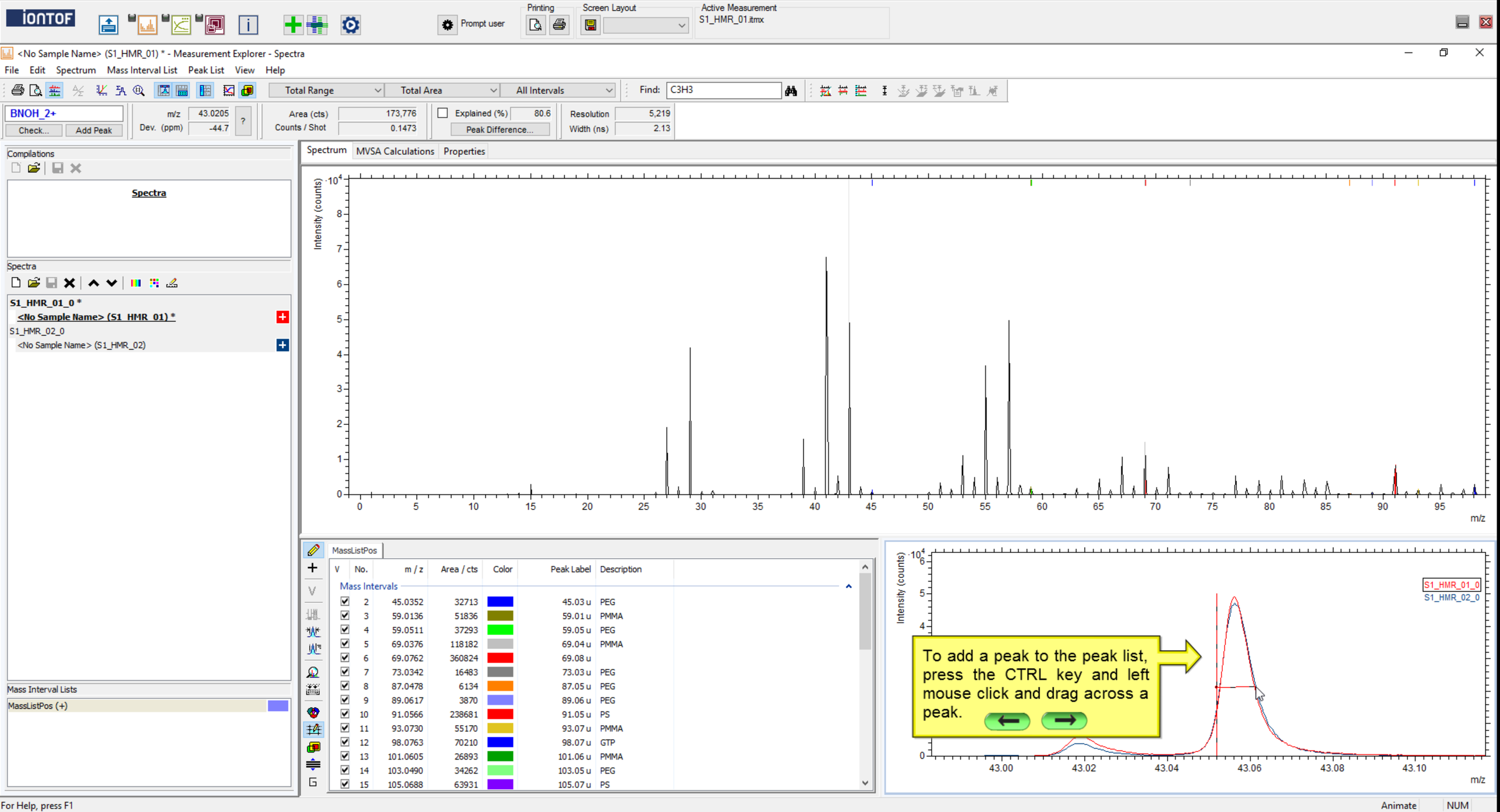

Prompt user
Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
C_3H_7+
Check... Add Peak
m/z 43.0572
Dev. (ppm) 68.6
Area (cts) 1,153,550
Counts / Shot 0.9779
Explained (%) 100.0
Peak Difference...
Resolution 5,856
Width (ns) 1.90
Compilations
Spectra
Spectra
S1_HMR_01_0
<No Sample Name> (S1_HMR_01)
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
Spectrum MVSA Calculations Properties
Intensity (counts)
m/z
MassListPos
V No. m / z Area / cts Color Peak Label Description
Mass Intervals
2 45.0352 32713 45.03 u PEG
3 59.0136 51836 59.01 u PMMA
4 59.0511 37293 59.05 u PEG
5 69.0376 118182 69.04 u PMMA
6 69.0762 360824 69.08 u
7 73.0342 16483 73.03 u PEG
8 87.0478 6134 87.05 u PEG
9 89.0617 3870 89.06 u PEG
10 91.0566 238681 91.05 u PS
11 93.0730 55170 93.07 u PMMA
12 98.0763 70210 98.07 u GTP
13 101.0605 26893 101.06 u PMMA
14 103.0490 34262 103.05 u PEG
15 105.0688 63931 105.07 u PS
To adjust the line positions, hover your mouse over the line until it turns into the shown icon.
S1_HMR_01_0
S1_HMR_02_0
For Help, press F1
Animate
NUM

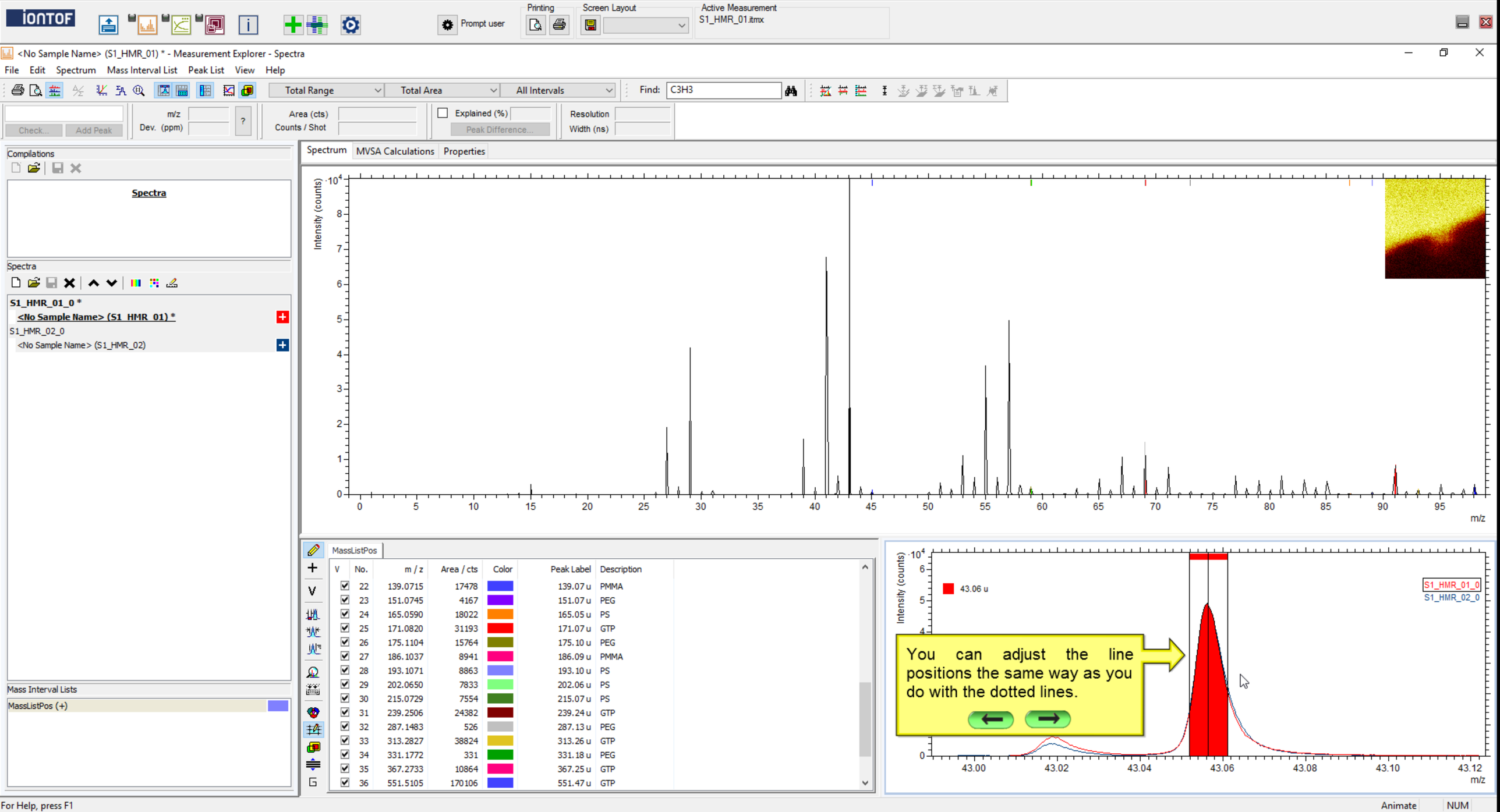

Prompt user
Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
C_3H_7+
Check...
Add Peak
m/z 43.0566
Dev. (ppm) 55.7
Area (cts) 1,015,984
Counts / Shot 0.8613
Explained (%) 100.0
Peak Difference...
Resolution 6,408
Width (ns) 1.74
Compilations
Spectra
Spectra
S1_HMR_01_0
<No Sample Name> (S1_HMR_01)
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
Spectrum
MVSA Calculations
Properties
Intensity (counts)
m/z
MassListPos
V No. m / z Area / cts Color Peak Label Description
Mass Intervals
2 45.0352 32713 45.03 u PEG
3 59.0136 51836 59.01 u PMMA
4 59.0511 37293 59.05 u PEG
5 69.0376 118182 69.04 u PMMA
6 69.0762 360824 69.08 u
7 73.0342 16483 73.03 u PEG
8 87.0478 6134 87.05 u PEG
9 89.0617 3870 89.06 u PEG
10 91.0566 238681 91.05 u PS
11 93.0730 55170 93.07 u PMMA
12 98.0763 70210 98.07 u GTP
13 101.0605 26893 101.06 u PMMA
14 103.0490 34262 103.05 u PEG
15 105.0688 63931 105.07 u PS
Then left click and drag to the new position.
S1_HMR_01_0
S1_HMR_02_0
For Help, press F1
Animate
NUM

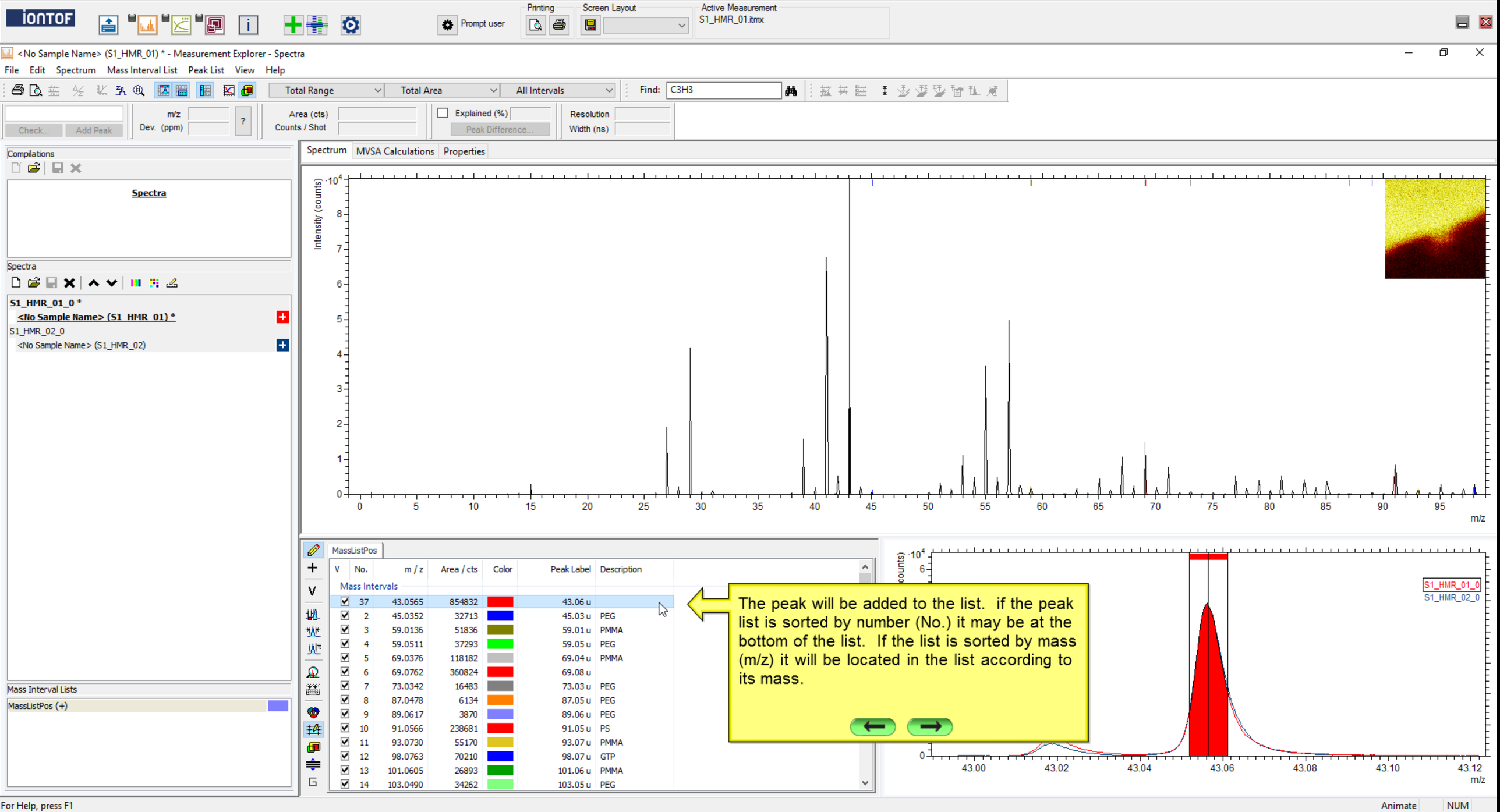

Prompt user
Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
C_3H_7+
Check...
Add Peak
m/z 43.0564
Dev. (ppm) 50.6
Area (cts) 960,738
Counts / Shot 0.8144
Explained (%) 100.0
Peak Difference...
Resolution 6,770
Width (ns) 1.65
Compilations
Spectra
Spectra
S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
Spectrum
MVSA Calculations
Properties
Intensity (counts)
m/z
MassListPos
V No. m / z Area / cts Color Peak Label Description
Mass Intervals
2 45.0352 32713 45.03 u PEG
3 59.0136 51836 59.01 u PMMA
4 59.0511 37293 59.05 u PEG
5 69.0376 118182 69.04 u PMMA
6 69.0762 360824 69.08 u
7 73.0342 16483 73.03 u PEG
8 87.0478 6134 87.05 u PEG
9 89.0617 3870 89.06 u PEG
10 91.0566 238681 91.05 u PS
11 93.0730 55170 93.07 u PMMA
12 98.0763 70210 98.07 u GTP
13 101.0605 26893 101.06 u PMMA
14 103.0490 34262 103.05 u PEG
15 105.0688 63931 105.07 u PS
If looking at the peak area you should adjust the position of both lines.
S1_HMR_01_0
S1_HMR_02_0
For Help, press F1
Animate
NUM

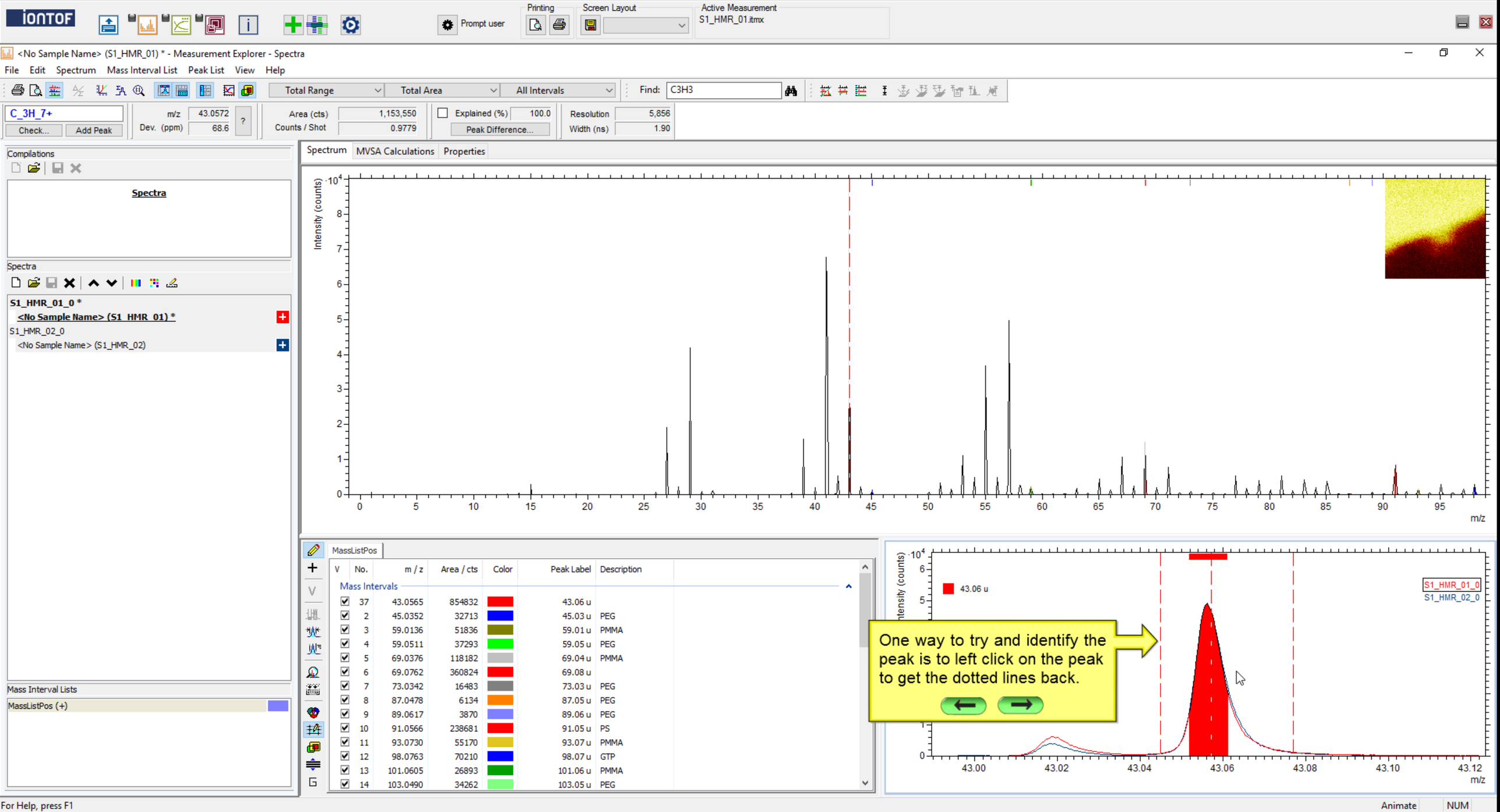

Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
Prompt user
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
C_3H_7+
Check...
Add Peak
m/z 43.0567
Dev. (ppm) 58.4
Area (cts) 876,855
Counts / Shot 0.7433
Explained (%) 100.0
Peak Difference...
Resolution 8,083
Width (ns) 1.38
Compilations
Spectra
Spectra
S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
Spectrum
MVSA Calculations
Properties
Intensity (counts)
m/z
MassListPos
V No. m / z Area / cts Color Peak Label Description
Mass Intervals
2 45.0352 32713 45.03 u PEG
3 59.0136 51836 59.01 u PMMA
4 59.0511 37293 59.05 u PEG
5 69.0376 118182 69.04 u PMMA
6 69.0762 360824 69.08 u
7 73.0342 16483 73.03 u PEG
8 87.0478 6134 87.05 u PEG
9 89.0617 3870 89.06 u PEG
10 91.0566 238681 91.05 u PS
11 93.0730 55170 93.07 u PMMA
12 98.0763 70210 98.07 u GTP
13 101.0605 26893 101.06 u PMMA
14 103.0490 34262 103.05 u PEG
15 105.0688 63931 105.07 u PS
If looking at peak areas you should set the peak limits at the full width at half maximum. This will make sure the peak areas are measured consistently and will minimize integrating area from overlapping peaks.
S1_HMR_01_0
S1_HMR_02_0
For Help, press F1
Animate
NUM

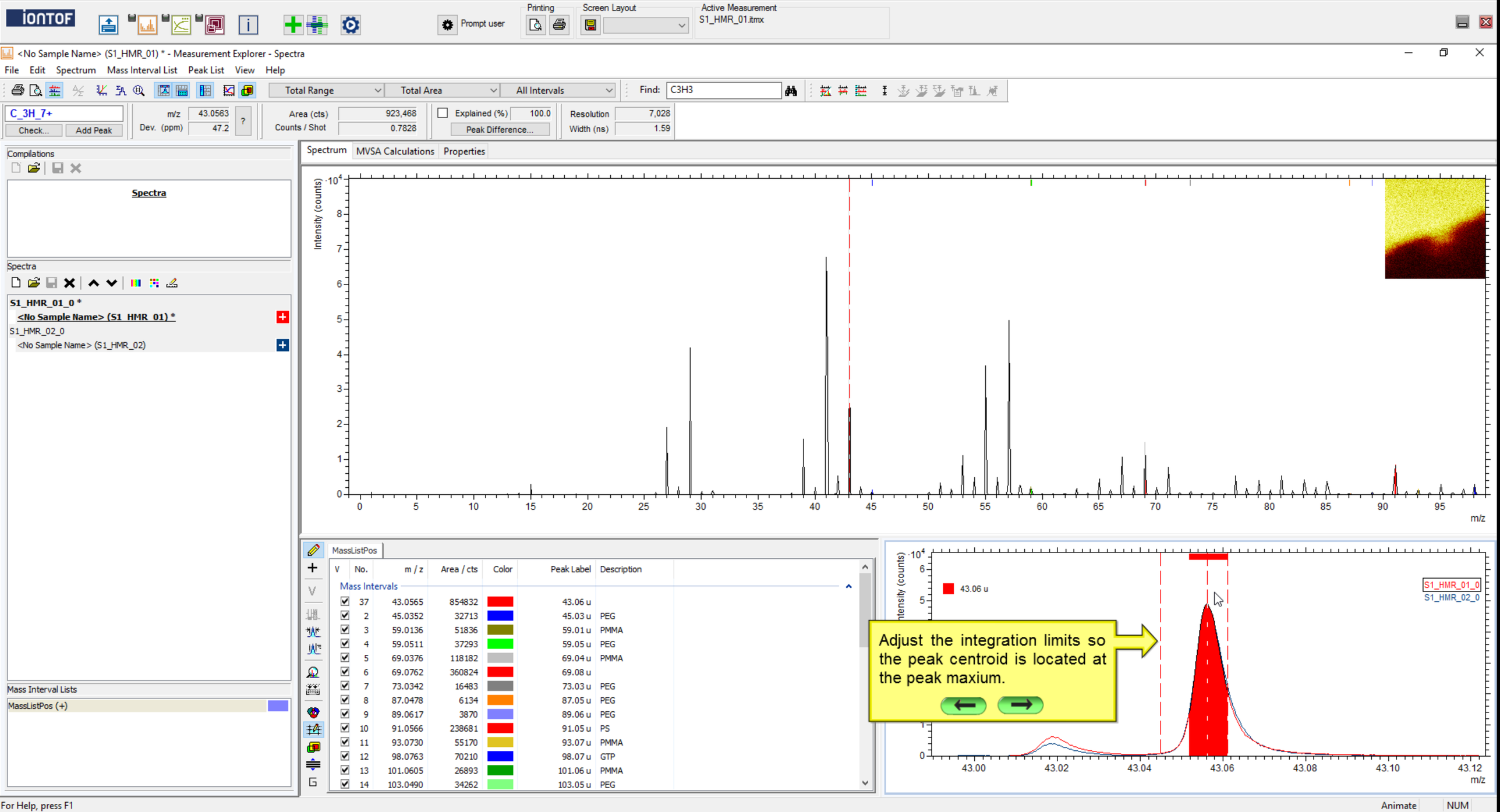

Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
Prompt user
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
C_3H_7+
Check...
Add Peak
m/z 43.0564
Dev. (ppm) 50.3
Area (cts) 845,732
Counts / Shot 0.7169
Explained (%) 100.0
Peak Difference...
Resolution 8,116
Width (ns) 1.37
Compilations
Spectra
Spectra
S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
Spectrum
MVSA Calculations
Properties
Intensity (counts)
m/z
MassListPos
V No. m / z Area / cts Color Peak Label Description
Mass Intervals
2 45.0352 32713 45.03 u PEG
3 59.0136 51836 59.01 u PMMA
4 59.0511 37293 59.05 u PEG
5 69.0376 118182 69.04 u PMMA
6 69.0762 360824 69.08 u
7 73.0342 16483 73.03 u PEG
8 87.0478 6134 87.05 u PEG
9 89.0617 3870 89.06 u PEG
10 91.0566 238681 91.05 u PS
11 93.0730 55170 93.07 u PMMA
12 98.0763 70210 98.07 u GTP
13 101.0605 26893 101.06 u PMMA
14 103.0490 34262 103.05 u PEG
15 105.0688 63931 105.07 u PS
After setting the integration limits you should check the location of the centroid line before trying to identify the peak.
S1_HMR_01_0
S1_HMR_02_0
For Help, press F1
Animate
NUM

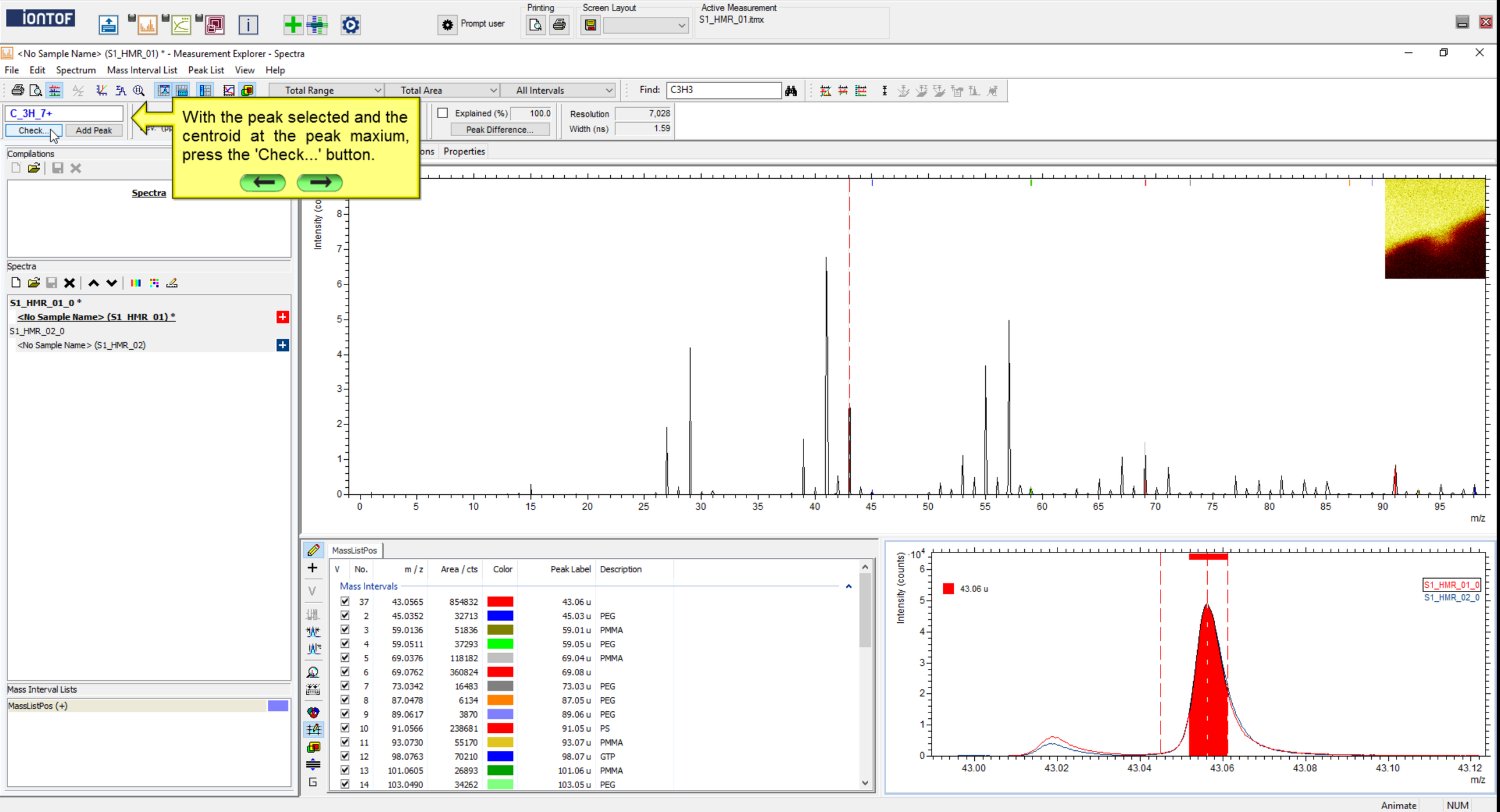

Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
Prompt user
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
BNOH_2+
Check... Add Peak
m/z 43.0205
Dev. (ppm) -44.7
Area (cts) 173,776
Counts / Shot 0.1473
Explained (%) 80.6
Peak Difference...
Resolution 5,219
Width (ns) 2.13
Compilations
Spectra
Spectra
S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
Spectrum MVSA Calculations Properties
Intensity (counts)
m/z
MassListPos
V No. m / z Area / cts Color Peak Label Description
Mass Intervals
2 45.0352 32713 45.03 u PEG
3 59.0136 51836 59.01 u PMMA
4 59.0511 37293 59.05 u PEG
5 69.0376 118182 69.04 u PMMA
6 69.0762 360824 69.08 u
7 73.0342 16483 73.03 u PEG
8 87.0478 6134 87.05 u PEG
9 89.0617 3870 89.06 u PEG
10 91.0566 238681 91.05 u PS
11 93.0730 55170 93.07 u PMMA
12 98.0763 70210 98.07 u GTP
13 101.0605 26893 101.06 u PMMA
14 103.0490 34262 103.05 u PEG
15 105.0688 63931 105.07 u PS
S1_HMR_01_0
S1_HMR_02_0
To add a peak to the peak list, press the CTRL key and left mouse click and drag across a peak.
For Help, press F1
Animate
NUM

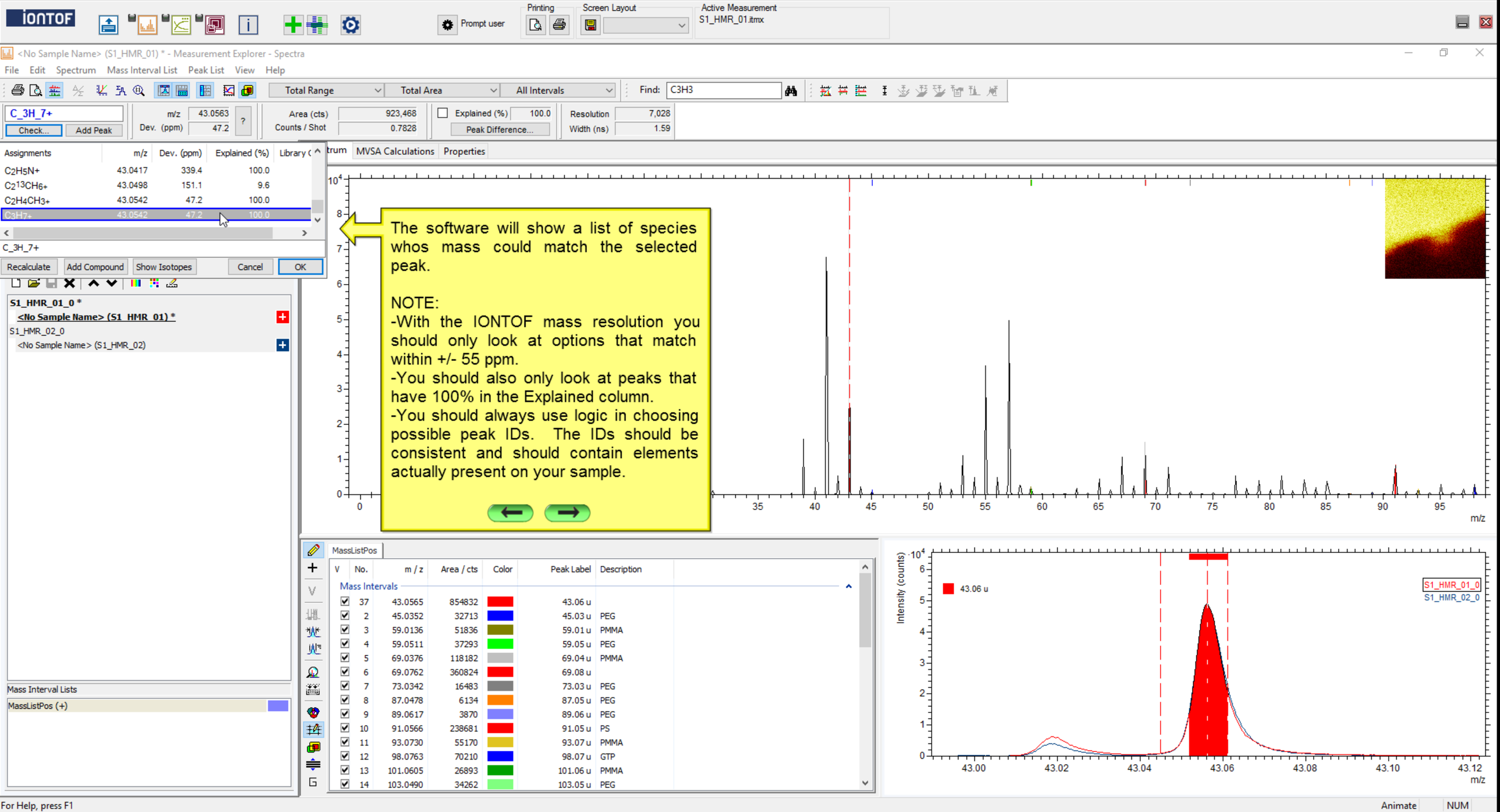

Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
Prompt user
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
Check... Add Peak
m/z
Dev. (ppm)
Area (cts)
Counts / Shot
Explained (%)
Peak Difference...
Resolution
Width (ns)
Compilations
Spectra
Spectra
S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
Spectrum
MVSA Calculations
Properties
Intensity (counts)
m/z
MassListPos
V No. m / z Area / cts Color Peak Label Description
22 139.0715 17478 139.07 u PMMA
23 151.0745 4167 151.07 u PEG
24 165.0590 18022 165.05 u PS
25 171.0820 31193 171.07 u GTP
26 175.1104 15764 175.10 u PEG
27 186.1037 8941 186.09 u PMMA
28 193.1071 8863 193.10 u PS
29 202.0650 7833 202.06 u PS
30 215.0729 7554 215.07 u PS
31 239.2506 24382 239.24 u GTP
32 287.1483 526 287.13 u PEG
33 313.2827 38824 313.26 u GTP
34 331.1772 331 331.18 u PEG
35 367.2733 10864 367.25 u GTP
36 551.5105 170106 551.47 u GTP
43.06 u
S1_HMR_01_0
S1_HMR_02_0
You can adjust the line positions the same way as you do with the dotted lines.
For Help, press F1
Animate
NUM

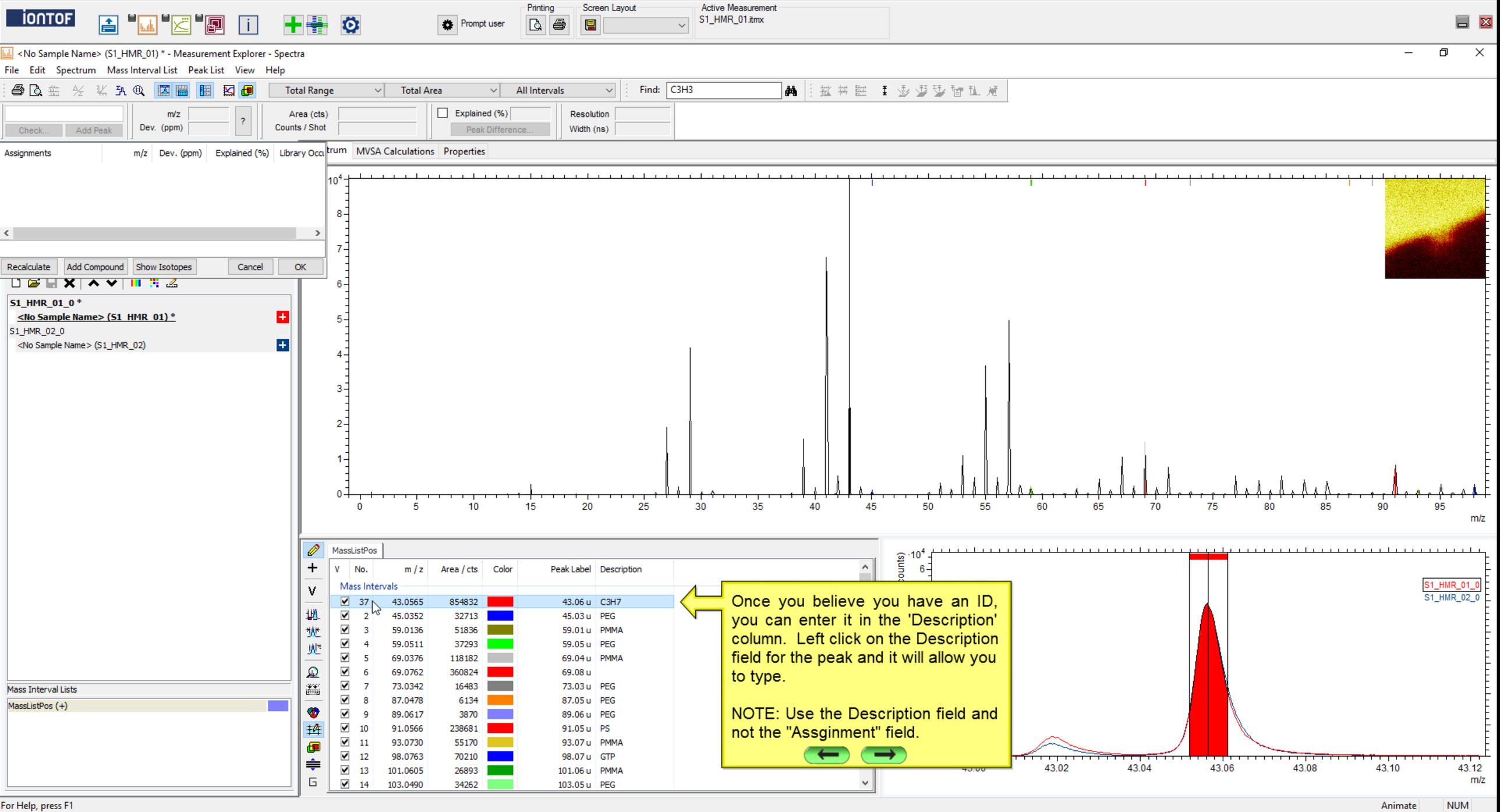

Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
Prompt user
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
m/z
Dev. (ppm)
Area (cts)
Counts / Shot
Explained (%)
Peak Difference...
Resolution
Width (ns)
Check...
Add Peak
Compilations
Spectra
Spectra
S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
Spectrum
MVSA Calculations
Properties
Intensity (counts)
m/z
MassListPos
V No. m / z Area / cts Color Peak Label Description
Mass Intervals
37 43.0565 854832 43.06 u
2 45.0352 32713 45.03 u PEG
3 59.0136 51836 59.01 u PMMA
4 59.0511 37293 59.05 u PEG
5 69.0376 118182 69.04 u PMMA
6 69.0762 360824 69.08 u
7 73.0342 16483 73.03 u PEG
8 87.0478 6134 87.05 u PEG
9 89.0617 3870 89.06 u PEG
10 91.0566 238681 91.05 u PS
11 93.0730 55170 93.07 u PMMA
12 98.0763 70210 98.07 u GTP
13 101.0605 26893 101.06 u PMMA
14 103.0490 34262 103.05 u PEG
The peak will be added to the list. if the peak list is sorted by number (No.) it may be at the bottom of the list. If the list is sorted by mass (m/z) it will be located in the list according to its mass.
S1_HMR_01_0
S1_HMR_02_0
For Help, press F1
Animate
NUM

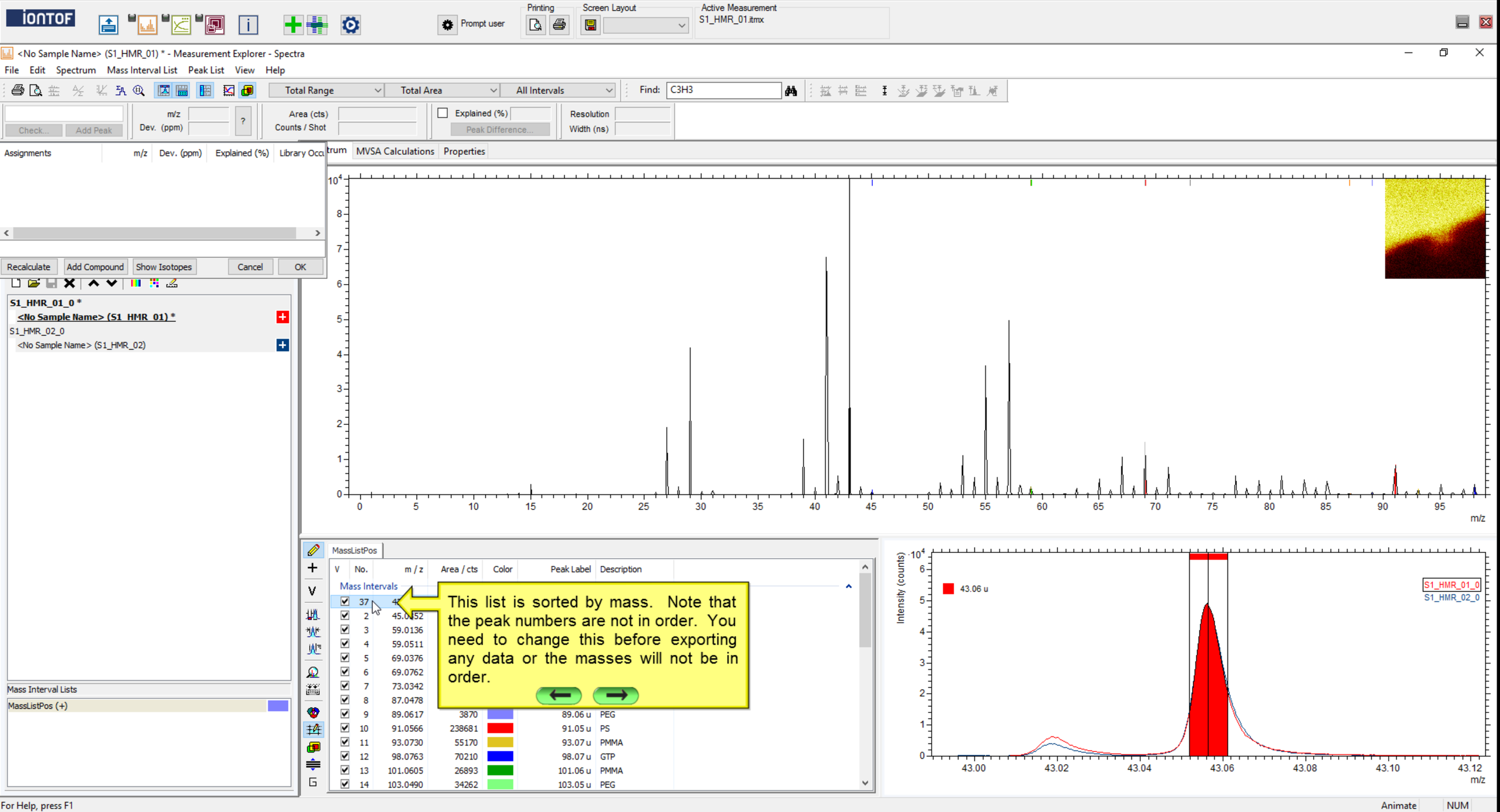

Prompt user
Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
C_3H_7+
Check...
Add Peak
m/z 43.0572
Dev. (ppm) 68.6
Area (cts) 1,153,550
Counts / Shot 0.9779
Explained (%) 100.0
Peak Difference...
Resolution 5,856
Width (ns) 1.90
Compilations
Spectra
Spectra
S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
Spectrum
MVSA Calculations
Properties
Intensity (counts)
m/z
MassListPos
V No. m / z Area / cts Color Peak Label Description
Mass Intervals
37 43.0565 854832 43.06 u
2 45.0352 32713 45.03 u PEG
3 59.0136 51836 59.01 u PMMA
4 59.0511 37293 59.05 u PEG
5 69.0376 118182 69.04 u PMMA
6 69.0762 360824 69.08 u
7 73.0342 16483 73.03 u PEG
8 87.0478 6134 87.05 u PEG
9 89.0617 3870 89.06 u PEG
10 91.0566 238681 91.05 u PS
11 93.0730 55170 93.07 u PMMA
12 98.0763 70210 98.07 u GTP
13 101.0605 26893 101.06 u PMMA
14 103.0490 34262 103.05 u PEG
43.06 u
S1_HMR_01_0
S1_HMR_02_0
One way to try and identify the peak is to left click on the peak to get the dotted lines back.
For Help, press F1
Animate
NUM

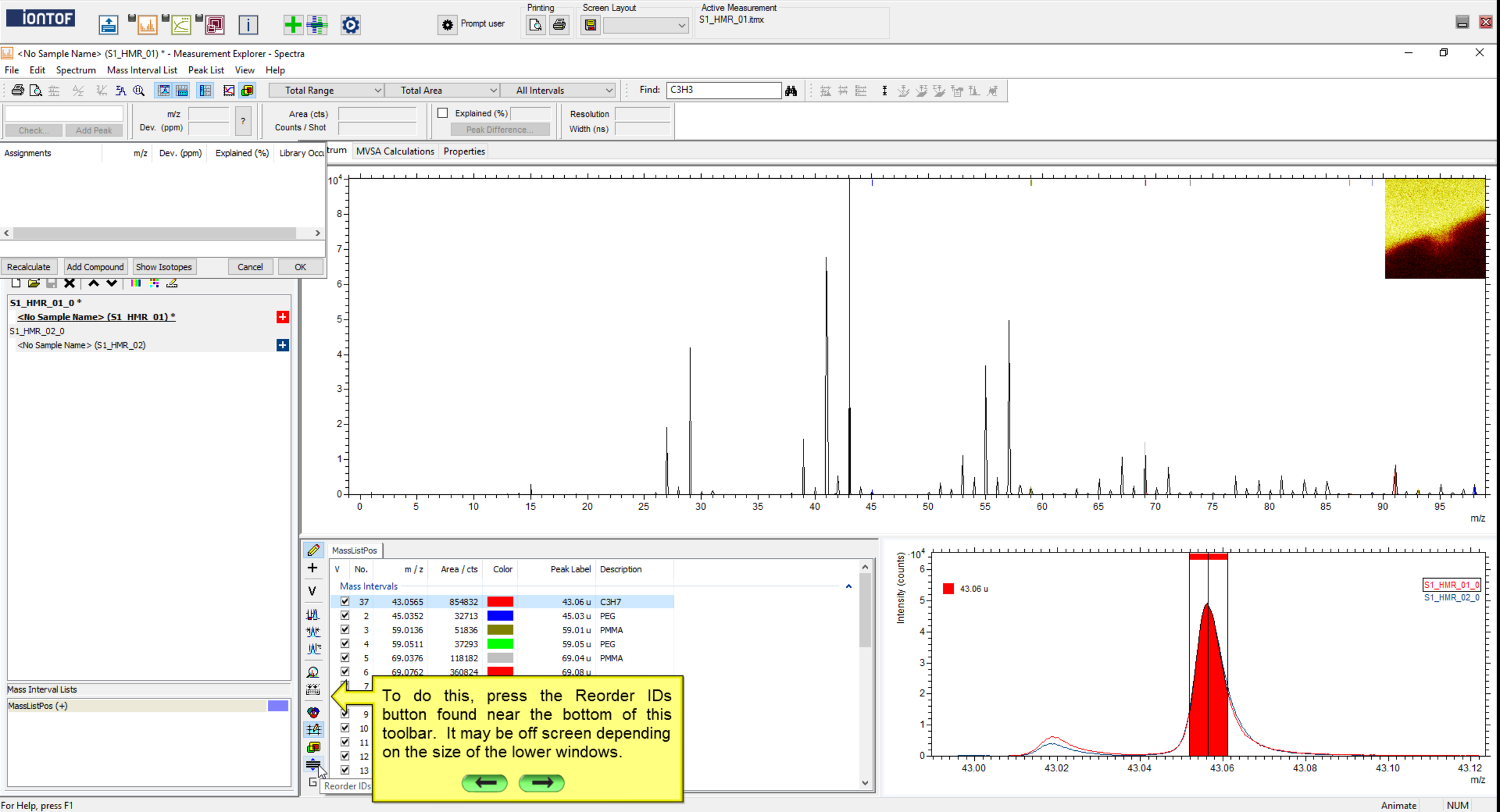

Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
Prompt user
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
C_3H_7+
Check...
Add Peak
m/z 43.0563
Dev. (ppm) 47.2
Area (cts) 923,468
Counts / Shot 0.7828
Explained (%) 100.0
Peak Difference...
Resolution 7,028
Width (ns) 1.59
Compilations
Spectra
Spectra
S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
Spectrum
MVSA Calculations
Properties
Intensity (counts)
m/z
MassListPos
V No. m / z Area / cts Color Peak Label Description
Mass Intervals
37 43.0565 854832 43.06 u
2 45.0352 32713 45.03 u PEG
3 59.0136 51836 59.01 u PMMA
4 59.0511 37293 59.05 u PEG
5 69.0376 118182 69.04 u PMMA
6 69.0762 360824 69.08 u
7 73.0342 16483 73.03 u PEG
8 87.0478 6134 87.05 u PEG
9 89.0617 3870 89.06 u PEG
10 91.0566 238681 91.05 u PS
11 93.0730 55170 93.07 u PMMA
12 98.0763 70210 98.07 u GTP
13 101.0605 26893 101.06 u PMMA
14 103.0490 34262 103.05 u PEG
43.06 u
S1_HMR_01_0
S1_HMR_02_0
Adjust the integration limits so the peak centroid is located at the peak maxium.
For Help, press F1
Animate
NUM

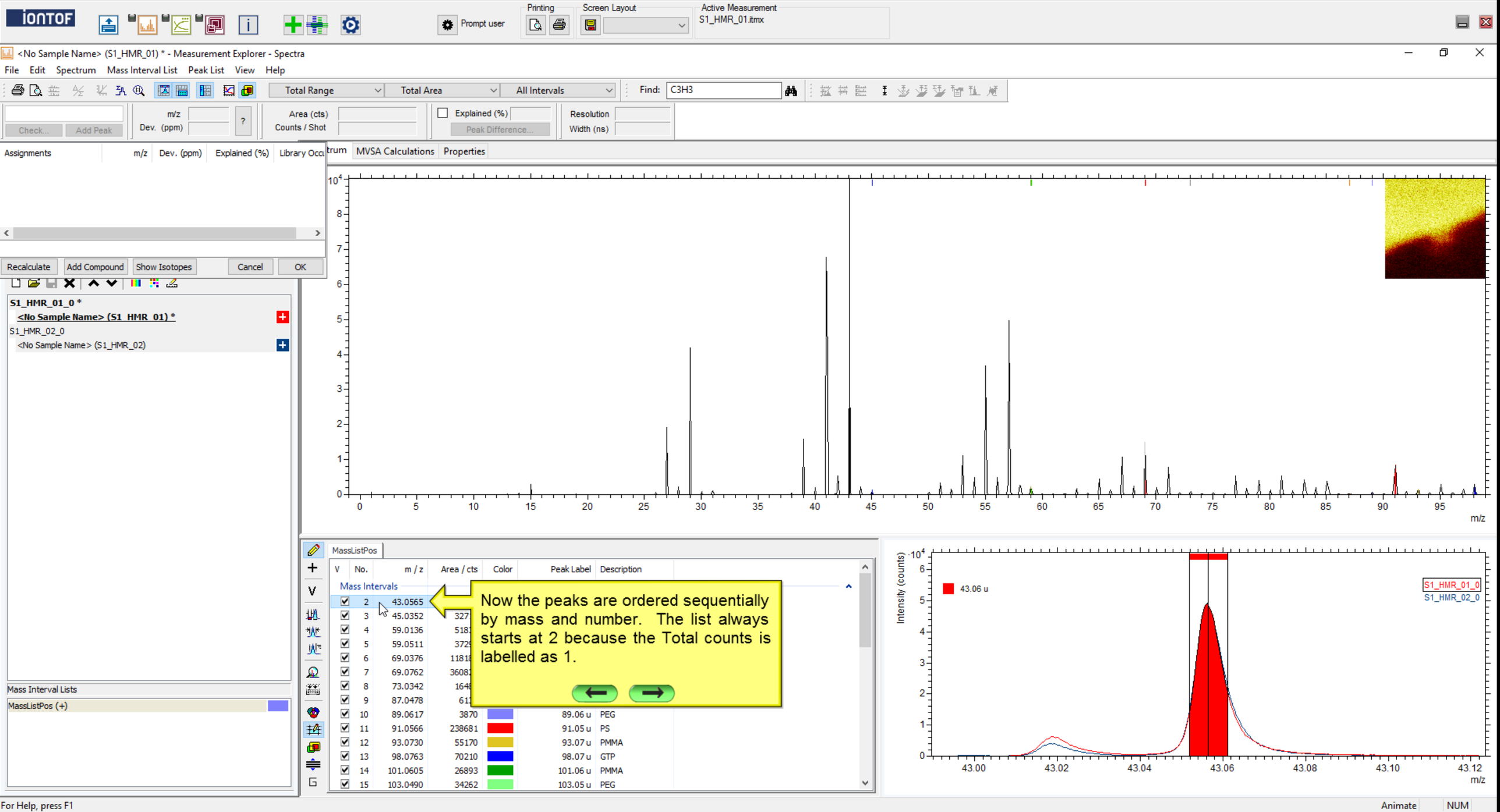

Prompt user
Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
C_3H_7+
Check...
Add Peak
Explained (%) 100.0
Peak Difference...
Resolution 7,028
Width (ns) 1.59
With the peak selected and the centroid at the peak maxium, press the 'Check...' button.
Compilations
Spectra
Properties
Intensity (co
m/z
Spectra
S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
MassListPos
V No. m / z Area / cts Color Peak Label Description
Mass Intervals
37 43.0565 854832 43.06 u
2 45.0352 32713 45.03 u PEG
3 59.0136 51836 59.01 u PMMA
4 59.0511 37293 59.05 u PEG
5 69.0376 118182 69.04 u PMMA
6 69.0762 360824 69.08 u
7 73.0342 16483 73.03 u PEG
8 87.0478 6134 87.05 u PEG
9 89.0617 3870 89.06 u PEG
10 91.0566 238681 91.05 u PS
11 93.0730 55170 93.07 u PMMA
12 98.0763 70210 98.07 u GTP
13 101.0605 26893 101.06 u PMMA
14 103.0490 34262 103.05 u PEG
Intensity (counts)
43.06 u
S1_HMR_01_0
S1_HMR_02_0
m/z
Animate
NUM

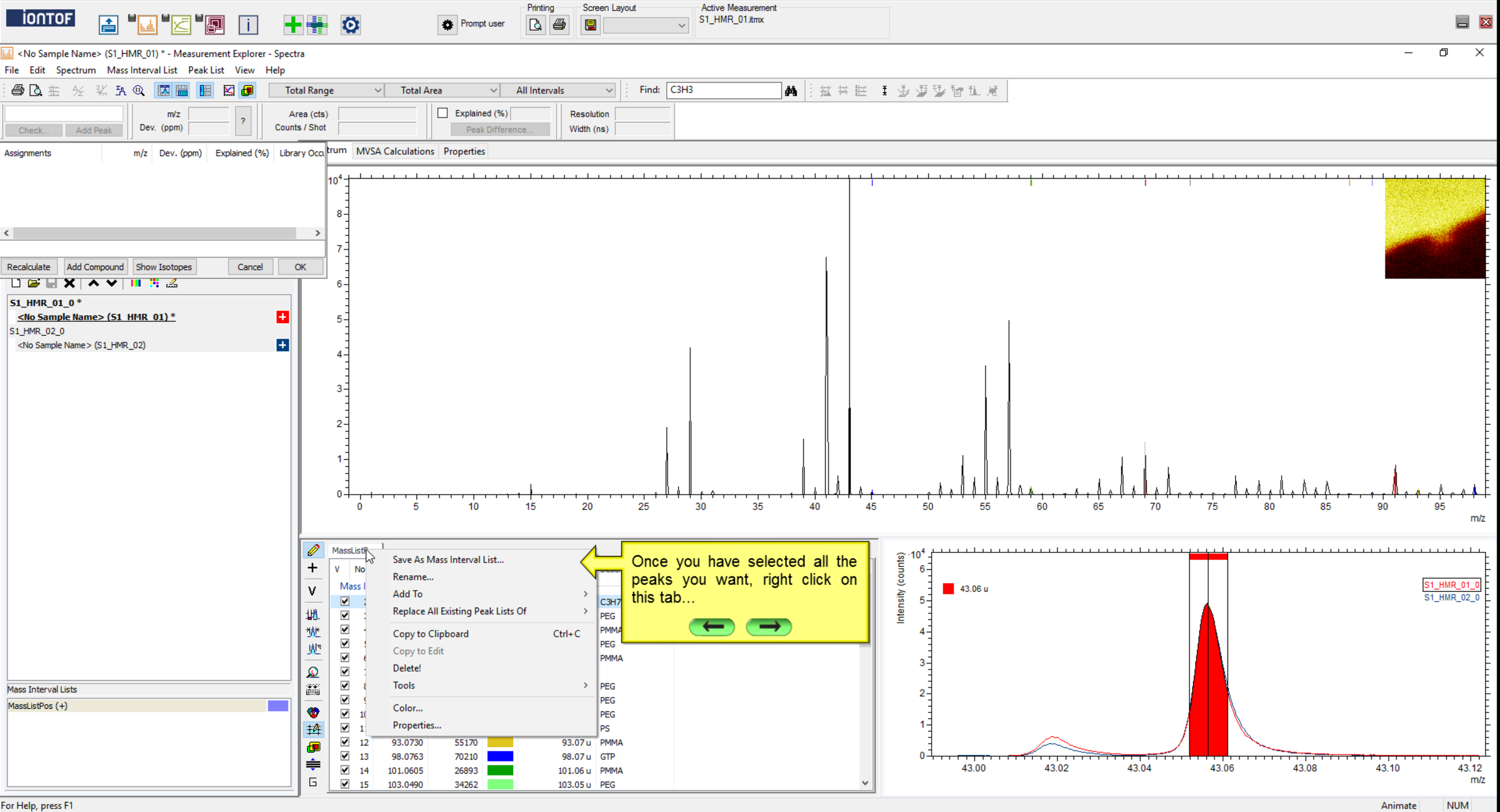

Prompt user
Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
C_3H_7+
Check... Add Peak
m/z 43.0563
Dev. (ppm) 47.2
Area (cts) 923,468
Counts / Shot 0.7828
Explained (%) 100.0
Peak Difference...
Resolution 7,028
Width (ns) 1.59
Assignments m/z Dev. (ppm) Explained (%) Library
C2H5N+ 43.0417 339.4 100.0
C2 13CH6+ 43.0498 151.1 9.6
C2H4CH3+ 43.0542 47.2 100.0
C3H7+ 43.0542 47.2 100.0
C_3H_7+
Recalculate Add Compound Show Isotopes Cancel OK
MVSA Calculations Properties
The software will show a list of species whos mass could match the selected peak.
NOTE:
-With the IONTOF mass resolution you should only look at options that match within +/- 55 ppm.
-You should also only look at peaks that have 100% in the Explained column.
-You should always use logic in choosing possible peak IDs. The IDs should be consistent and should contain elements actually present on your sample.
S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
MassListPos
V No. m / z Area / cts Color Peak Label Description
Mass Intervals
37 43.0565 854832 43.06 u
2 45.0352 32713 45.03 u PEG
3 59.0136 51836 59.01 u PMMA
4 59.0511 37293 59.05 u PEG
5 69.0376 118182 69.04 u PMMA
6 69.0762 360824 69.08 u
7 73.0342 16483 73.03 u PEG
8 87.0478 6134 87.05 u PEG
9 89.0617 3870 89.06 u PEG
10 91.0566 238681 91.05 u PS
11 93.0730 55170 93.07 u PMMA
12 98.0763 70210 98.07 u GTP
13 101.0605 26893 101.06 u PMMA
14 103.0490 34262 103.05 u PEG
Intensity (counts)
43.06 u
S1_HMR_01_0
S1_HMR_02_0
m/z
For Help, press F1
Animate
NUM

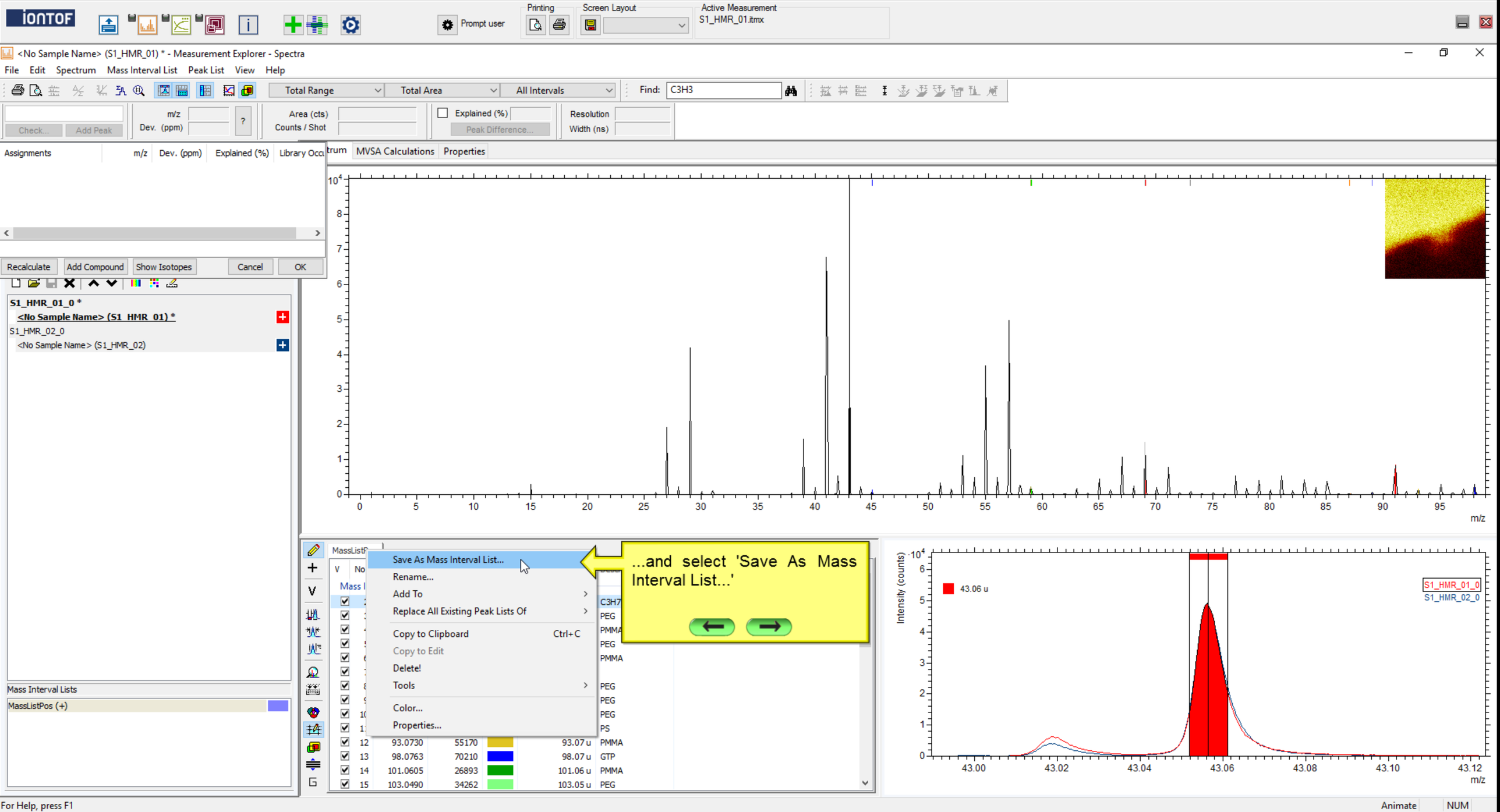

Prompt user
Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
Check... Add Peak
m/z
Dev. (ppm)
Area (cts)
Counts / Shot
Explained (%)
Peak Difference...
Resolution
Width (ns)
Assignments m/z Dev. (ppm) Explained (%) Library Occ
MVSA Calculations
Properties
Recalculate Add Compound Show Isotopes Cancel OK
S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
MassListPos
V No. m / z Area / cts Color Peak Label Description
Mass Intervals
37 43.0565 854832 43.06 u C3H7
2 45.0352 32713 45.03 u PEG
3 59.0136 51836 59.01 u PMMA
4 59.0511 37293 59.05 u PEG
5 69.0376 118182 69.04 u PMMA
6 69.0762 360824 69.08 u
7 73.0342 16483 73.03 u PEG
8 87.0478 6134 87.05 u PEG
9 89.0617 3870 89.06 u PEG
10 91.0566 238681 91.05 u PS
11 93.0730 55170 93.07 u PMMA
12 98.0763 70210 98.07 u GTP
13 101.0605 26893 101.06 u PMMA
14 103.0490 34262 103.05 u PEG
Once you believe you have an ID, you can enter it in the 'Description' column. Left click on the Description field for the peak and it will allow you to type.
NOTE: Use the Description field and not the "Assginment" field.
S1_HMR_01_0
S1_HMR_02_0
m/z
For Help, press F1
Animate
NUM

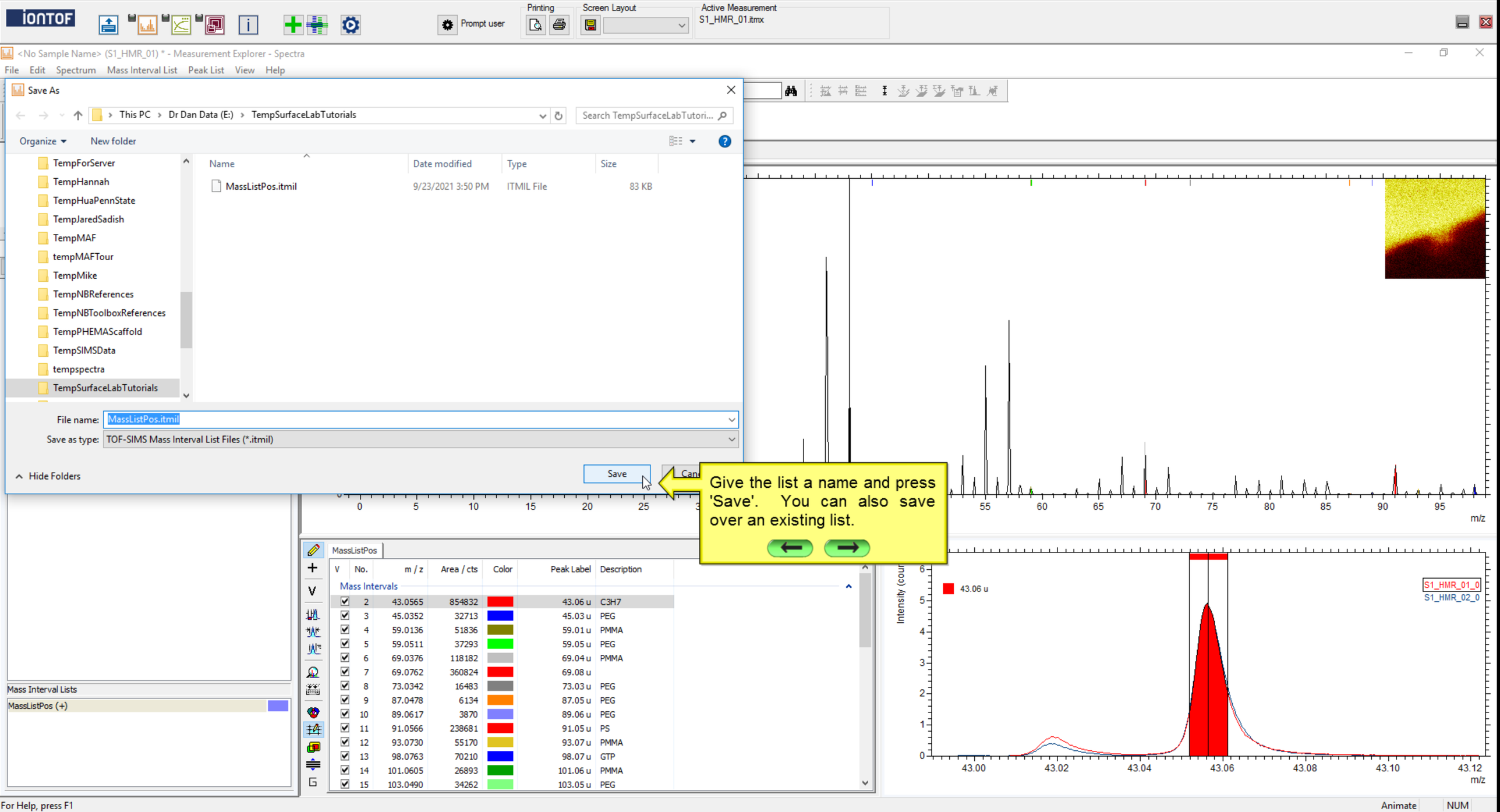

Prompt user
Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
Check... Add Peak
m/z
Dev. (ppm)
Area (cts)
Counts / Shot
Explained (%)
Peak Difference...
Resolution
Width (ns)
Assignments m/z Dev. (ppm) Explained (%) Library Occ
MVSA Calculations
Properties
Recalculate Add Compound Show Isotopes Cancel OK
S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
MassListPos
V No. m / z Area / cts Color Peak Label Description
Mass Intervals
37
2 45.0152
3 59.0136
4 59.0511
5 69.0376
6 69.0762
7 73.0342
8 87.0478
9 89.0617 3870 89.06 u PEG
10 91.0566 238681 91.05 u PS
11 93.0730 55170 93.07 u PMMA
12 98.0763 70210 98.07 u GTP
13 101.0605 26893 101.06 u PMMA
14 103.0490 34262 103.05 u PEG
This list is sorted by mass. Note that the peak numbers are not in order. You need to change this before exporting any data or the masses will not be in order.
m/z
Intensity (counts)
43.06 u
S1_HMR_01_0
S1_HMR_02_0
For Help, press F1
Animate
NUM

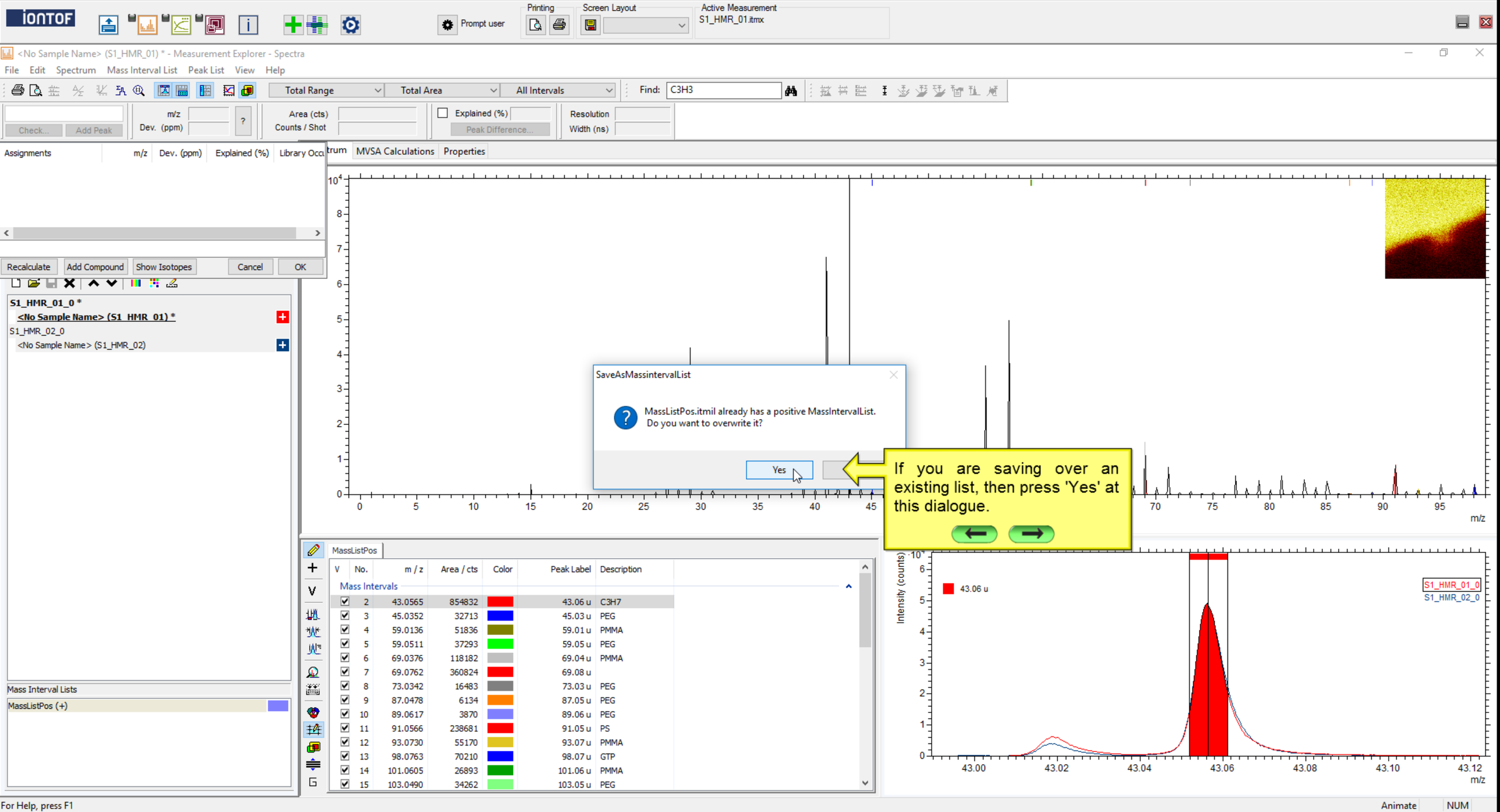

Prompt user
Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
Check... Add Peak
m/z
Dev. (ppm)
Area (cts)
Counts / Shot
Explained (%)
Peak Difference...
Resolution
Width (ns)
Assignments m/z Dev. (ppm) Explained (%) Library Occ
MVSA Calculations
Properties
Recalculate Add Compound Show Isotopes Cancel OK
S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
MassListPos
V No. m / z Area / cts Color Peak Label Description
Mass Intervals
37 43.0565 854832 43.06 u C3H7
2 45.0352 32713 45.03 u PEG
3 59.0136 51836 59.01 u PMMA
4 59.0511 37293 59.05 u PEG
5 69.0376 118182 69.04 u PMMA
6 69.0762 360824 69.08 u
Reorder IDs
To do this, press the Reorder IDs button found near the bottom of this toolbar. It may be off screen depending on the size of the lower windows.
Intensity (counts)
43.06 u
S1_HMR_01_0
S1_HMR_02_0
m/z
For Help, press F1
Animate
NUM

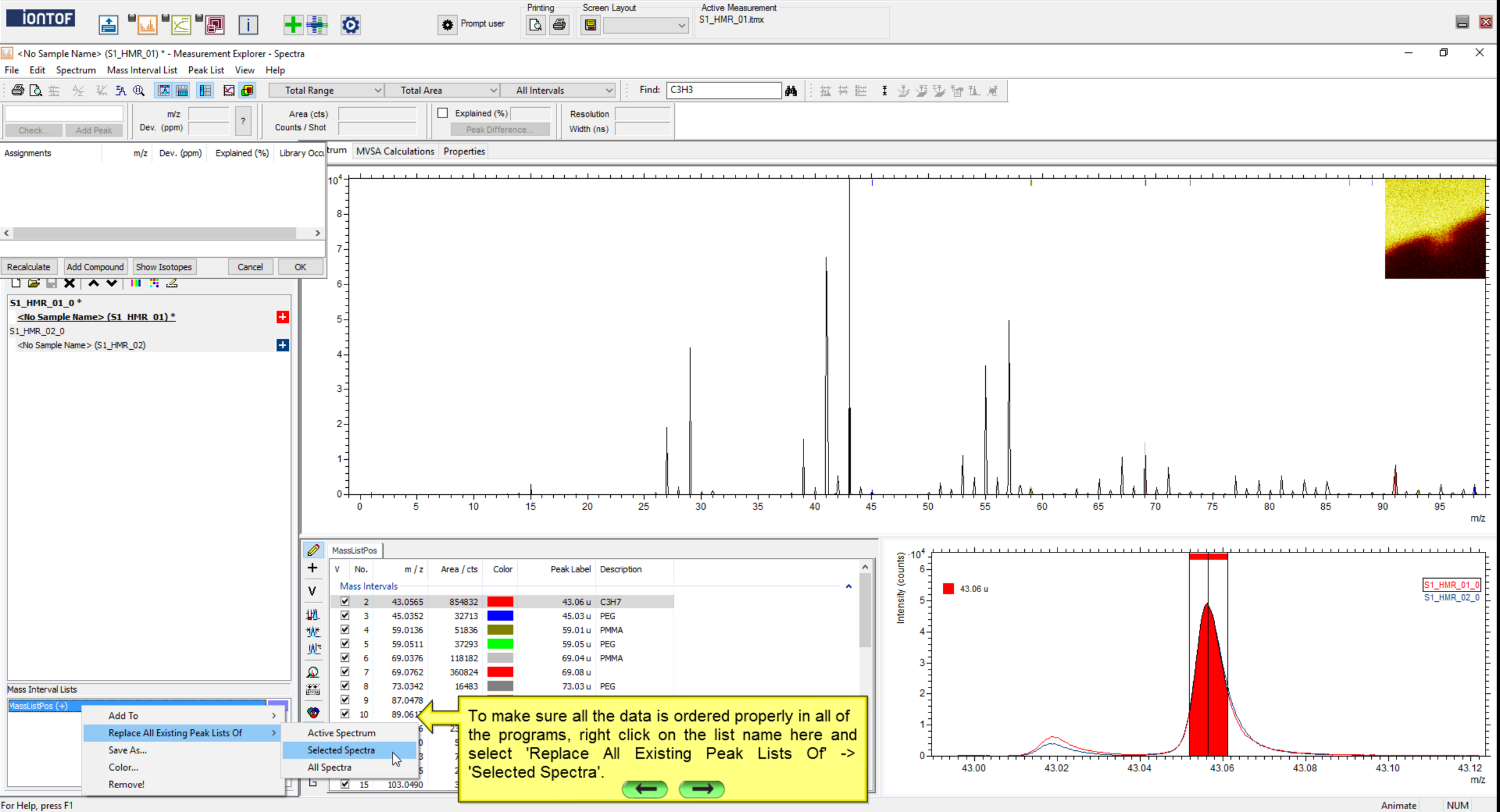

Prompt user
Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
Check... Add Peak
m/z
Dev. (ppm)
Area (cts)
Counts / Shot
Explained (%)
Peak Difference...
Resolution
Width (ns)
Assignments m/z Dev. (ppm) Explained (%) Library Occ
Recalculate Add Compound Show Isotopes Cancel OK
MVSA Calculations
Properties
S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
MassListPos
V No. m / z Area / cts Color Peak Label Description
Mass Intervals
2 43.0565
3 45.0352
4 59.0136
5 59.0511
6 69.0376
7 69.0762
8 73.0342
9 87.0478
10 89.0617 3870 89.06 u PEG
11 91.0566 238681 91.05 u PS
12 93.0730 55170 93.07 u PMMA
13 98.0763 70210 98.07 u GTP
14 101.0605 26893 101.06 u PMMA
15 103.0490 34262 103.05 u PEG
Now the peaks are ordered sequentially by mass and number. The list always starts at 2 because the Total counts is labelled as 1.
m/z
Intensity (counts)
43.06 u
S1_HMR_01_0
S1_HMR_02_0
For Help, press F1
Animate
NUM

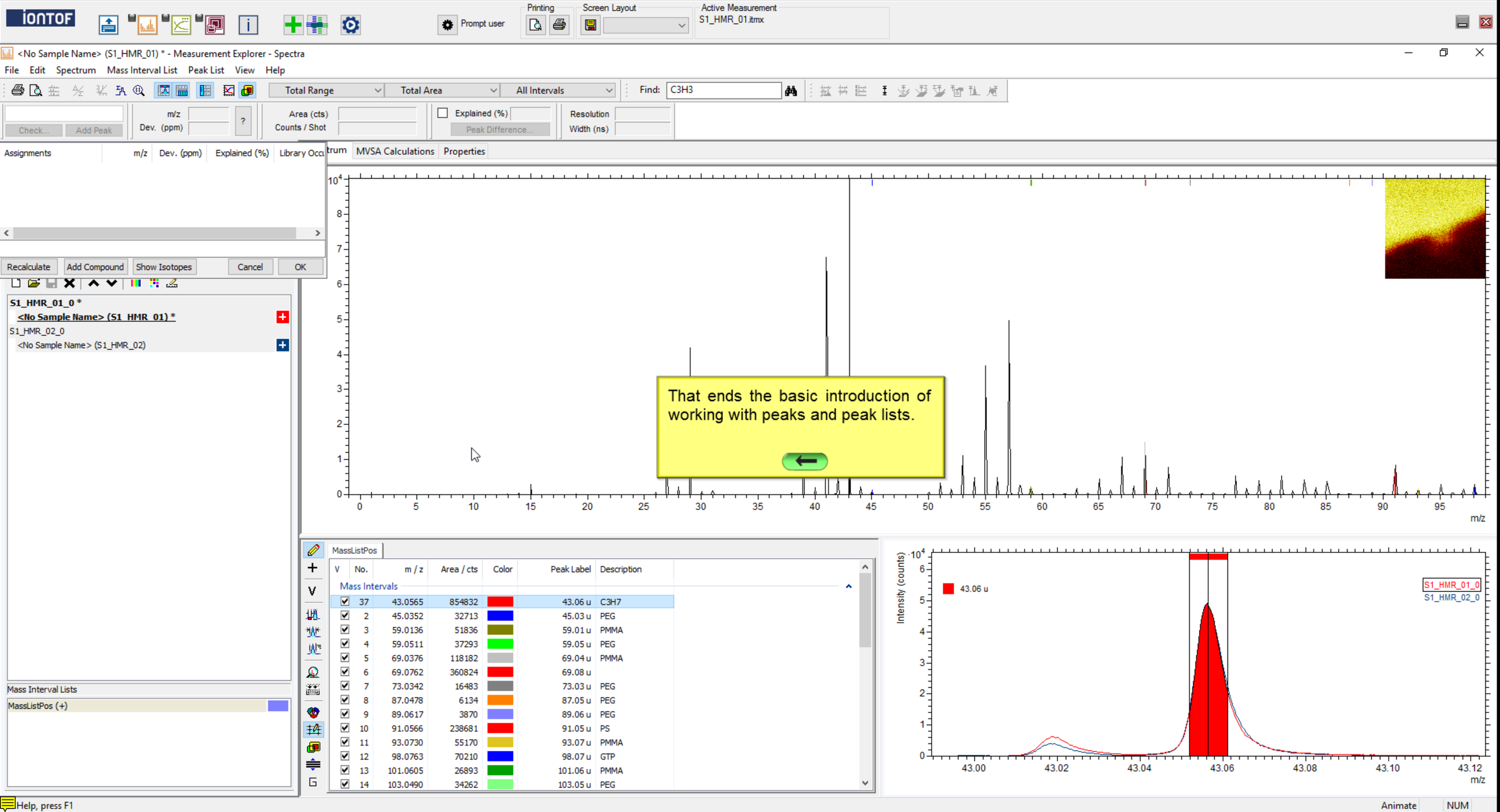

Prompt user
Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
Check... Add Peak
m/z
Dev. (ppm)
Area (cts)
Counts / Shot
Explained (%)
Peak Difference...
Resolution
Width (ns)
Assignments
m/z
Dev. (ppm)
Explained (%)
Library Occ
MVSA Calculations
Properties
Recalculate
Add Compound
Show Isotopes
Cancel
OK
S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
Save As Mass Interval List...
Rename...
Add To
Replace All Existing Peak Lists Of
Copy to Clipboard Ctrl+C
Copy to Edit
Delete!
Tools
Color...
Properties...
Once you have selected all the peaks you want, right click on this tab...
m/z
Intensity (counts)
43.06 u
S1_HMR_01_0
S1_HMR_02_0
For Help, press F1
Animate
NUM


Prompt user
Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
Check... Add Peak
m/z
Dev. (ppm)
Area (cts)
Counts / Shot
Explained (%)
Peak Difference...
Resolution
Width (ns)
Assignments
m/z
Dev. (ppm)
Explained (%)
Library Occu
MVSA Calculations
Properties
Recalculate
Add Compound
Show Isotopes
Cancel
OK
S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
Save As Mass Interval List...
Rename...
Add To
Replace All Existing Peak Lists Of
Copy to Clipboard Ctrl+C
Copy to Edit
Delete!
Tools
Color...
Properties...
...and select 'Save As Mass Interval List...'
Intensity (counts)
43.06 u
S1_HMR_01_0
S1_HMR_02_0
m/z
For Help, press F1
Animate
NUM


Prompt user
Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Save As
This PC › Dr Dan Data (E:) › TempSurfaceLabTutorials
Search TempSurfaceLabTutori...
Organize
New folder
TempForServer
TempHannah
TempHuaPennState
TempJaredSadish
TempMAF
tempMAFTour
TempMike
TempNBReferences
TempNBToolboxReferences
TempPHEMAScaffold
TempSIMSData
tempspectra
TempSurfaceLabTutorials
Name
Date modified
Type
Size
MassListPos.itmil
9/23/2021 3:50 PM
ITMIL File
83 KB
File name: MassListPos.itmil
Save as type: TOF-SIMS Mass Interval List Files (*.itmil)
Hide Folders
Save
Give the list a name and press 'Save'. You can also save over an existing list.
MassListPos
V No. m / z Area / cts Color Peak Label Description
Mass Intervals
2 43.0565 854832 43.06 u C3H7
3 45.0352 32713 45.03 u PEG
4 59.0136 51836 59.01 u PMMA
5 59.0511 37293 59.05 u PEG
6 69.0376 118182 69.04 u PMMA
7 69.0762 360824 69.08 u
8 73.0342 16483 73.03 u PEG
9 87.0478 6134 87.05 u PEG
10 89.0617 3870 89.06 u PEG
11 91.0566 238681 91.05 u PS
12 93.0730 55170 93.07 u PMMA
13 98.0763 70210 98.07 u GTP
14 101.0605 26893 101.06 u PMMA
15 103.0490 34262 103.05 u PEG
Mass Interval Lists
MassListPos (+)
43.06 u
S1_HMR_01_0
S1_HMR_02_0
Intensity (cou
m/z
For Help, press F1
Animate
NUM


Prompt user
Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
Check... Add Peak
m/z
Dev. (ppm)
Area (cts)
Counts / Shot
Explained (%)
Peak Difference...
Resolution
Width (ns)
Assignments m/z Dev. (ppm) Explained (%) Library Occ
MVSA Calculations
Properties
Recalculate Add Compound Show Isotopes Cancel OK
S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
SaveAsMassintervalList
MassListPos.itmil already has a positive MassIntervalList.
Do you want to overwrite it?
Yes
If you are saving over an existing list, then press 'Yes' at this dialogue.
MassListPos
Mass Intervals
V No. m / z Area / cts Color Peak Label Description
2 43.0565 854832 43.06 u C3H7
3 45.0352 32713 45.03 u PEG
4 59.0136 51836 59.01 u PMMA
5 59.0511 37293 59.05 u PEG
6 69.0376 118182 69.04 u PMMA
7 69.0762 360824 69.08 u
8 73.0342 16483 73.03 u PEG
9 87.0478 6134 87.05 u PEG
10 89.0617 3870 89.06 u PEG
11 91.0566 238681 91.05 u PS
12 93.0730 55170 93.07 u PMMA
13 98.0763 70210 98.07 u GTP
14 101.0605 26893 101.06 u PMMA
15 103.0490 34262 103.05 u PEG
Intensity (counts)
43.06 u
S1_HMR_01_0
S1_HMR_02_0
m/z
For Help, press F1
Animate
NUM


Prompt user
Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
Check... Add Peak
m/z
Dev. (ppm)
Area (cts)
Counts / Shot
Explained (%)
Peak Difference...
Resolution
Width (ns)
Assignments m/z Dev. (ppm) Explained (%) Library Occ
MVSA Calculations
Properties
Recalculate Add Compound Show Isotopes Cancel OK
S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
Mass Interval Lists
MassListPos (+)
Add To
Replace All Existing Peak Lists Of
Save As...
Color...
Remove!
Active Spectrum
Selected Spectra
All Spectra
MassListPos
V No. m / z Area / cts Color Peak Label Description
Mass Intervals
2 43.0565 854832 43.06 u C3H7
3 45.0352 32713 45.03 u PEG
4 59.0136 51836 59.01 u PMMA
5 59.0511 37293 59.05 u PEG
6 69.0376 118182 69.04 u PMMA
7 69.0762 360824 69.08 u
8 73.0342 16483 73.03 u PEG
9 87.0478
10 89.061
15 103.0490
To make sure all the data is ordered properly in all of the programs, right click on the list name here and select 'Replace All Existing Peak Lists Of' -> 'Selected Spectra'.
Intensity (counts)
43.06 u
S1_HMR_01_0
S1_HMR_02_0
m/z
For Help, press F1
Animate
NUM


Prompt user
Printing
Screen Layout
Active Measurement
S1_HMR_01.itmx
<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra
File Edit Spectrum Mass Interval List Peak List View Help
Total Range
Total Area
All Intervals
Find: C3H3
Check... Add Peak
m/z
Dev. (ppm)
Area (cts)
Counts / Shot
Explained (%)
Peak Difference...
Resolution
Width (ns)
Assignments m/z Dev. (ppm) Explained (%) Library Occ
trum MVSA Calculations Properties
Recalculate Add Compound Show Isotopes Cancel OK
S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
That ends the basic introduction of working with peaks and peak lists.
m/z
Mass Interval Lists
MassListPos (+)
MassListPos
V No. m / z Area / cts Color Peak Label Description
Mass Intervals
37 43.0565 854832 43.06 u C3H7
2 45.0352 32713 45.03 u PEG
3 59.0136 51836 59.01 u PMMA
4 59.0511 37293 59.05 u PEG
5 69.0376 118182 69.04 u PMMA
6 69.0762 360824 69.08 u
7 73.0342 16483 73.03 u PEG
8 87.0478 6134 87.05 u PEG
9 89.0617 3870 89.06 u PEG
10 91.0566 238681 91.05 u PS
11 93.0730 55170 93.07 u PMMA
12 98.0763 70210 98.07 u GTP
13 101.0605 26893 101.06 u PMMA
14 103.0490 34262 103.05 u PEG
Intensity (counts)
43.06 u
S1_HMR_01_0
S1_HMR_02_0
m/z
Help, press F1
Animate
NUM