

C ₃ H ₅ ⁺	m/z	41.0409	Area (cts)	368	Explained (%)	100.0	Resolution	2,149
Check... Add Peak	Dev. (ppm)	56.4	Counts / Shot	0.0003	Peak Difference...		Width (ns)	7.45

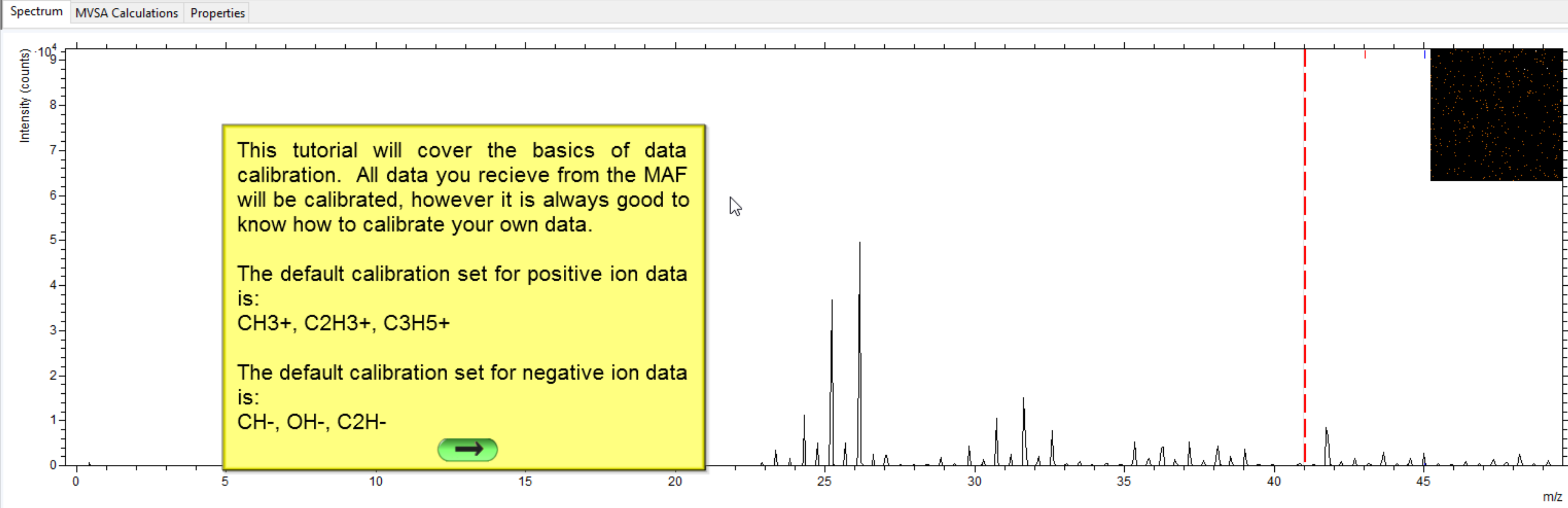
Compilations

Spectra

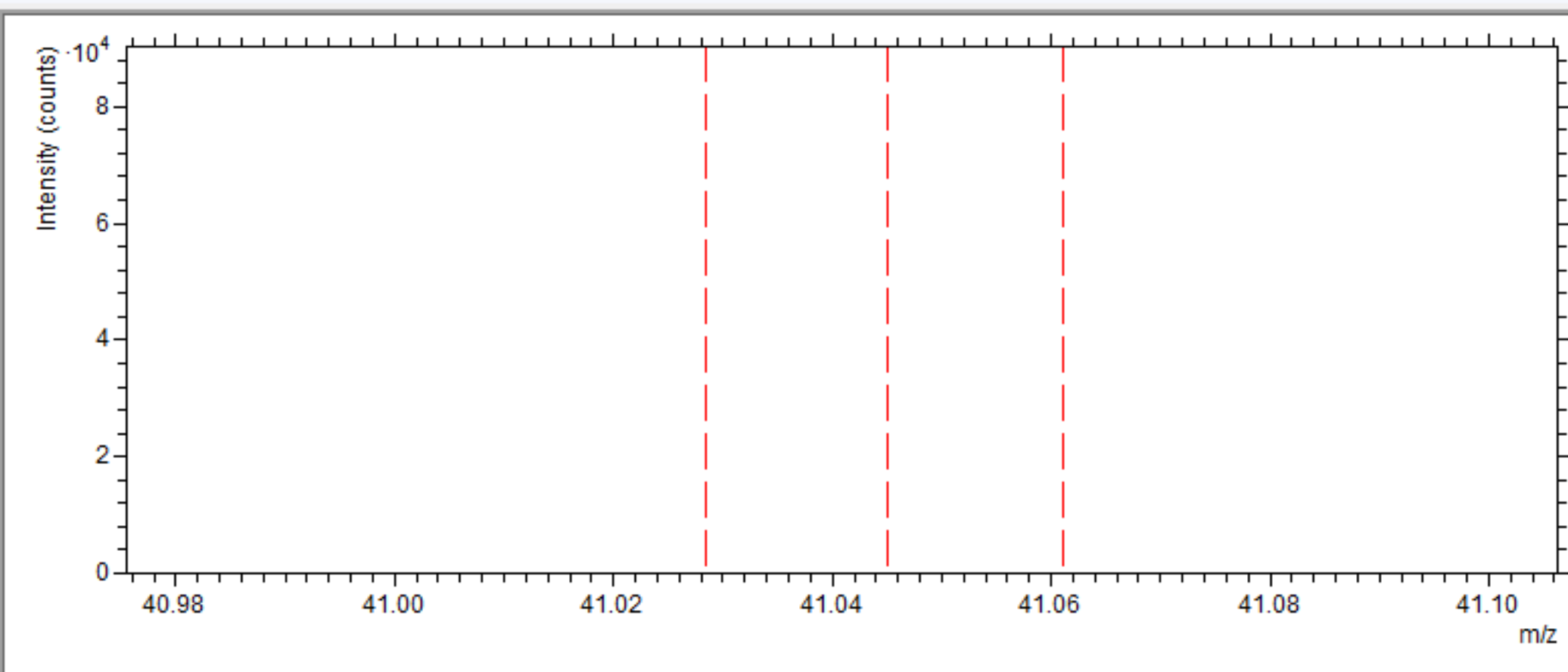
Spectra

S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *

S1_HMR_02_0
<No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
<input checked="" type="checkbox"/>	2	43.0569	248	Red	43.06 u	C ₃ H ₇
<input checked="" type="checkbox"/>	3	45.0333	5989	Blue	45.03 u	PEG
<input checked="" type="checkbox"/>	4	59.0125	945	Olive	59.01 u	PMMA
<input checked="" type="checkbox"/>	5	59.0520	1168	Green	59.05 u	PEG
<input checked="" type="checkbox"/>	6	69.0353	727	Grey	69.04 u	PMMA
<input checked="" type="checkbox"/>	7	69.0770	390	Red	69.08 u	
<input checked="" type="checkbox"/>	8	73.0391	3021	Grey	73.03 u	PEG
<input checked="" type="checkbox"/>	9	87.0494	3388	Orange	87.05 u	PEG
<input checked="" type="checkbox"/>	10	89.0670	643	Blue	89.06 u	PEG
<input checked="" type="checkbox"/>	11	91.0554	2212	Red	91.05 u	PS
<input checked="" type="checkbox"/>	12	93.0712	2472	Yellow	93.07 u	PMMA
<input checked="" type="checkbox"/>	13	98.0721	1370	Blue	98.07 u	GTP
<input checked="" type="checkbox"/>	14	101.0567	1869	Green	101.06 u	PMMA
<input checked="" type="checkbox"/>	15	103.0389	713	Light Green	103.05 u	PEG



m/z Area (cts) Explained (%) Resolution
 Dev. (ppm) Counts / Shot Peak Difference... Width (ns)

Compilations

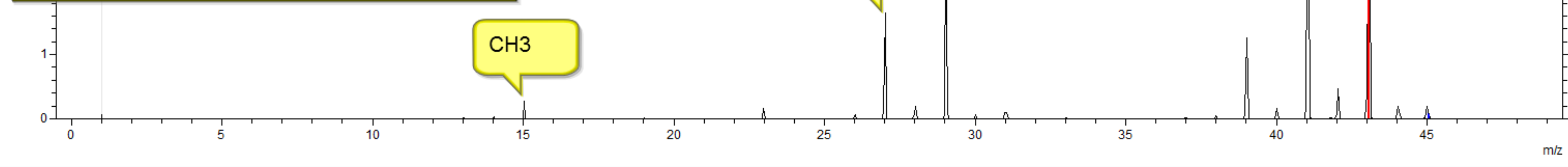
Spectra

S1_HMR_01_0
<No Sample Name> (S1_HMR_01)

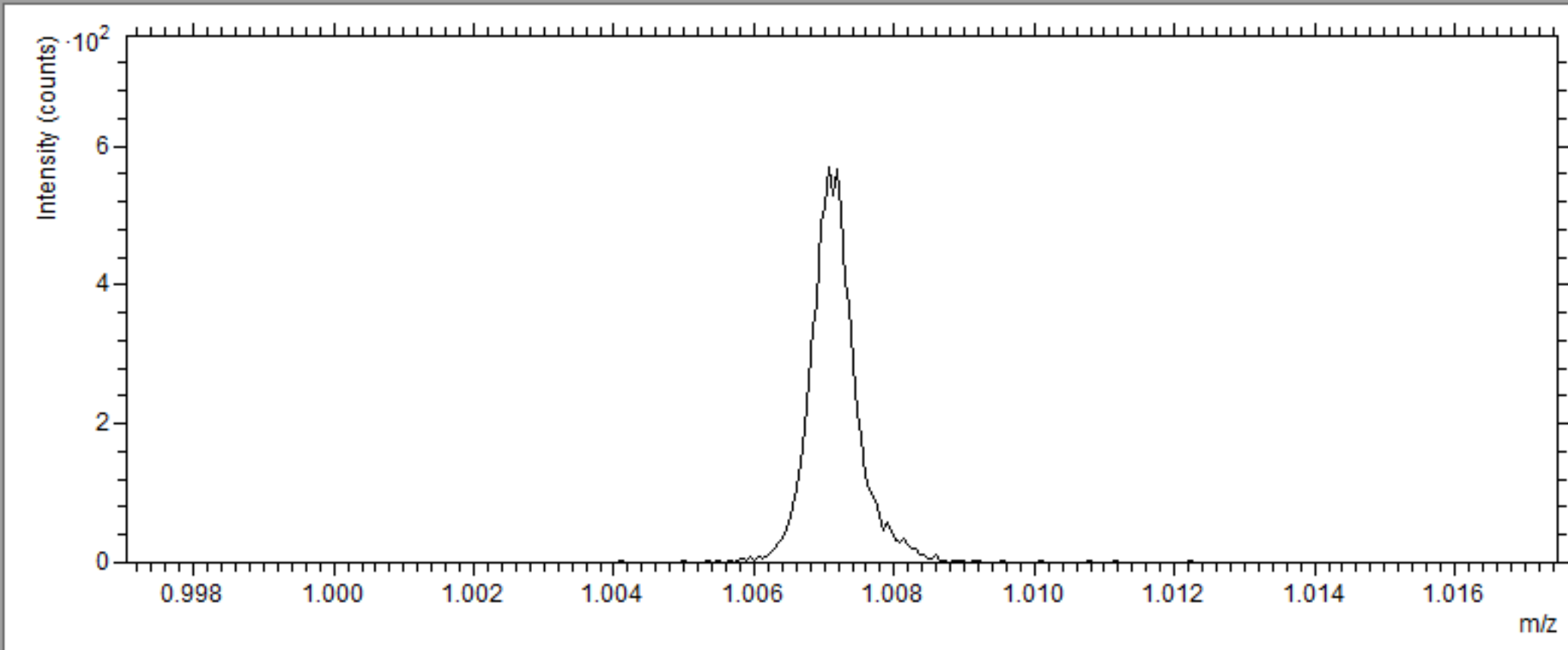
S1_HMR_02_0
<No Sample Name> (S1_HMR_02)

This slide shows the m/z 0 to 50 region from a positive ion spectrum. Almost all positive ion spectra will have a similar pattern of peaks. This can help when identifying the default calibration peaks.

CH3 is typically the tallest peak in the first cluster of peaks.
 C2H3 is typically the first tall peak in the next cluster of peaks.
 C3H5 is typically the middle peak in the next cluster of peaks.



V	No.	m/z	Area / cts	Color	Peak Label	Description
Mass Intervals						
<input checked="" type="checkbox"/>	2	43.0566	850449	Red	43.06 u	C3H7
<input checked="" type="checkbox"/>	3	45.0348	41872	Blue	45.03 u	PEG
<input checked="" type="checkbox"/>	4	59.0138	42768	Olive	59.01 u	PMMA
<input checked="" type="checkbox"/>	5	59.0512	25029	Green	59.05 u	PEG
<input checked="" type="checkbox"/>	6	69.0376	92774	Grey	69.04 u	PMMA
<input checked="" type="checkbox"/>	7	69.0761	289533	Red	69.08 u	
<input checked="" type="checkbox"/>	8	73.0342	15305	Grey	73.03 u	PEG
<input checked="" type="checkbox"/>	9	87.0477	5488	Orange	87.05 u	PEG
<input checked="" type="checkbox"/>	10	89.0605	3641	Blue	89.06 u	PEG
<input checked="" type="checkbox"/>	11	91.0587	586826	Red	91.05 u	PS
<input checked="" type="checkbox"/>	12	93.0731	40934	Yellow	93.07 u	PMMA
<input checked="" type="checkbox"/>	13	98.0765	65028	Blue	98.07 u	GTP
<input checked="" type="checkbox"/>	14	101.0604	18365	Green	101.06 u	PMMA
<input checked="" type="checkbox"/>	15	103.0514	58432	Light Green	103.05 u	PEG



m/z Area (cts) Explained (%) Resolution
 Dev. (ppm) Counts / Shot Peak Difference... Width (ns)

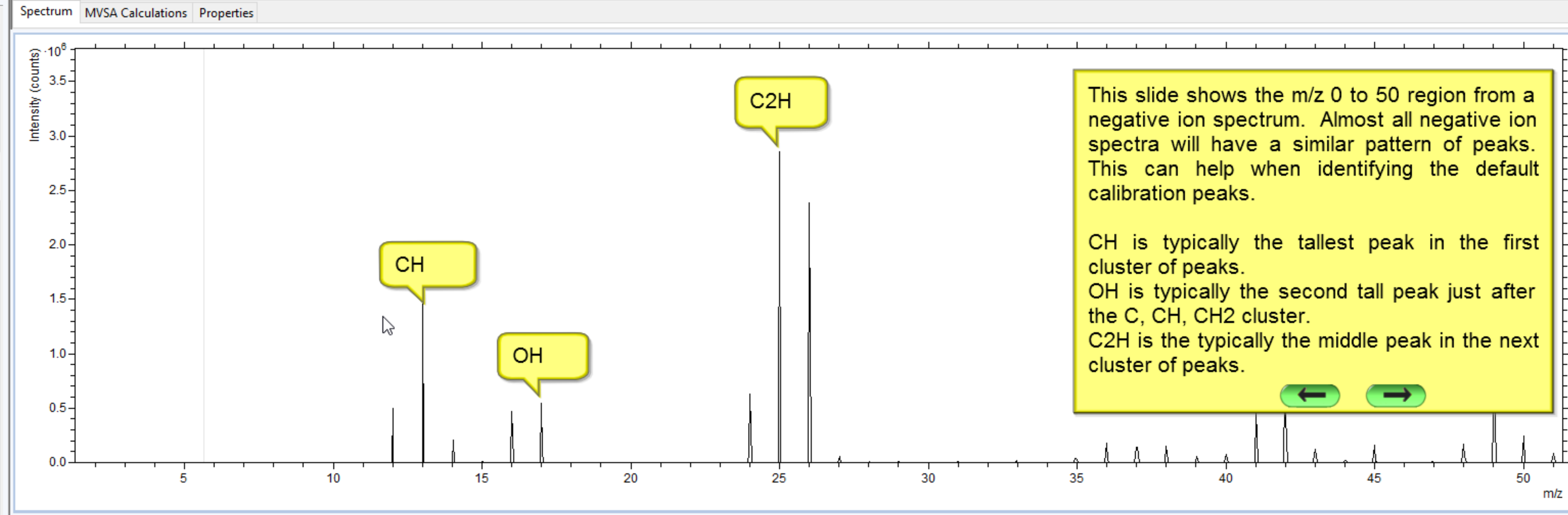
Compilations

Spectra

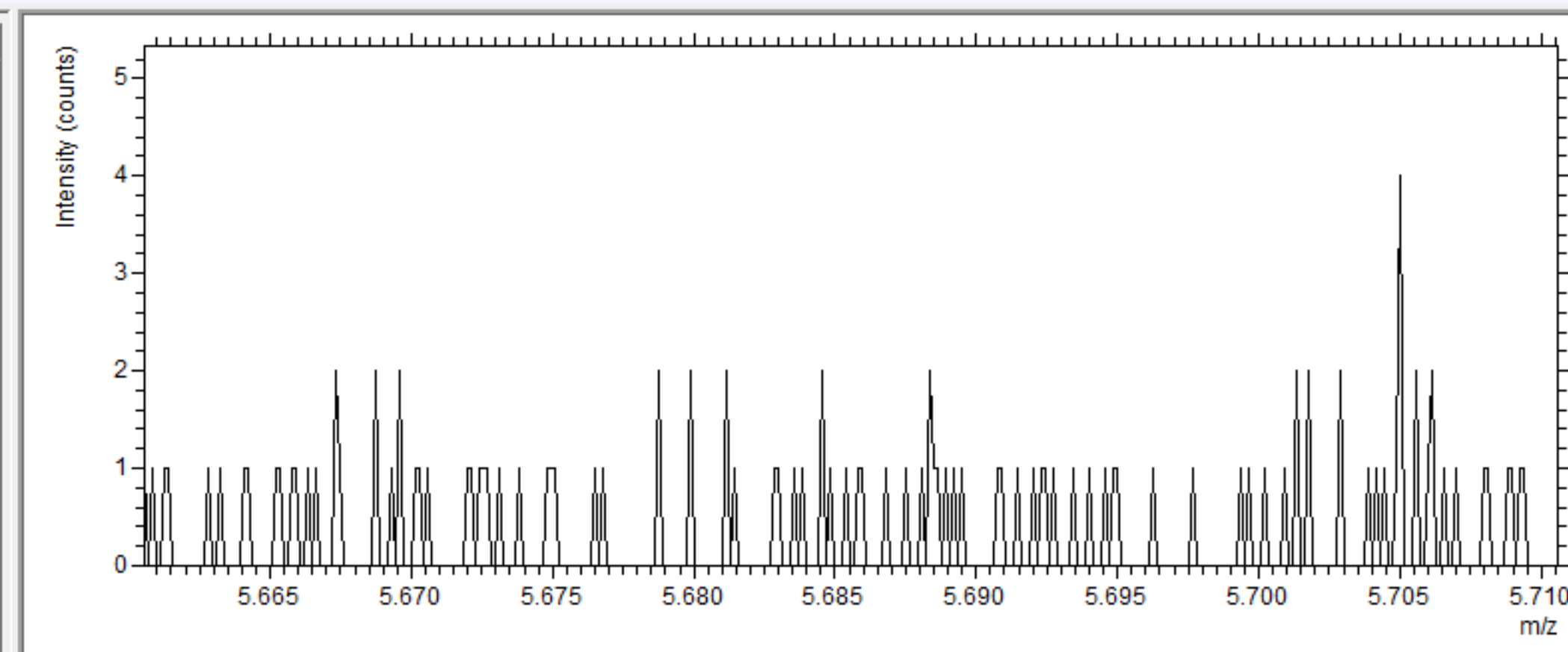
- Spectra
- S1_HMR_01_0
<No Sample Name> (S1_HMR_01)
 - S1_HMR_02_0
<No Sample Name> (S1_HMR_02)
 - ThyroidLow_HMR_06_0***
<No Sample Name> (ThyroidLow_HMR_06)*

Mass Interval Lists

MassListPos (+)

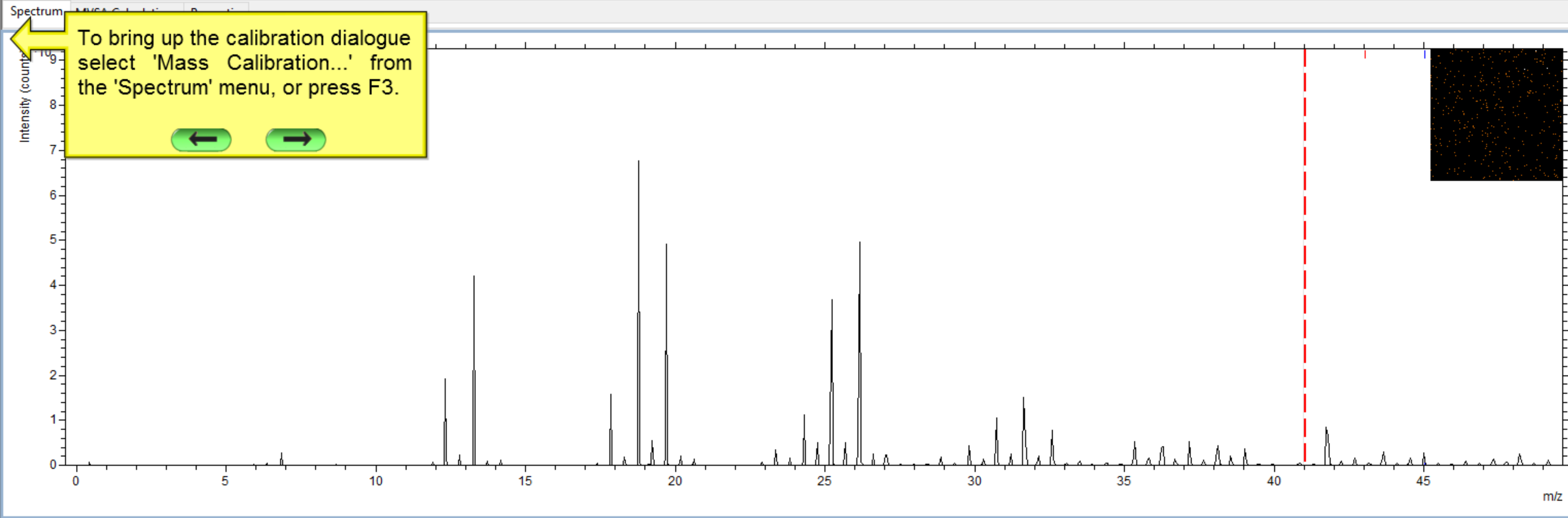


V	No.	m / z	Area / cts	Color	Peak Label	Description
Special Intervals						
<input type="checkbox"/>	1		832203974	■	total	total

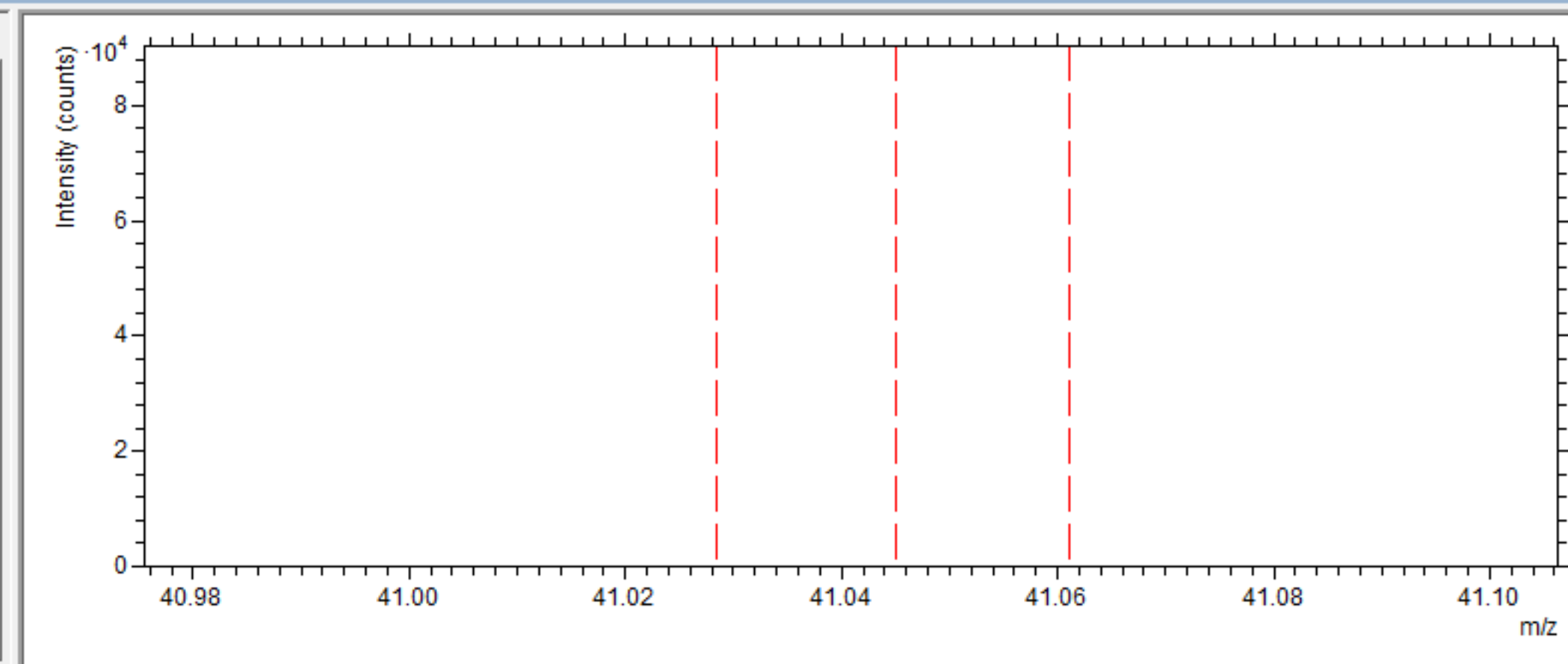


Display Spectra As Line Spectra S
 Combine Line Spectra...
 Display Spectra as Overlay Z
 Spectra Overlay Options >
Mass Calibration ... F3
 Apply Mass Calibration To >
 Find Mass Ctrl+F
 Find Compound... Ctrl+G
 Add selected Peak Ctrl+A
 Add Background to selected Peak(s)
 Recalibrate Peak Searcher
 Search Peaks...
 Search Elements...
 Search Compounds...
 Mass Shift Correction...
 Add Lateral ROIs To >
 Replace Lateral ROIs Of >
 Copy z-ROIs To >
 Add Interval Subsets To >
 Replace Interval Subsets Of >
 Show Analysis Peaklists
 Create G-SIMS Spectrum...
 Show G-SIMS Spectrum...
 Apply Smooth
 Smooth Properties...
 Element Information...
 Isotope Cluster Calculator...
 Spectra Library
 Add to Spectra Library
 Scale Spectra
 Scale Spectra by >

Total Range Total Area All Intervals Find: c7h7
 Area (cts) 368 Explained (%) 100.0 Resolution 2,149
 Shots / Shot 0.0003 Peak Difference... Width (ns) 7.45



V	No.	m/z	Area / cts	Color	Peak Label	Description
Mass Intervals						
✓	2	43.0569	248	Red	43.06 u	C3H7
✓	3	45.0333	5989	Blue	45.03 u	PEG
✓	4	59.0125	945	Olive	59.01 u	PMMA
✓	5	59.0520	1168	Green	59.05 u	PEG
✓	6	69.0353	727	Grey	69.04 u	PMMA
✓	7	69.0770	390	Red	69.08 u	
✓	8	73.0391	3021	Grey	73.03 u	PEG
✓	9	87.0494	3388	Orange	87.05 u	PEG
✓	10	89.0670	643	Blue	89.06 u	PEG
✓	11	91.0554	2212	Red	91.05 u	PS
✓	12	93.0712	2472	Yellow	93.07 u	PMMA
✓	13	98.0721	1370	Blue	98.07 u	GTP
✓	14	101.0567	1869	Green	101.06 u	PMMA
✓	15	103.0389	713	Light Green	103.05 u	PEG



C_3H_5+	m/z	41.0409	Area (cts)	368	Explained (%)	100.0	Resolution	2,149
Check...	Dev. (ppm)	56.4	Counts / Shot	0.0003	Peak Difference...		Width (ns)	7.45

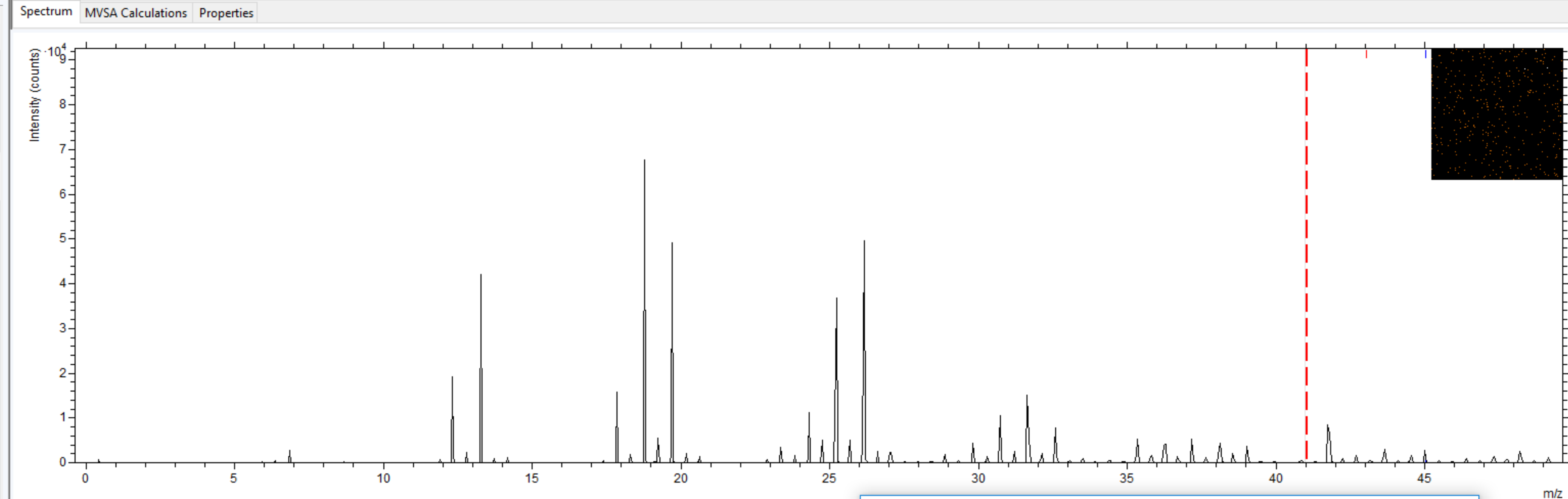
Compilations

Icons for file operations

Spectra

Icons for spectrum management

- S1_HMR_01_0 *
 - <No Sample Name> (S1_HMR_01) *
 - S1_HMR_02_0
 - <No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts	Color	Peak Label
Mass Intervals					
<input checked="" type="checkbox"/>	2	43.0569	248	Red	43.06 u
<input checked="" type="checkbox"/>	3	45.0333	5989	Blue	45.03 u
<input checked="" type="checkbox"/>	4	59.0125	945	Olive	59.01 u
<input checked="" type="checkbox"/>	5	59.0520	1168	Green	59.05 u
<input checked="" type="checkbox"/>	6	69.0353	727	Grey	69.04 u
<input checked="" type="checkbox"/>	7	69.0770	390	Red	69.08 u
<input checked="" type="checkbox"/>	8	73.0391	3021	Grey	73.03 u PEG
<input checked="" type="checkbox"/>	9	87.0494	3388	Orange	87.05 u PEG
<input checked="" type="checkbox"/>	10	89.0670	643	Blue	89.06 u PEG
<input checked="" type="checkbox"/>	11	91.0554	2212	Red	91.05 u PS
<input checked="" type="checkbox"/>	12	93.0712	2472	Yellow	93.07 u PMMA
<input checked="" type="checkbox"/>	13	98.0721	1370	Blue	98.07 u GTP
<input checked="" type="checkbox"/>	14	101.0567	1869	Green	101.06 u PMMA
<input checked="" type="checkbox"/>	15	103.0389	713	Light Green	103.05 u PEG

This is the calibration dialogue. Typically you will see the default set of calibration peaks. The calibration has been cleared to illustrate how you can calibrate the data.

← →

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: left click Add

use selected channel Delete All

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...

SF = 100000.000, K0 = 0.000, Positive

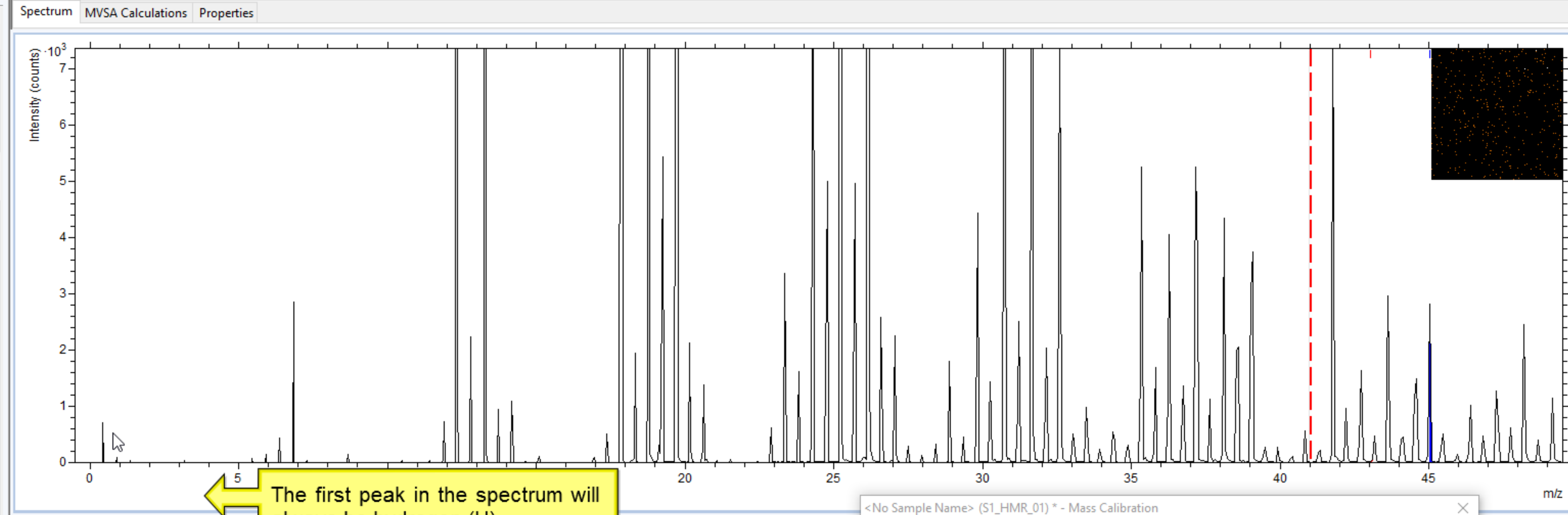
Options... Autocalibrate As Default... Revoke Recalibrate

C_3H_5+	m/z	41.0409	Area (cts)	368	Explained (%)	100.0	Resolution	2,149
Check...	Dev. (ppm)	56.4	Counts / Shot	0.0003	Peak Difference...		Width (ns)	7.45

Compilations

Spectra

- S1_HMR_01_0 *
 - <No Sample Name> (S1_HMR_01) *
 - S1_HMR_02_0
 - <No Sample Name> (S1_HMR_02)



The first peak in the spectrum will always be hydrogen (H).

V	No.	m / z	Area / cts		
Mass Intervals					
✓	2	43.0569	248		
✓	3	45.0333	5989	45.03 u	PEG
✓	4	59.0125	945	59.01 u	PMMA
✓	5	59.0520	1168	59.05 u	PEG
✓	6	69.0353	727	69.04 u	PMMA
✓	7	69.0770	390	69.08 u	
✓	8	73.0391	3021	73.03 u	PEG
✓	9	87.0494	3388	87.05 u	PEG
✓	10	89.0670	643	89.06 u	PEG
✓	11	91.0554	2212	91.05 u	PS
✓	12	93.0712	2472	93.07 u	PMMA
✓	13	98.0721	1370	98.07 u	GTP
✓	14	101.0567	1869	101.06 u	PMMA
✓	15	103.0389	713	103.05 u	PEG

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: left click Add

use selected channel Delete All

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...

SF = 100000.000, K0 = 0.000, Positive

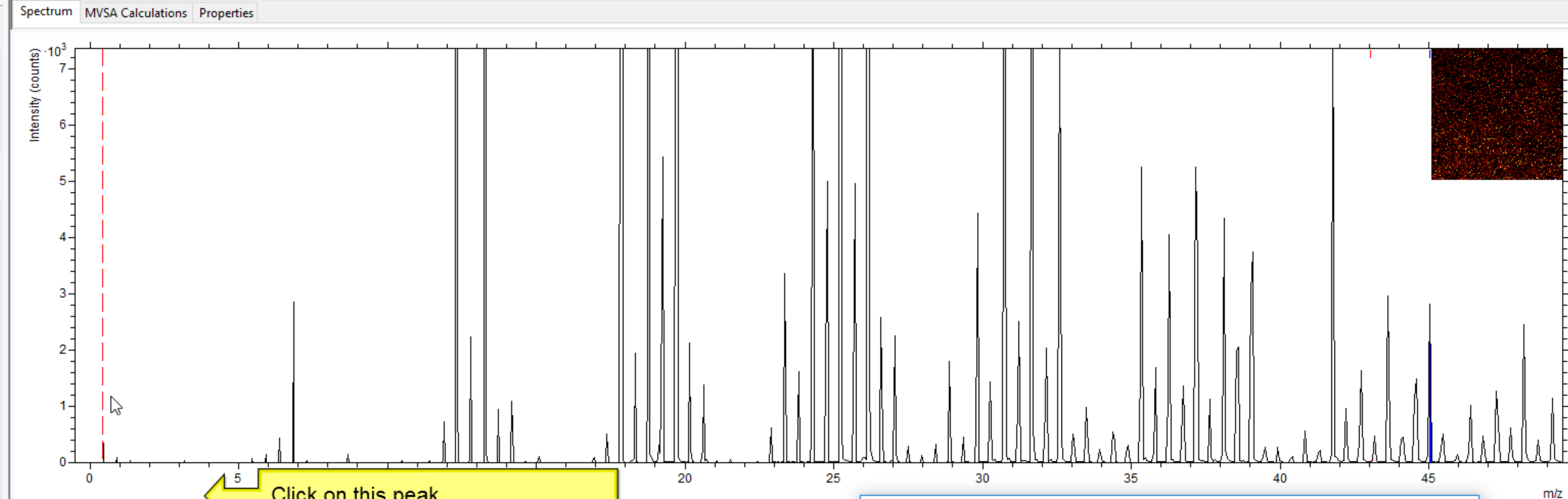
Options... Autocalibrate As Default... Revoke Recalibrate

m/z 0.4415 Area (cts) 8,642 Explained (%) 0.0 Resolution 1,672
 Dev. (ppm) ? Counts / Shot 0.0073 Peak Difference... Width (ns) 0.99

Compilations

Spectra

S1_HMR_01_0 *
 <No Sample Name> (S1_HMR_01) *
 S1_HMR_02_0
 <No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts		
Mass Intervals					
<input checked="" type="checkbox"/>	2	43.0569	248		
<input checked="" type="checkbox"/>	3	45.0333	5989	45.03 u	PEG
<input checked="" type="checkbox"/>	4	59.0125	945	59.01 u	PMMA
<input checked="" type="checkbox"/>	5	59.0520	1168	59.05 u	PEG
<input checked="" type="checkbox"/>	6	69.0353	727	69.04 u	PMMA
<input checked="" type="checkbox"/>	7	69.0770	390	69.08 u	
<input checked="" type="checkbox"/>	8	73.0391	3021	73.03 u	PEG
<input checked="" type="checkbox"/>	9	87.0494	3388	87.05 u	PEG
<input checked="" type="checkbox"/>	10	89.0670	643	89.06 u	PEG
<input checked="" type="checkbox"/>	11	91.0554	2212	91.05 u	PS
<input checked="" type="checkbox"/>	12	93.0712	2472	93.07 u	PMMA
<input checked="" type="checkbox"/>	13	98.0721	1370	98.07 u	GTP
<input checked="" type="checkbox"/>	14	101.0567	1869	101.06 u	PMMA
<input checked="" type="checkbox"/>	15	103.0389	713	103.05 u	PEG

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion:

use selected channel

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...

SF = 100000.000, K0 = 0.000, Positive

Channel: 33222.80

Options... Autocalibrate As Default... Revoke Recalibrate

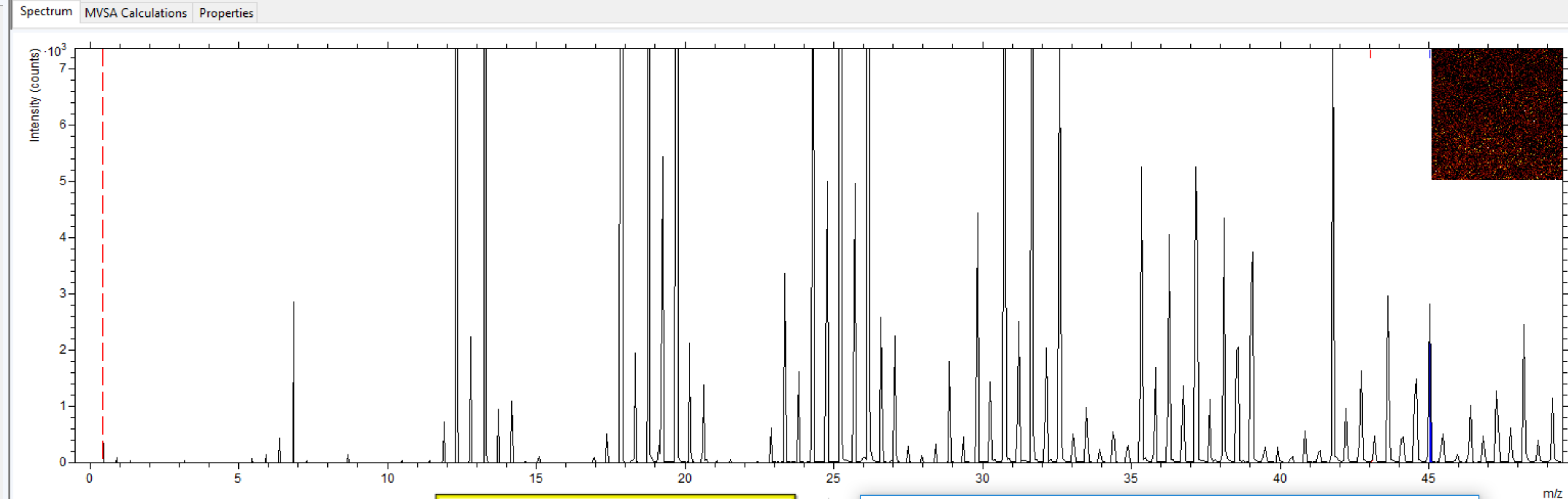
m/z 0.4415 Area (cts) 8,642 Explained (%) 0.0 Resolution 1,672
 Dev. (ppm) ? Counts / Shot 0.0073 Peak Difference... Width (ns) 0.99

Compilations

Spectra

Spectra

S1_HMR_01_0 *
 <No Sample Name> (S1_HMR_01) *
 S1_HMR_02_0
 <No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts	Color	Peak Label	Descri
Mass Intervals						
<input checked="" type="checkbox"/>	2	43.0569	248	Red	43.06 u	C3H7
<input checked="" type="checkbox"/>	3	45.0333	5989	Blue	45.03 u	PEG
<input checked="" type="checkbox"/>	4	59.0125	945	Olive	59.01 u	PMMA
<input checked="" type="checkbox"/>	5	59.0520	1168	Green	59.05 u	PEG
<input checked="" type="checkbox"/>	6	69.0353	727	Grey	69.04 u	PMMA
<input checked="" type="checkbox"/>	7	69.0770	390	Red	69.08 u	
<input checked="" type="checkbox"/>	8	73.0391	3021	Grey	73.03 u	PEG
<input checked="" type="checkbox"/>	9	87.0494	3388	Orange	87.05 u	PEG
<input checked="" type="checkbox"/>	10	89.0670	643	Blue	89.06 u	PEG
<input checked="" type="checkbox"/>	11	91.0554	2212	Red	91.05 u	PS
<input checked="" type="checkbox"/>	12	93.0712	2472	Yellow	93.07 u	PMMA
<input checked="" type="checkbox"/>	13	98.0721	1370	Blue	98.07 u	GTP
<input checked="" type="checkbox"/>	14	101.0567	1869	Green	101.06 u	PMMA
<input checked="" type="checkbox"/>	15	103.0389	713	Light Green	103.05 u	PEG

Then type 'H' in the 'Ion' box and press the 'Add' button. You can also just hit <Enter>.

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: [H]

use selected channel

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...

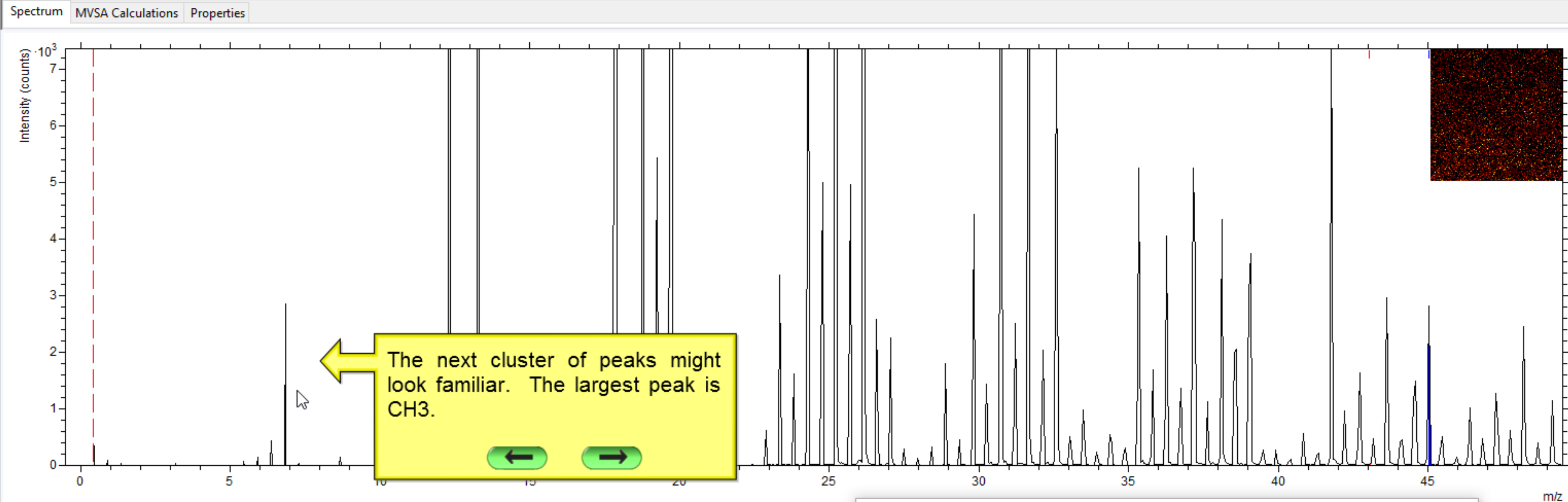
SF = 100000.000, K0 = 0.000, Positive

Channel: 33222.80

Compilations

Spectra

S1_HMR_01_0 *
 <No Sample Name> (S1_HMR_01) *
 S1_HMR_02_0
 <No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
<input checked="" type="checkbox"/>	2	43.0569	248	Red	43.06 u	C3H7
<input checked="" type="checkbox"/>	3	45.0333	5989	Blue	45.03 u	PEG
<input checked="" type="checkbox"/>	4	59.0125	945	Olive	59.01 u	PMMA
<input checked="" type="checkbox"/>	5	59.0520	1168	Green	59.05 u	PEG
<input checked="" type="checkbox"/>	6	69.0353	727	Grey	69.04 u	PMMA
<input checked="" type="checkbox"/>	7	69.0770	390	Red	69.08 u	
<input checked="" type="checkbox"/>	8	73.0391	3021	Grey	73.03 u	PEG
<input checked="" type="checkbox"/>	9	87.0494	3388	Orange	87.05 u	PEG
<input checked="" type="checkbox"/>	10	89.0670	643	Blue	89.06 u	PEG
<input checked="" type="checkbox"/>	11	91.0554	2212	Red	91.05 u	PS
<input checked="" type="checkbox"/>	12	93.0712	2472	Yellow	93.07 u	PMMA
<input checked="" type="checkbox"/>	13	98.0721	1370	Blue	98.07 u	GTP
<input checked="" type="checkbox"/>	14	101.0567	1869	Green	101.06 u	PMMA
<input checked="" type="checkbox"/>	15	103.0389	713	Light Green	103.05 u	PEG

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: Add

use selected channel Delete All

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...
H+	30	1...	1.\$	1.\$	0.01

SF = 100000.000, K0 = 0.000, Positive

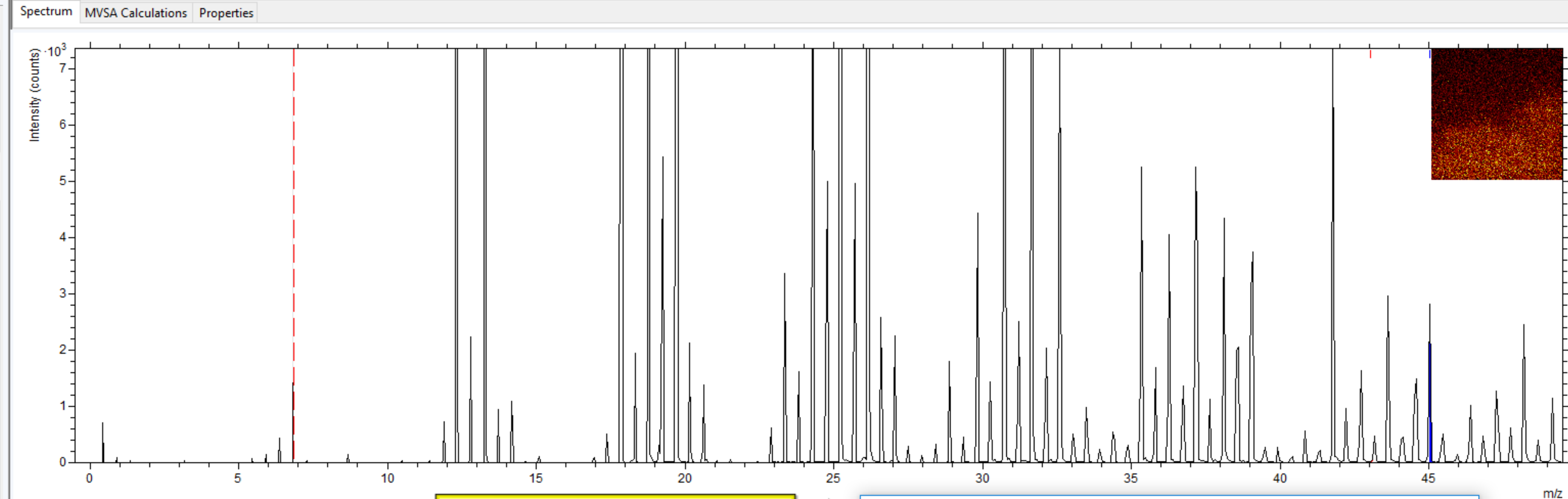
Options... Autocalibrate As Default... Revoke Recalibrate

m/z 6.8396 Area (cts) 51,600 Explained (%) 0.0 Resolution 4,290
 Dev. (ppm) ? Counts / Shot 0.0437 Peak Difference... Width (ns) 1.52

Compilations

Spectra

- Spectra
- S1_HMR_01_0 *
 - <No Sample Name> (S1_HMR_01) * +
 - S1_HMR_02_0
 - <No Sample Name> (S1_HMR_02) +



V	No.	m / z	Area / cts	Color	Peak Label	Descri
Mass Intervals						
<input checked="" type="checkbox"/>	2	43.0569	248	Red	43.06 u	C3H7
<input checked="" type="checkbox"/>	3	45.0333	5989	Blue	45.03 u	PEG
<input checked="" type="checkbox"/>	4	59.0125	945	Olive	59.01 u	PMMA
<input checked="" type="checkbox"/>	5	59.0520	1168	Green	59.05 u	PEG
<input checked="" type="checkbox"/>	6	69.0353	727	Grey	69.04 u	PMMA
<input checked="" type="checkbox"/>	7	69.0770	390	Red	69.08 u	
<input checked="" type="checkbox"/>	8	73.0391	3021	Grey	73.03 u	PEG
<input checked="" type="checkbox"/>	9	87.0494	3388	Orange	87.05 u	PEG
<input checked="" type="checkbox"/>	10	89.0670	643	Blue	89.06 u	PEG
<input checked="" type="checkbox"/>	11	91.0554	2212	Red	91.05 u	PS
<input checked="" type="checkbox"/>	12	93.0712	2472	Yellow	93.07 u	PMMA
<input checked="" type="checkbox"/>	13	98.0721	1370	Blue	98.07 u	GTP
<input checked="" type="checkbox"/>	14	101.0567	1869	Green	101.06 u	PMMA
<input checked="" type="checkbox"/>	15	103.0389	713	Light Green	103.05 u	PEG

Click on the CH3 peak, type the name in the 'Ion' box and press 'Add' (or hit <enter>).

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: CH3

use selected channel

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...
H+	30	1...	1.\$	1.\$	0.01

SF = 100000.000, K0 = 0.000, Positive

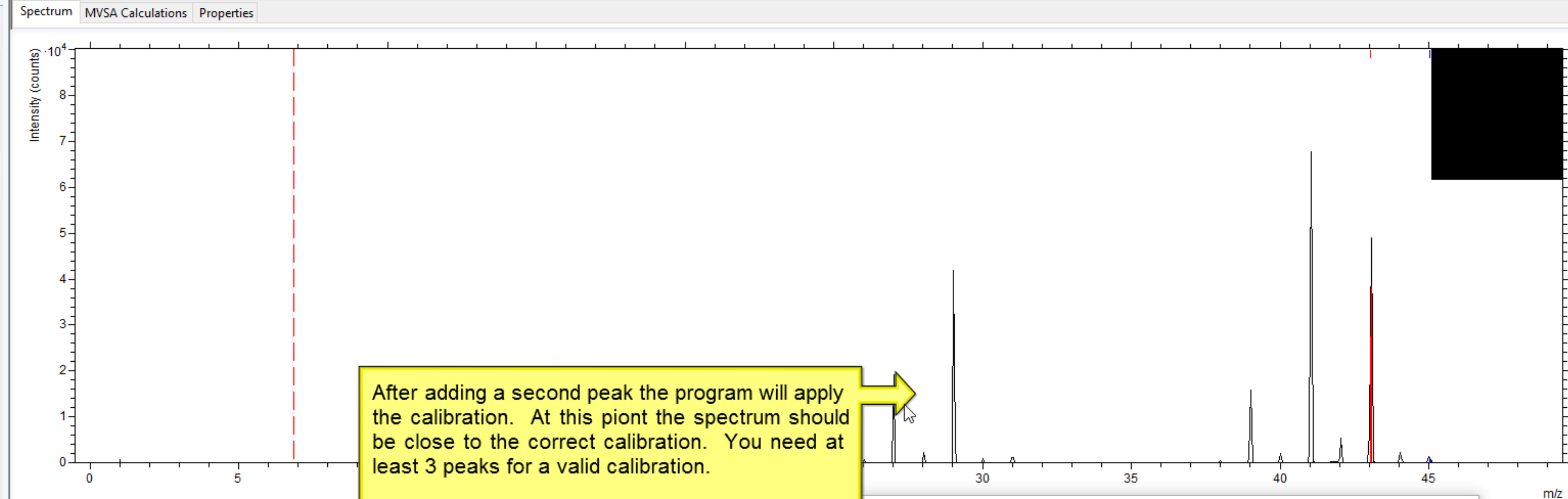
Channel: 130763.33

m/z 6.8396 Area (cts) Explained (%) 0.0 Resolution
 Dev. (ppm) Counts / Shot Peak Difference... Width (ns) 0.00

Compilations

Spectra

- Spectra
- S1_HMR_01_0 *
 - <No Sample Name> (S1_HMR_01) *
 - S1_HMR_02_0
 - <No Sample Name> (S1_HMR_02)



After adding a second peak the program will apply the calibration. At this point the spectrum should be close to the correct calibration. You need at least 3 peaks for a valid calibration.

V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
<input checked="" type="checkbox"/>	2	43.0558	873874	Red	43.06 u	C3H7
<input checked="" type="checkbox"/>	3	45.0342	32389	Blue	45.03 u	PEG
<input checked="" type="checkbox"/>	4	59.0121	53409	Olive	59.01 u	PMMA
<input checked="" type="checkbox"/>	5	59.0496	37584	Green	59.05 u	PEG
<input checked="" type="checkbox"/>	6	69.0356	122335	Grey	69.04 u	PMMA
<input checked="" type="checkbox"/>	7	69.0749	351368	Red	69.08 u	
<input checked="" type="checkbox"/>	8	73.0327	17312	Grey	73.03 u	PEG
<input checked="" type="checkbox"/>	9	87.0455	5925	Orange	87.05 u	PEG
<input checked="" type="checkbox"/>	10	89.0605	3378	Blue	89.06 u	PEG
<input checked="" type="checkbox"/>	11	91.0539	236503	Red	91.05 u	PS
<input checked="" type="checkbox"/>	12	93.0705	56308	Yellow	93.07 u	PMMA
<input checked="" type="checkbox"/>	13	98.0732	73400	Blue	98.07 u	GTP
<input checked="" type="checkbox"/>	14	101.0576	27812	Green	101.06 u	PMMA
<input checked="" type="checkbox"/>	15	103.0471	37193	Light Green	103.05 u	PEG

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion:

use selected channel

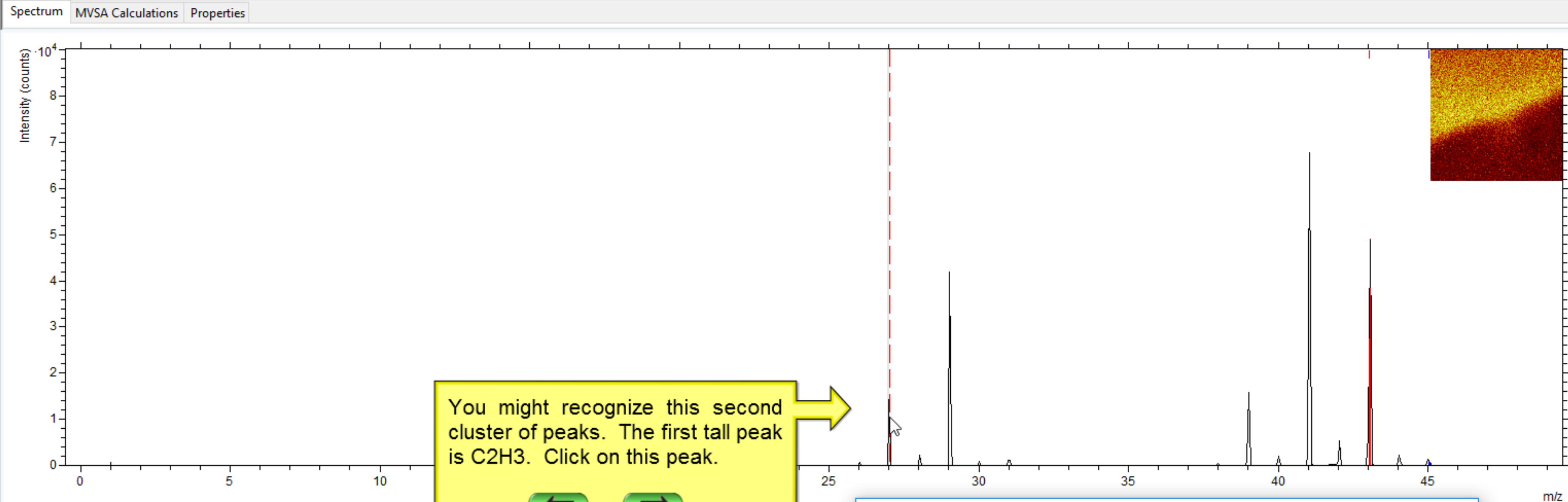
Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...	
H+	30	1...	-0.0	-0.0	0.01	✓
CH ₃ ⁺	10	15...	-0.0	-0.0	0.04	✓

SF = 67917.824, K0 = -1718.879, Positive

BeH_20+ m/z 27.0223 Area (cts) 352,554 Explained (%) 100.0 Resolution 5,572
 Check... Add Peak Dev. (ppm) 3.9 Counts / Shot 0.2989 Peak Difference... Width (ns) 1.58

Compilations Spectra

S1_HMR_01_0 *
 <No Sample Name> (S1_HMR_01) *
 S1_HMR_02_0
 <No Sample Name> (S1_HMR_02)



You might recognize this second cluster of peaks. The first tall peak is C2H3. Click on this peak.

V	No.	m / z	Area / cts	Color	Peak Label	Description
✓	2	43.0558	873874	Red	43.06 u	C3H7
✓	3	45.0342	32389	Blue	45.03 u	PEG
✓	4	59.0121	53409	Olive	59.01 u	PMMA
✓	5	59.0496	37584	Green	59.05 u	PEG
✓	6	69.0356	122335	Grey	69.04 u	PMMA
✓	7	69.0749	351368	Red	69.08 u	
✓	8	73.0327	17312	Grey	73.03 u	PEG
✓	9	87.0455	5925	Orange	87.05 u	PEG
✓	10	89.0605	3378	Blue	89.06 u	PEG
✓	11	91.0539	236503	Red	91.05 u	PS
✓	12	93.0705	56308	Yellow	93.07 u	PMMA
✓	13	98.0732	73400	Blue	98.07 u	GTP
✓	14	101.0576	27812	Green	101.06 u	PMMA
✓	15	103.0471	37193	Light Green	103.05 u	PEG

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: BeH_20+ Add Delete All

use selected channel

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...
H+	30	1...	-0.0	-0.0	0.01 ✓
CH_3+	10	15...	-0.0	-0.0	0.04 ✓

SF = 67917.824, K0 = -1718.879, Positive

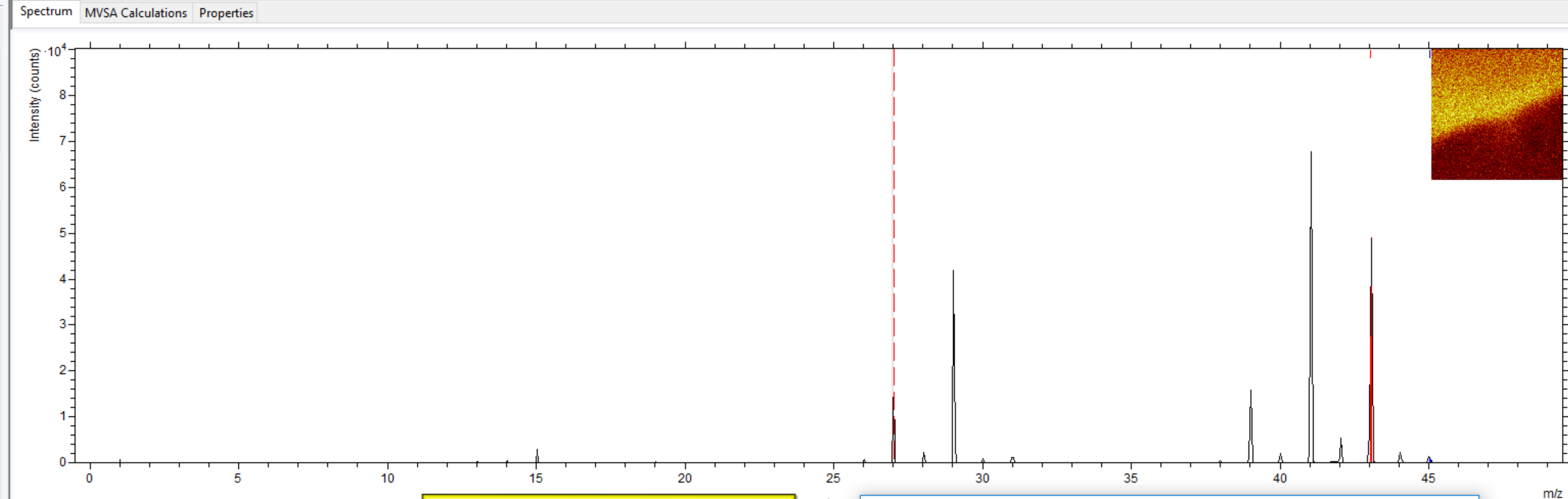
Channel: 175669.11

Options... Autocalibrate As Default... Revoke Recalibrate

BeH_20+ m/z 27.0223 Area (cts) 352,554 Explained (%) 100.0 Resolution 5,572
 Check... Add Peak Dev. (ppm) 3.9 Counts / Shot 0.2989 Peak Difference... Width (ns) 1.58

Compilations
 Spectra

Spectra
 S1_HMR_01_0 *
 <No Sample Name> (S1_HMR_01) *
 S1_HMR_02_0
 <No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts	Color	Peak Label	Des
✓	2	43.0558	873874	Red	43.06 u	C3H
✓	3	45.0342	32389	Blue	45.03 u	PEG
✓	4	59.0121	53409	Olive	59.01 u	PMMA
✓	5	59.0496	37584	Green	59.05 u	PEG
✓	6	69.0356	122335	Grey	69.04 u	PMMA
✓	7	69.0749	351368	Red	69.08 u	
✓	8	73.0327	17312	Grey	73.03 u	PEG
✓	9	87.0455	5925	Orange	87.05 u	PEG
✓	10	89.0605	3378	Blue	89.06 u	PEG
✓	11	91.0539	236503	Red	91.05 u	PS
✓	12	93.0705	56308	Yellow	93.07 u	PMMA
✓	13	98.0732	73400	Blue	98.07 u	GTP
✓	14	101.0576	27812	Green	101.06 u	PMMA
✓	15	103.0471	37193	Light Green	103.05 u	PEG

After at least 2 peaks have been added the software will try to predict the identity of the peak you clicked on. Here it has guessed wrong.

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: BeH_20+ Add Delete All

use selected channel

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...
H+	30	1...	-0.0	-0.0	0.01 ✓
CH_3+	10	15...	-0.0	-0.0	0.04 ✓

SF = 67917.824, K0 = -1718.879, Positive

Channel: 175669.11

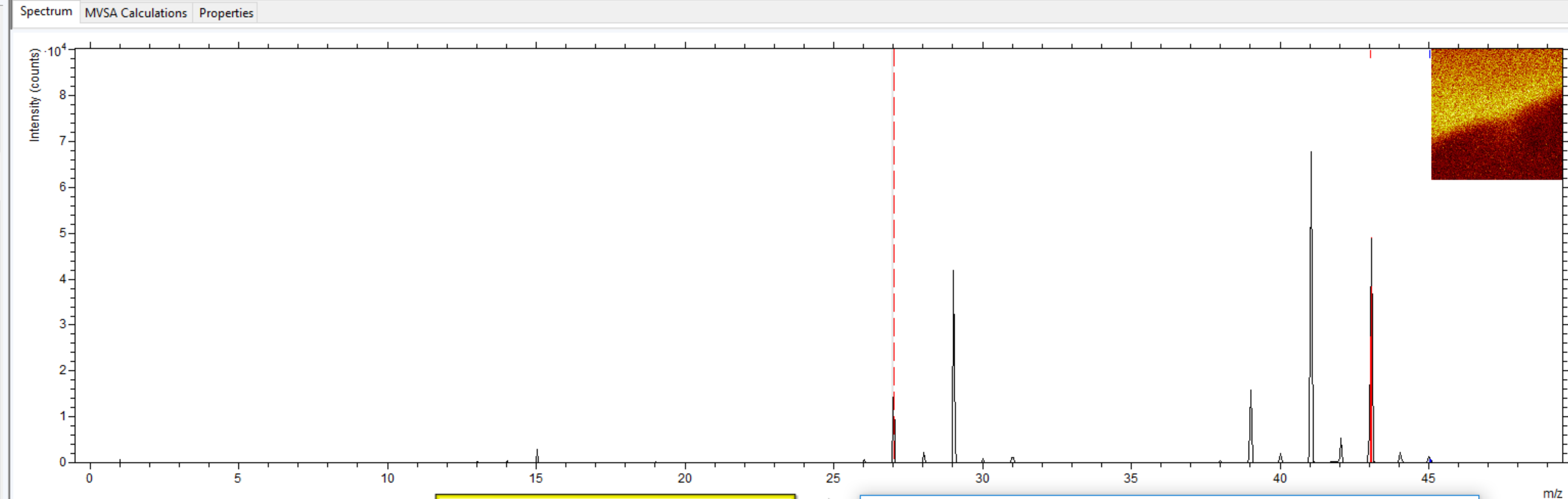
Options... Autocalibrate As Default... Revoke Recalibrate

BeH_20+ m/z 27.0223 Area (cts) 352,554 Explained (%) 100.0 Resolution 5,572
 Check... Add Peak Dev. (ppm) 3.9 Counts / Shot 0.2989 Peak Difference... Width (ns) 1.58

Compilations Spectra

Spectra

S1_HMR_01_0 *
 <No Sample Name> (S1_HMR_01) *
 S1_HMR_02_0
 <No Sample Name> (S1_HMR_02)



MassListPos

V	No.	m / z	Area / cts	Color	Peak Label	Descri
Mass Intervals						
<input checked="" type="checkbox"/>	2	43.0558	873874	Red	43.06 u	C3H7
<input checked="" type="checkbox"/>	3	45.0342	32389	Blue	45.03 u	PEG
<input checked="" type="checkbox"/>	4	59.0121	53409	Olive	59.01 u	PMMA
<input checked="" type="checkbox"/>	5	59.0496	37584	Green	59.05 u	PEG
<input checked="" type="checkbox"/>	6	69.0356	122335	Grey	69.04 u	PMMA
<input checked="" type="checkbox"/>	7	69.0749	351368	Red	69.08 u	
<input checked="" type="checkbox"/>	8	73.0327	17312	Grey	73.03 u	PEG
<input checked="" type="checkbox"/>	9	87.0455	5925	Orange	87.05 u	PEG
<input checked="" type="checkbox"/>	10	89.0605	3378	Blue	89.06 u	PEG
<input checked="" type="checkbox"/>	11	91.0539	236503	Red	91.05 u	PS
<input checked="" type="checkbox"/>	12	93.0705	56308	Yellow	93.07 u	PMMA
<input checked="" type="checkbox"/>	13	98.0732	73400	Blue	98.07 u	GTP
<input checked="" type="checkbox"/>	14	101.0576	27812	Green	101.06 u	PMMA
<input checked="" type="checkbox"/>	15	103.0471	37193	Light Green	103.05 u	PEG

Correct the text to say C2H3 and press 'Add' (or hit <Enter>).

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: C2H3 Add Delete All

use selected channel

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...
H+	30	1...	-0.0	-0.0	0.01 ✓
CH_3+	10	15...	-0.0	-0.0	0.04 ✓

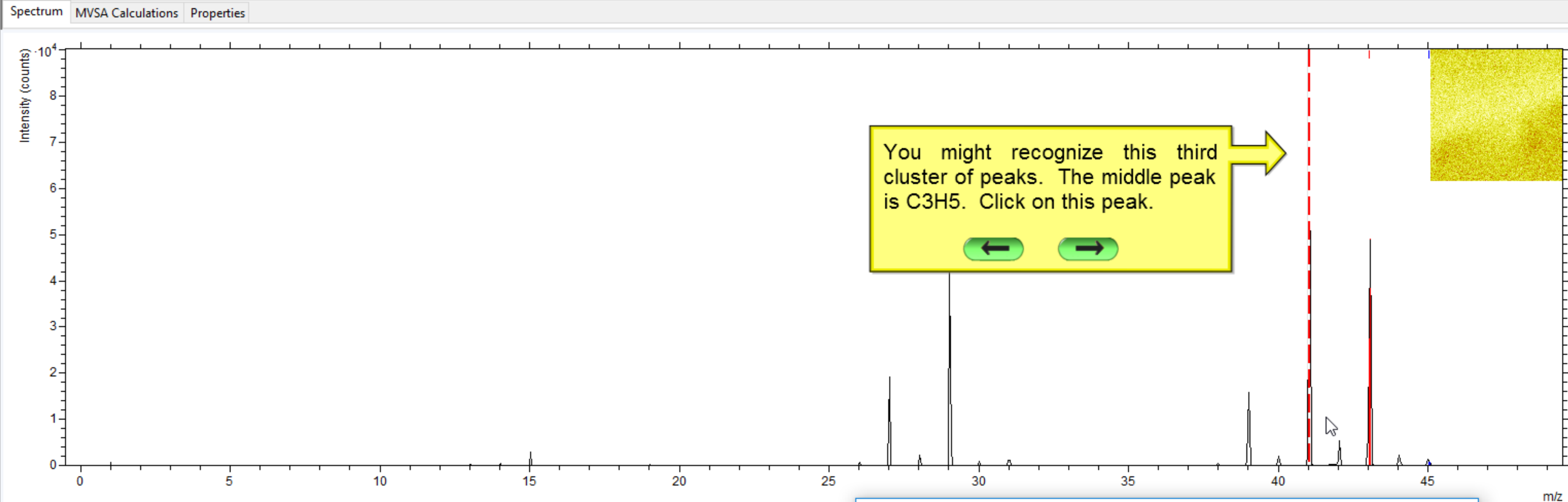
SF = 67917.824, K0 = -1718.879, Positive

Channel: 175669.11

Options... Autocalibrate As Default... Revoke Recalibrate

C_3H_5+ m/z 41.0401 Area (cts) 1,548,829 Explained (%) 100.0 Resolution 5,836
 Check... Add Peak Dev. (ppm) 38.3 Counts / Shot 1.3130 Peak Difference... Width (ns) 1.86

Compilations Spectra S1_HMR_01_0 * <No Sample Name> (S1_HMR_01) * S1_HMR_02_0 <No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
✓	2	43.0563	874524	Red	43.06 u	C3H7
✓	3	45.0349	32640	Blue	45.03 u	PEG
✓	4	59.0131	52707	Olive	59.01 u	PMMA
✓	5	59.0506	37453	Green	59.05 u	PEG
✓	6	69.0368	120075	Grey	69.04 u	PMMA
✓	7	69.0757	358653	Red	69.08 u	
✓	8	73.0335	16832	Grey	73.03 u	PEG
✓	9	87.0468	6050	Orange	87.05 u	PEG
✓	10	89.0612	3651	Blue	89.06 u	PEG
✓	11	91.0555	238167	Red	91.05 u	PS
✓	12	93.0719	55716	Yellow	93.07 u	PMMA
✓	13	98.0749	71380	Blue	98.07 u	GTP
✓	14	101.0592	27408	Green	101.06 u	PMMA
✓	15	103.0483	35923	Light Green	103.05 u	PEG

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: C_3H_5+ Add Delete All

use selected channel

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...
H+	30	1...	-16.4	-0.0	0.01 ✓
CH_3+	10	15...	13.5	0.2	0.04 ✓
C_2H_3+	5	27...	-6.9	-0.2	0.30 ✓

SF = 67917.010, K0 = -1717.501, Positive

Channel: 216688.21

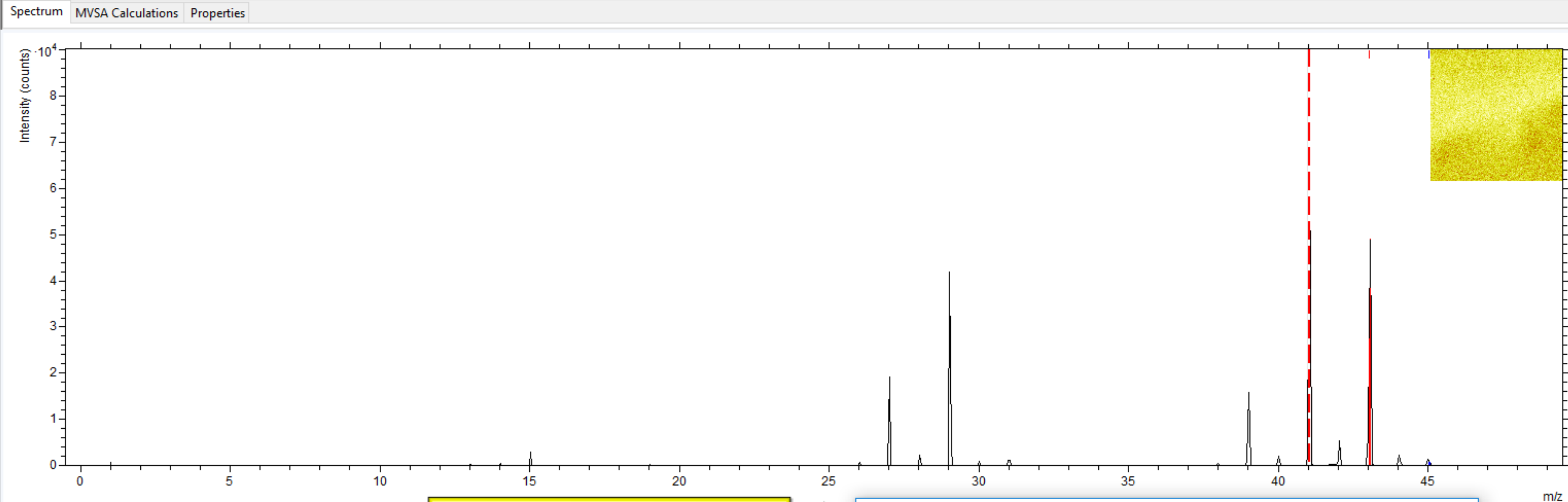
Options... Autocalibrate As Default... Revoke Recalibrate

C_3H_5+	m/z	41.0401	Area (cts)	1,548,829	Explained (%)	100.0	Resolution	5,836
Check...	Dev. (ppm)	38.3	Counts / Shot	1.3130	Peak Difference...		Width (ns)	1.86

Compilations

Spectra

- S1_HMR_01_0 *
 - <No Sample Name> (S1_HMR_01) *
 - S1_HMR_02_0
 - <No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts	Color	Peak Label	Descri
Mass Intervals						
✓	2	43.0563	874524	Red	43.06 u	C3H7
✓	3	45.0349	32640	Blue	45.03 u	PEG
✓	4	59.0131	52707	Olive	59.01 u	PMMA
✓	5	59.0506	37453	Green	59.05 u	PEG
✓	6	69.0368	120075	Grey	69.04 u	PMMA
✓	7	69.0757	358653	Red	69.08 u	
✓	8	73.0335	16832	Grey	73.03 u	PEG
✓	9	87.0468	6050	Orange	87.05 u	PEG
✓	10	89.0612	3651	Blue	89.06 u	PEG
✓	11	91.0555	238167	Red	91.05 u	PS
✓	12	93.0719	55716	Yellow	93.07 u	PMMA
✓	13	98.0749	71380	Blue	98.07 u	GTP
✓	14	101.0592	27408	Green	101.06 u	PMMA
✓	15	103.0483	35923	Light Green	103.05 u	PEG

This time the software got it correct.

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: C_3H_5+

use selected channel

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...	
H+	30	1...	-16.4	-0.0	0.01	✓
CH_3+	10	15...	13.5	0.2	0.04	✓
C_2H_3+	5	27...	-6.9	-0.2	0.30	✓

SF = 67917.010, K0 = -1717.501, Positive

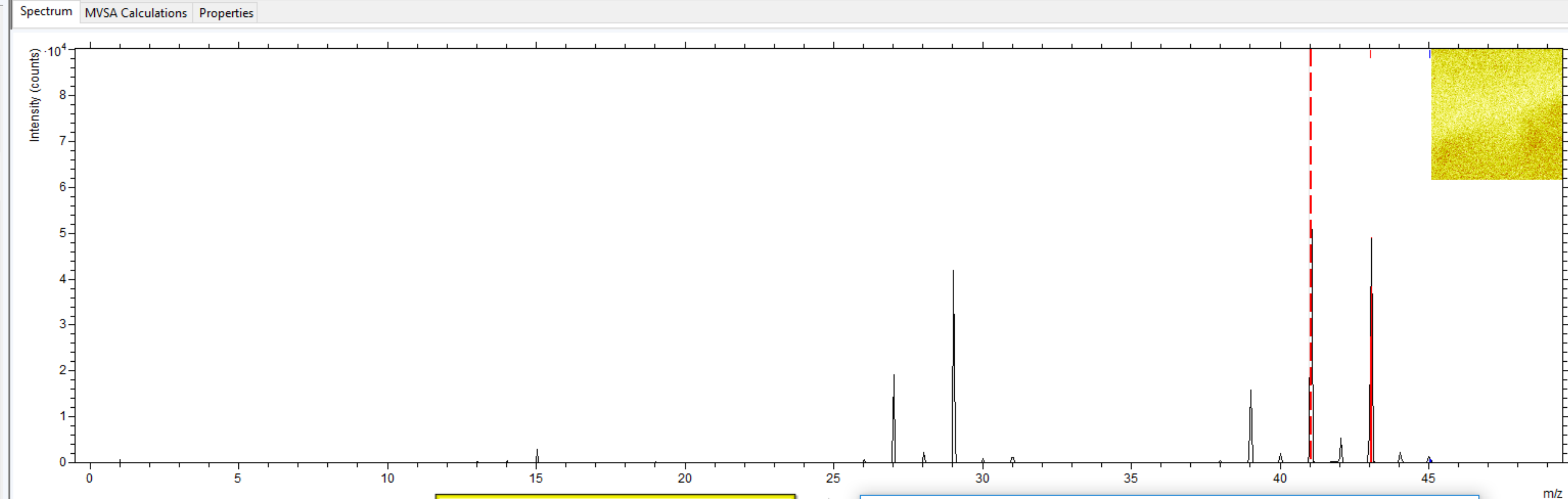
Channel: 216688.21

C ₃ H ₅ ⁺	m/z	41.0401	Area (cts)	1,548,829	Explained (%)	100.0	Resolution	5,836
Check...	Dev. (ppm)	38.3	Counts / Shot	1.3130	Peak Difference...		Width (ns)	1.86

Compilations

Spectra

- S1_HMR_01_0 *
 - <No Sample Name> (S1_HMR_01) *
 - S1_HMR_02_0
 - <No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts	Color	Peak Label	Descri
Mass Intervals						
✓	2	43.0563	874524	Red	43.06 u	C3H7
✓	3	45.0349	32640	Blue	45.03 u	PEG
✓	4	59.0131	52707	Olive	59.01 u	PMMA
✓	5	59.0506	37453	Green	59.05 u	PEG
✓	6	69.0368	120075	Grey	69.04 u	PMMA
✓	7	69.0757	358653	Red	69.08 u	
✓	8	73.0335	16832	Grey	73.03 u	PEG
✓	9	87.0468	6050	Orange	87.05 u	PEG
✓	10	89.0612	3651	Blue	89.06 u	PEG
✓	11	91.0555	238167	Red	91.05 u	PS
✓	12	93.0719	55716	Yellow	93.07 u	PMMA
✓	13	98.0749	71380	Blue	98.07 u	GTP
✓	14	101.0592	27408	Green	101.06 u	PMMA
✓	15	103.0483	35923	Light Green	103.05 u	PEG

Press 'Add' (or hit <Enter>) to add it to the calibration list.

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: C₃H₅⁺ Add

use selected channel Delete All

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...	
H ⁺	30	1...	-16.4	-0.0	0.01	✓
CH ₃ ⁺	10	15...	13.5	0.2	0.04	✓
C ₂ H ₃ ⁺	5	27...	-6.9	-0.2	0.30	✓

SF = 67917.010, K0 = -1717.501, Positive

Channel: 216688.21

Options... Autocalibrate As Default... Revoke Recalibrate

C_3H_5+	m/z	41.0401	Area (cts)	1,548,829	Explained (%)	100.0	Resolution	5,836
Check...	Dev. (ppm)	38.3	Counts / Shot	1.3130	Peak Difference...		Width (ns)	1.86

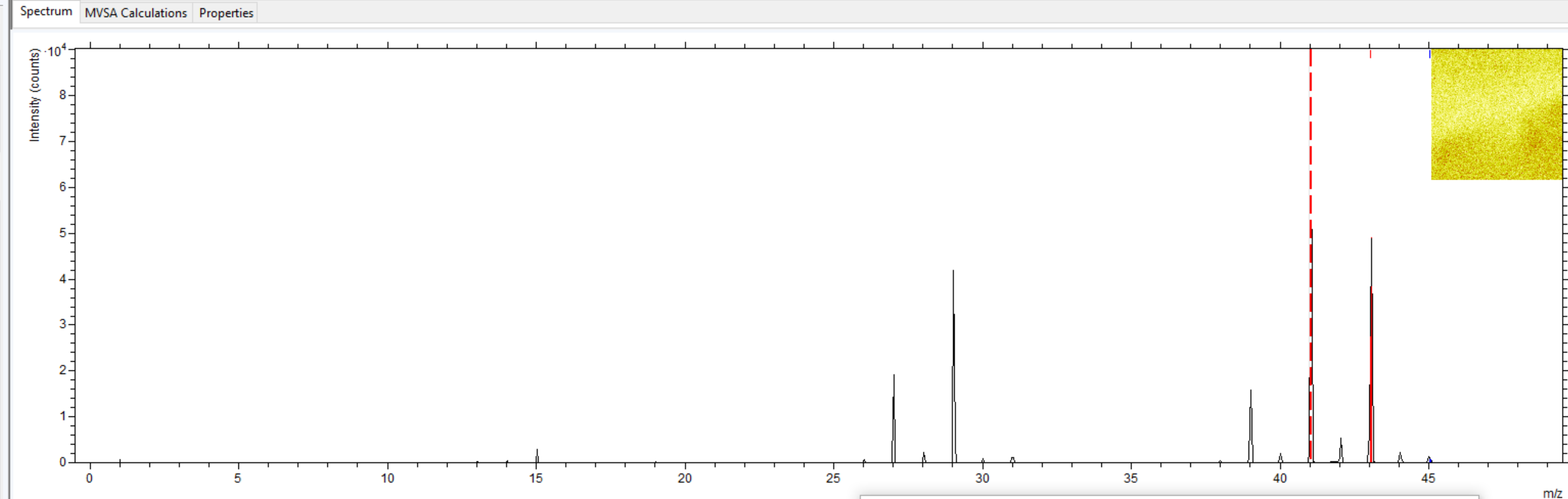
Compilations

Spectra

Spectra

S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *

S1_HMR_02_0
<No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
<input checked="" type="checkbox"/>	2	43.0563	874524	Red	43.06 u	C3H7
<input checked="" type="checkbox"/>	3	45.0349	32640	Blue	45.03 u	PEG
<input checked="" type="checkbox"/>	14	101.0592	27408	Green	101.06 u	PMMA
<input checked="" type="checkbox"/>	15	103.0483	35923	Light Green	103.05 u	PEG

If the newly added peak is highlighted in red, this means that the selected peak is saturated. Though it is in the list, it is not used in the calibration.

As seen here the 'Counts/' entry is above 1. If the Counts are below 2 you can still use the peak in the calibration.

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion:

use selected channel

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...
H+	30	1...	-16.4	-0.0	0.01
CH_3+	10	15...	13.5	0.2	0.04
C_2H_3+	5	27...	-6.9	-0.2	0.30
C_3H_5+	5	41...	38.3	1.6	1.31

SF = 67917.010, K0 = -1717.501, Positive

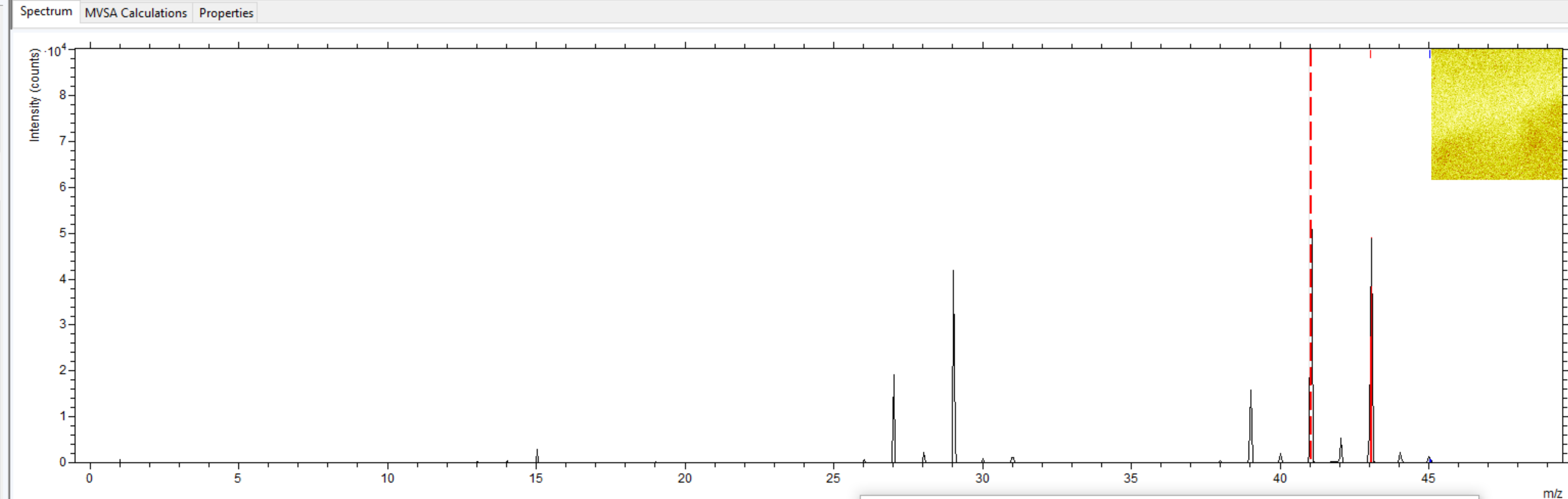
Options... Autocalibrate As Default... Revoke Recalibrate

C_3H_5+	m/z	41.0401	Area (cts)	1,548,829	Explained (%)	100.0	Resolution	5,836
Check...	Dev. (ppm)	38.3	Counts / Shot	1.3130	Peak Difference...		Width (ns)	1.86

Compilations

Spectra

- S1_HMR_01_0 *
 - <No Sample Name> (S1_HMR_01) *
 - S1_HMR_02_0
 - <No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
✓	2	43.0563	874524	Red	43.06 u	C3H7
✓	3	45.0349	32640	Blue	45.03 u	PEG
✓	4	59.0131	52707	Olive	59.01 u	PMMA
✓	5	59.0506	37453	Green	59.05 u	PEG
✓	6	69.0368	120075	Grey	69.04 u	PMMA
✓	7	69.0757	358653	Red	69.08 u	
✓	8	73.0335	16832	Grey	73.03 u	PEG
✓	9	87.0468	6050	Orange	87.05 u	PEG
✓	10	89.0612	3651	Blue	89.06 u	PEG
✓	11	91.0555	238167	Red	91.05 u	PS
✓	12	93.0719	55716	Yellow	93.07 u	PMMA
✓	13	98.0749	71380	Blue	98.07 u	GTP
✓	14	101.0592	27408	Green	101.06 u	PMMA
✓	15	103.0483	35923	Light Green	103.05 u	PEG

To do so, press the 'Options...' button.

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion:

use selected channel

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...
H+	30	1...	-16.4	-0.0	0.01 ✓
CH_3+	10	15...	13.5	0.2	0.04 ✓
C_2H_3+	5	27...	-6.9	-0.2	0.30 ✓
C_3H_5+	5	41...	38.3	1.6	1.31

SF = 67917.010, K0 = -1717.501, Positive

Options... Autocalibrate As Default... Revoke Recalibrate

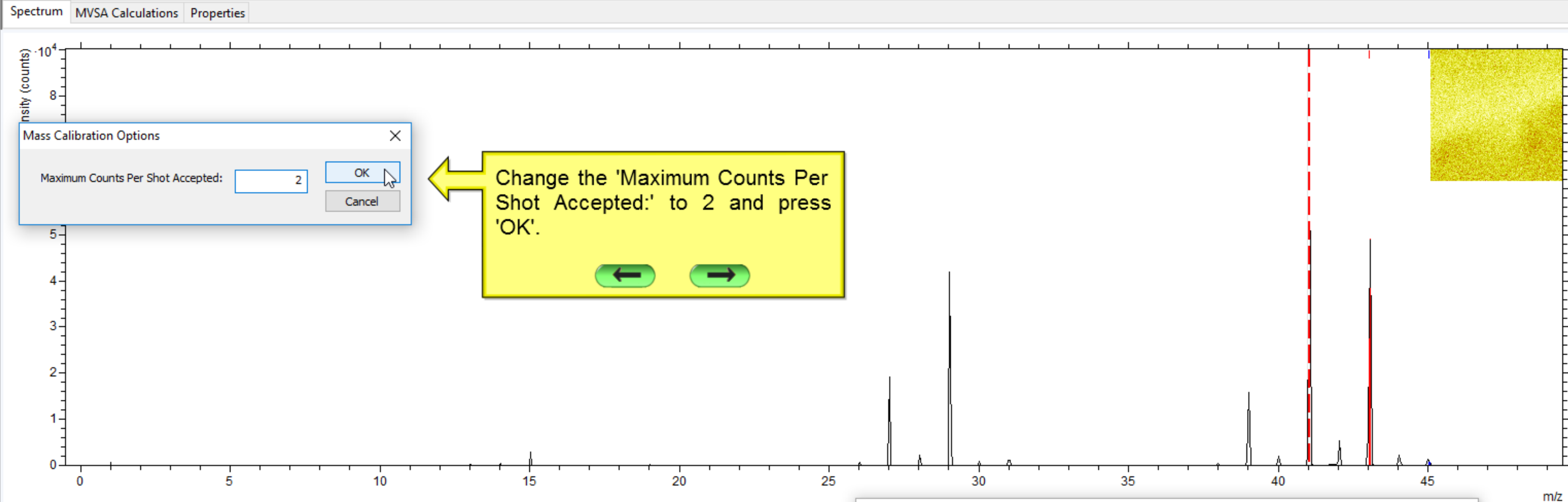
C_3H_5+	m/z	41.0401	Area (cts)	1,548,829	Explained (%)	100.0	Resolution	5,836
Check...	Dev. (ppm)	38.3	Counts / Shot	1.3130	Peak Difference...		Width (ns)	1.86

Compilations

Spectra

Spectra

S1_HMR_01_0 *
 <No Sample Name> (S1_HMR_01) *
 S1_HMR_02_0
 <No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
✓	2	43.0563	874524	Red	43.06 u	C3H7
✓	3	45.0349	32640	Blue	45.03 u	PEG
✓	4	59.0131	52707	Olive	59.01 u	PMMA
✓	5	59.0506	37453	Green	59.05 u	PEG
✓	6	69.0368	120075	Grey	69.04 u	PMMA
✓	7	69.0757	358653	Red	69.08 u	
✓	8	73.0335	16832	Grey	73.03 u	PEG
✓	9	87.0468	6050	Orange	87.05 u	PEG
✓	10	89.0612	3651	Blue	89.06 u	PEG
✓	11	91.0555	238167	Red	91.05 u	PS
✓	12	93.0719	55716	Yellow	93.07 u	PMMA
✓	13	98.0749	71380	Blue	98.07 u	GTP
✓	14	101.0592	27408	Green	101.06 u	PMMA
✓	15	103.0483	35923	Light Green	103.05 u	PEG

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion:

use selected channel

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...
H+	30	1...	-16.4	-0.0	0.01 ✓
CH_3+	10	15...	13.5	0.2	0.04 ✓
C_2H_3+	5	27...	-6.9	-0.2	0.30 ✓
C_3H_5+	5	41...	38.3	1.6	1.31

SF = 67917.010, K0 = -1717.501, Positive

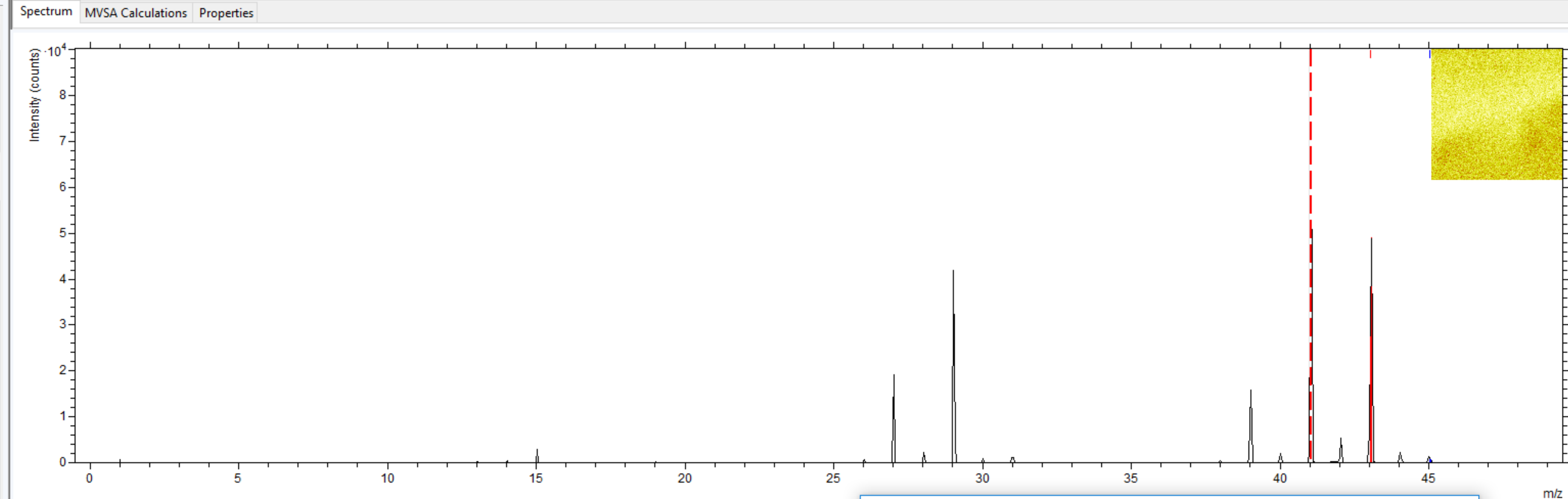
Options... Autocalibrate As Default... Revoke Recalibrate

C_3H_5+	m/z	41.0401	Area (cts)	1,548,829	Explained (%)	100.0	Resolution	5,836
Check...	Dev. (ppm)	38.3	Counts / Shot	1.3130	Peak Difference...		Width (ns)	1.86

Compilations

Spectra

- S1_HMR_01_0 *
 - <No Sample Name> (S1_HMR_01) *
 - S1_HMR_02_0
 - <No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
✓	2	43.0563	874524	Red	43.06 u	C3H7
✓	3	45.0349	32640	Blue	45.03 u	PEG
✓	4	59.0131	52707	Olive	59.01 u	PMMA
✓	5	59.0506	37453	Green	59.05 u	PEG
✓	6	69.0368	120075	Grey	69.04 u	PMMA
✓	7	69.0757	358653	Red	69.08 u	
✓	8	73.0335	16832	Grey	73.03 u	PEG
✓	9	87.0468	6050	Orange	87.05 u	PEG
✓	10	89.0612	3651	Blue	89.06 u	PEG
✓	11	91.0555	238167	Red	91.05 u	PS
✓	12	93.0719	55716	Yellow	93.07 u	PMMA
✓	13	98.0749	71380	Blue	98.07 u	GTP
✓	14	101.0592	27408	Green	101.06 u	PMMA
✓	15	103.0483	35923	Light Green	103.05 u	PEG

The entry is no longer red and will be used in the calibration.

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion:

use selected channel

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...
H+	30	1...	-16.4	-0.0	0.01 ✓
CH_3+	10	15...	13.5	0.2	0.04 ✓
C_2H_3+	5	27...	-6.9	-0.2	0.30 ✓
C_3H_5+	5	41...	38.3	1.6	1.31

SF = 67917.010, K0 = -1717.501, Positive

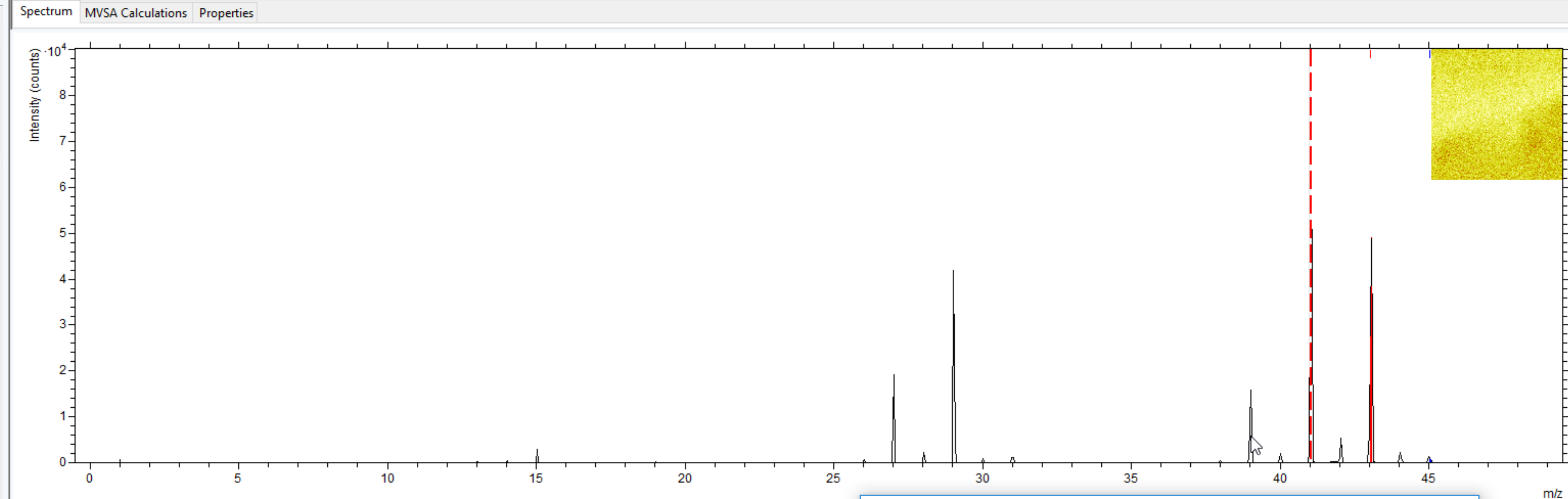
Options... Autocalibrate As Default... Revoke Recalibrate

C_3H_5+	m/z	41.0401	Area (cts)	1,548,829	Explained (%)	100.0	Resolution	5,836
Check...	Dev. (ppm)	38.3	Counts / Shot	1.3130	Peak Difference...		Width (ns)	1.86

Compilations

Spectra

- S1_HMR_01_0 *
 - <No Sample Name> (S1_HMR_01) *
 - S1_HMR_02_0
 - <No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
<input checked="" type="checkbox"/>	2	43.0563	874524	Red	43.06 u	C3H7
<input checked="" type="checkbox"/>	3	45.0349	32640	Blue	45.03 u	PEG
<input checked="" type="checkbox"/>	4	59.0131	52707	Olive	59.01 u	PMMA
<input checked="" type="checkbox"/>	5	59.0506	37453	Green	59.05 u	PEG
<input checked="" type="checkbox"/>	6	69.0368	120075	Grey	69.04 u	PMMA
<input checked="" type="checkbox"/>	7	69.0757	358653	Red	69.08 u	
<input checked="" type="checkbox"/>	8	73.0335	16832	Grey	73.03 u	PEG
<input checked="" type="checkbox"/>	9	87.0468	6050	Orange	87.05 u	PEG
<input checked="" type="checkbox"/>	10	89.0612	3651	Blue	89.06 u	PEG
<input checked="" type="checkbox"/>	11	91.0555	238167	Red	91.05 u	PS
<input checked="" type="checkbox"/>	12	93.0719	55716	Yellow	93.07 u	PMMA
<input checked="" type="checkbox"/>	13	98.0749	71380	Blue	98.07 u	GTP
<input checked="" type="checkbox"/>	14	101.0592	27408	Green	101.06 u	PMMA
<input checked="" type="checkbox"/>	15	103.0483	35923	Light Green	103.05 u	PEG

If the Counts/Shot is too high (>2) or you do not want to use the peak in the calibration, look for an alternate peak to include.

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion:

use selected channel

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...	
H+	30	1...	-16.4	-0.0	0.01	✓
CH_3+	10	15...	13.5	0.2	0.04	✓
C_2H_3+	5	27...	-6.9	-0.2	0.30	✓
C_3H_5+	5	41...	38.3	1.6	1.31	

SF = 67917.010, K0 = -1717.501, Positive

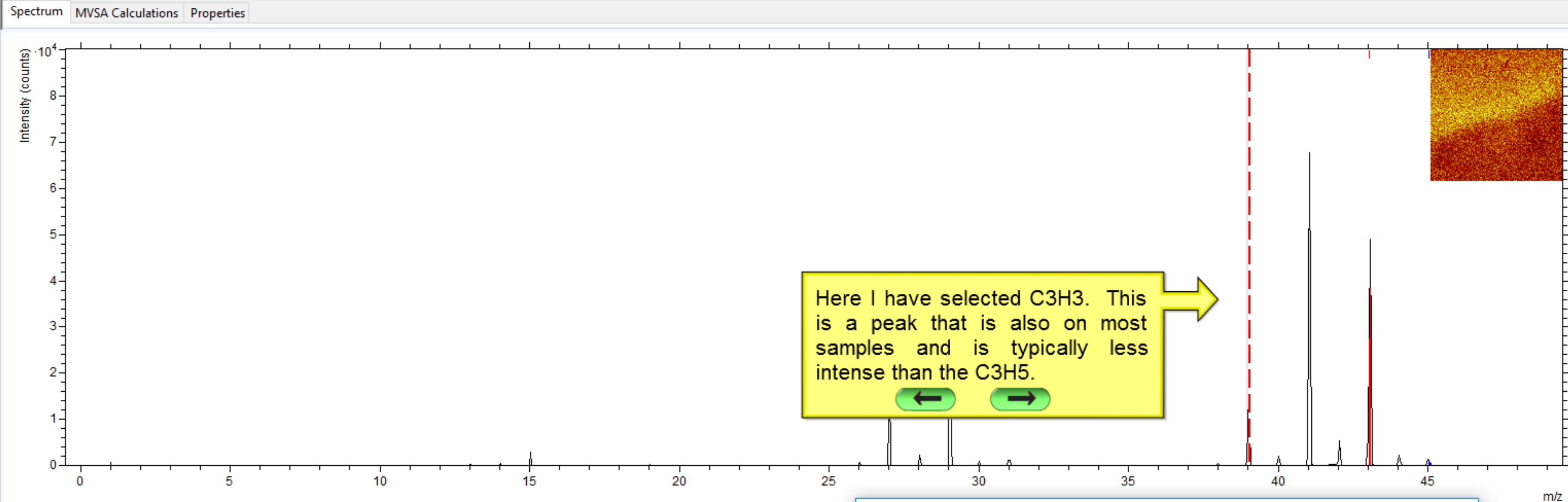
Options... Autocalibrate As Default... Revoke Recalibrate

C ₃ H ₃ ⁺	m/z	39.0228	Area (cts)	337,035	Explained (%)	100.0	Resolution	5,947
Check... Add Peak	Dev. (ppm)	-3.5	Counts / Shot	0.2857	Peak Difference...		Width (ns)	1.78

Compilations

Spectra

- Spectra
- S1_HMR_01_0 *
 - <No Sample Name> (S1_HMR_01) *
 - S1_HMR_02_0
 - <No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
✓	2	43.0563	874524	Red	43.06 u	C3H7
✓	3	45.0349	32640	Blue	45.03 u	PEG
✓	4	59.0131	52707	Olive	59.01 u	PMMA
✓	5	59.0506	37453	Green	59.05 u	PEG
✓	6	69.0368	120075	Grey	69.04 u	PMMA
✓	7	69.0757	358653	Red	69.08 u	
✓	8	73.0335	16832	Grey	73.03 u	PEG
✓	9	87.0468	6050	Orange	87.05 u	PEG
✓	10	89.0612	3651	Blue	89.06 u	PEG
✓	11	91.0555	238167	Red	91.05 u	PS
✓	12	93.0719	55716	Yellow	93.07 u	PMMA
✓	13	98.0749	71380	Blue	98.07 u	GTP
✓	14	101.0592	27408	Green	101.06 u	PMMA
✓	15	103.0483	35923	Light Green	103.05 u	PEG

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: C₃H₃⁺ Add

use selected channel Delete All

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...
H+	30	1...	-16.4	-0.0	0.01 ✓
CH ₃ ⁺	10	15...	13.5	0.2	0.04 ✓
C ₂ H ₃ ⁺	5	27...	-6.9	-0.2	0.30 ✓
C ₃ H ₅ ⁺	5	41...	38.3	1.6	1.31

SF = 67917.010, K0 = -1717.501, Positive

Channel: 211274.00

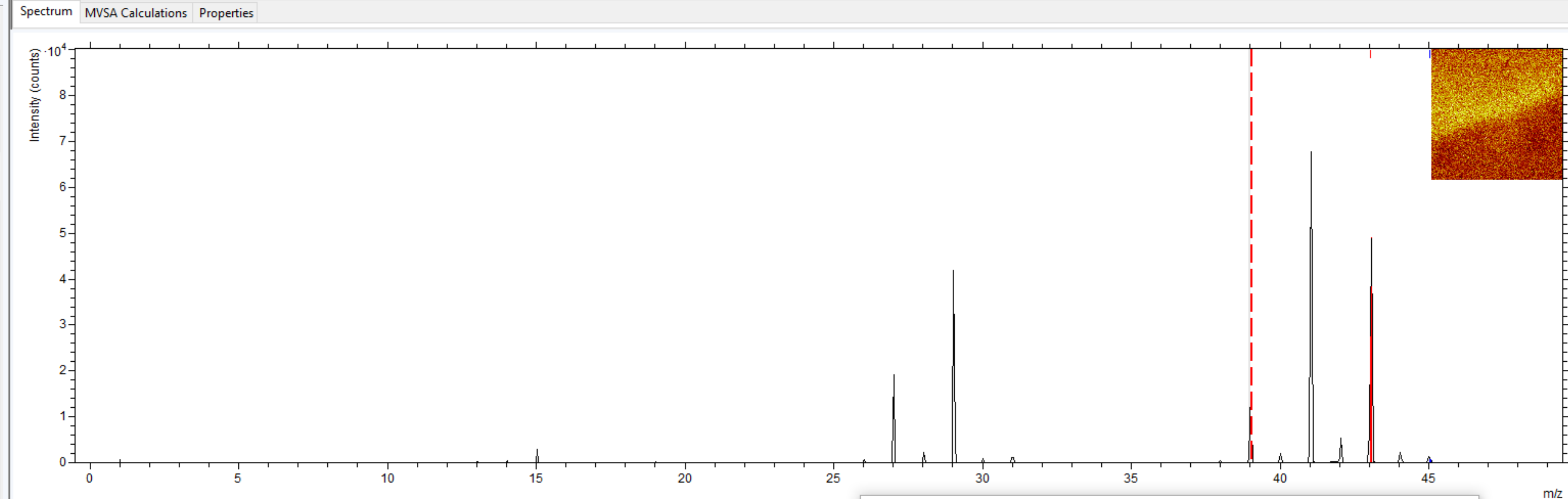
Options... Autocalibrate As Default... Revoke Recalibrate

C_3H_3+	m/z	39.0228	Area (cts)	336,560	Explained (%)	100.0	Resolution	5,957
Check...	Dev. (ppm)	-3.5	Counts / Shot	0.2853	Peak Difference...		Width (ns)	1.78

Compilations

Spectra

- S1_HMR_01_0 *
 - <No Sample Name> (S1_HMR_01) *
 - S1_HMR_02_0
 - <No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
✓	2	43.0559	858049	Red	43.06 u	C3H7
✓	3	45.0344	32551	Blue	45.03 u	PEG
✓	4	59.0124	53409	Olive	59.01 u	PMMA
✓	5	59.0499	37584	Green	59.05 u	PEG
✓	6	69.0359	121654	Grey	69.04 u	PMMA
✓	7	69.0751	351368	Red	69.08 u	
✓	8	73.0327	17157	Grey	73.03 u	PEG
✓	9	87.0457	5981	Orange	87.05 u	PEG
✓	10	89.0609	3378	Blue	89.06 u	PEG
✓	11	91.0542	237252	Red	91.05 u	PS
✓	12	93.0708	56308	Yellow	93.07 u	PMMA
✓	13	98.0735	72995	Blue	98.07 u	GTP
✓	14	101.0579	27710	Green	101.06 u	PMMA
✓	15	103.0475	37193	Light Green	103.05 u	PEG

We now have 5 peaks in our calibration set. We only need 3 and the extra peaks are not going to help with the calibration.

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: Add

use selected channel Delete All

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...	
H+	30	1...	13.8	0.0	0.01	✓
CH_3+	10	15...	5.7	0.1	0.04	✓
C_2H_3+	5	27...	-18.1	-0.5	0.30	✓
C_3H_3+	5	39...	-16.4	-0.6	0.29	✓
C_3H_5+	5	41...	25.1	1.0	1.31	✓

SF = 67917.729, K0 = -1719.254, Positive

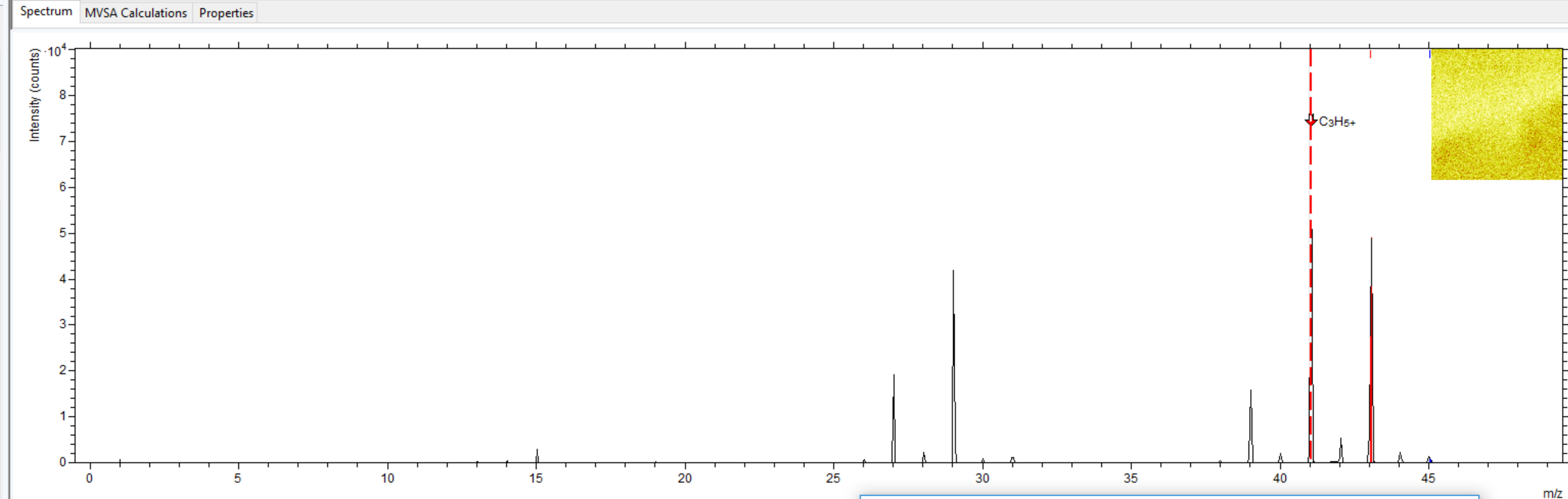
Options... Autocalibrate As Default... Revoke Recalibrate

C_3H_5+ m/z 41.0396 Area (cts) 1,548,829 Explained (%) 100.0 Resolution 5,836
 Check... Add Peak Dev. (ppm) 25.1 Counts / Shot 1.3130 Peak Difference... Width (ns) 1.86

Compilations

Spectra

S1_HMR_01_0 *
 <No Sample Name> (S1_HMR_01) *
 S1_HMR_02_0
 <No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
✓	2	43.0559	858049	Red	43.06 u	C3H7
✓	3	45.0344	32551	Blue	45.03 u	PEG
✓	4	59.0124	53409	Olive	59.01 u	PMMA
✓	5	59.0499	37584	Green	59.05 u	PEG
✓	6	69.0359	121654	Grey	69.04 u	PMMA
✓	7	69.0751	351368	Red	69.08 u	
✓	8	73.0327	17157	Grey	73.03 u	PEG
✓	9	87.0457	5981	Orange	87.05 u	PEG
✓	10	89.0609	3378	Blue	89.06 u	PEG
✓	11	91.0542	237252	Red	91.05 u	PS
✓	12	93.0708	56308	Yellow	93.07 u	PMMA
✓	13	98.0735	72995	Blue	98.07 u	GTP
✓	14	101.0579	27710	Green	101.06 u	PMMA
✓	15	103.0475	37193	Light Green	103.05 u	PEG

Right click on a peak and select 'Delete' to remove the peak from the calibration list. Here we remove C3H5.

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: C_3H_5+ Deviation: 25.1 ppm

use selected channel

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts / ...
H+	30	1...	13.8	0.0	0.01 ✓
CH_3+	10	15...	5.7	0.1	0.04 ✓
C_2H_3+	5	27...	-18.1	-0.5	0.30 ✓
C_3H_3+	5	39...	-16.4	-0.6	0.29 ✓
C_3H_5+			25.1	1.0	1.31 ✓

SF = 679

Channel: 216688.21

Options... Autocalibrate As Default... Revoke Recalibrate

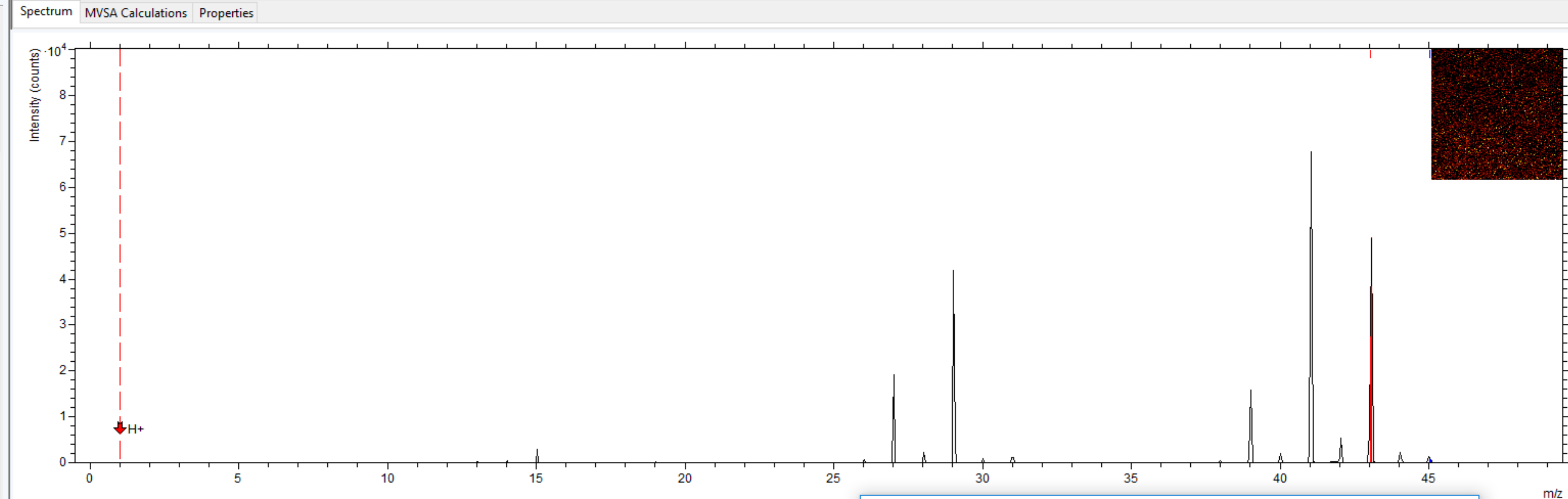
m/z 1.0073 Area (cts) 8,642 Explained (%) 100.0 Resolution 1,715
 Dev. (ppm) -20.4 Counts / Shot 0.0073 Peak Difference... Width (ns) 0.99

Compilations

Spectra

Spectra

- S1_HMR_01_0 *
 - <No Sample Name> (S1_HMR_01) *
 - S1_HMR_02_0
 - <No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
<input checked="" type="checkbox"/>	2	43.0564	874524	Red	43.06 u	C3H7
<input checked="" type="checkbox"/>	3	45.0350	32640	Blue	45.03 u	PEG
<input checked="" type="checkbox"/>	4	59.0132	52707	Olive	59.01 u	PMMA
<input checked="" type="checkbox"/>	5	59.0507	37453	Green	59.05 u	PEG
<input checked="" type="checkbox"/>	6	69.0369	120075	Grey	69.04 u	PMMA
<input checked="" type="checkbox"/>	7	69.0756	360124	Red	69.08 u	
<input checked="" type="checkbox"/>	8	73.0336	16832	Grey	73.03 u	PEG
<input checked="" type="checkbox"/>	9	87.0470	6050	Orange	87.05 u	PEG
<input checked="" type="checkbox"/>	10	89.0614	3651	Blue	89.06 u	PEG
<input checked="" type="checkbox"/>	11	91.0557	238167	Red	91.05 u	PS
<input checked="" type="checkbox"/>	12	93.0721	55716	Yellow	93.07 u	PMMA
<input checked="" type="checkbox"/>	13	98.0751	71380	Blue	98.07 u	GTP
<input checked="" type="checkbox"/>	14	101.0594	27408	Green	101.06 u	PMMA
<input checked="" type="checkbox"/>	15	103.0485	35923	Light Green	103.05 u	PEG

We'll also remove 'H' from the list. H is too low of a mass to help with the calibration.

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: H+ Deviation: -20.4 ppm

use selected channel

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...	
H+	20.4	1	-20.4	-0.0	0.01	<input checked="" type="checkbox"/>
CH ₃ ⁺	4.8	0.2	4.8	0.2	0.04	<input checked="" type="checkbox"/>
C ₂ H ₃ ⁺	5.2	-0.1	5.2	-0.1	0.30	<input checked="" type="checkbox"/>
C ₃ H ₃ ⁺	1.6	-0.1	1.6	-0.1	0.29	<input checked="" type="checkbox"/>

SF = 67916.906, K0 = -1717.263, Positive

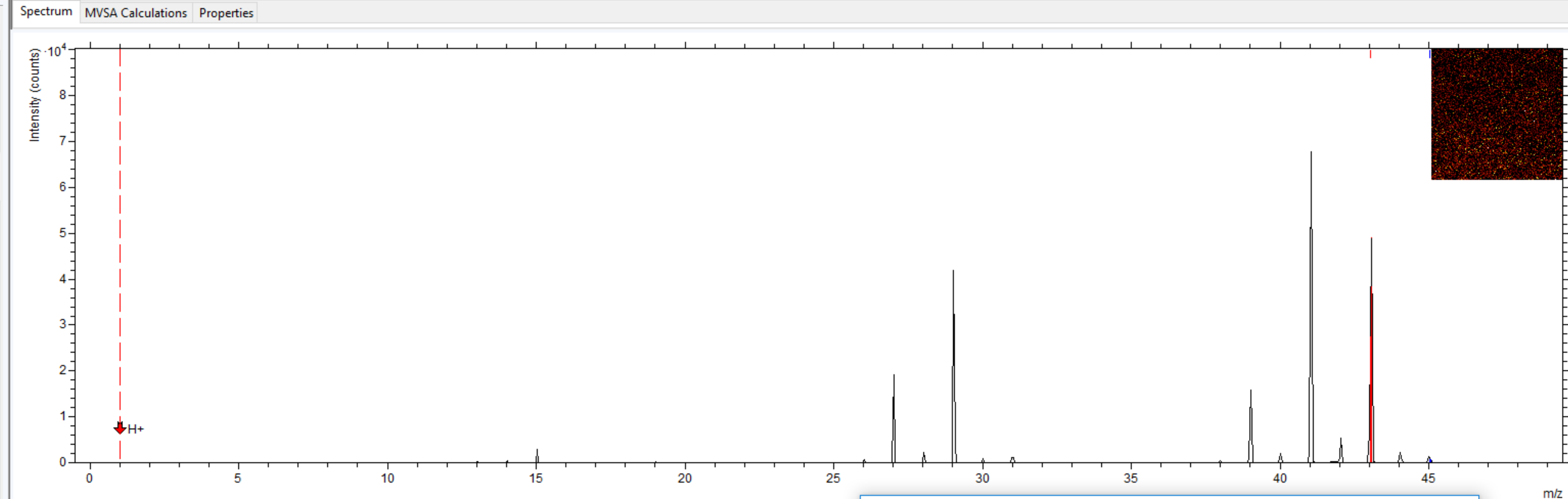
Channel: 33222.80

m/z 1.0073
 Dev. (ppm) -20.4
 Area (cts) 8,651
 Counts / Shot 0.0073
 Explained (%) 100.0
 Resolution 1,711
 Width (ns) 1.00

Compilations

Spectra

S1_HMR_01_0 *
 <No Sample Name> (S1_HMR_01) *
 S1_HMR_02_0
 <No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
<input checked="" type="checkbox"/>	2	43.0565	854832	Red	43.06 u	C3H7
<input checked="" type="checkbox"/>	3	45.0352	32713	Blue	45.03 u	PEG
<input checked="" type="checkbox"/>	4	59.0136	51836	Olive	59.01 u	PMMA
<input checked="" type="checkbox"/>	5	59.0511	37293	Green	59.05 u	PEG
<input checked="" type="checkbox"/>	6	69.0376	118182	Grey	69.04 u	PMMA
<input checked="" type="checkbox"/>	7	69.0762	360824	Red	69.08 u	
<input checked="" type="checkbox"/>	8	73.0342	16483	Grey	73.03 u	PEG
<input checked="" type="checkbox"/>	9	87.0478	6134	Orange	87.05 u	PEG
<input checked="" type="checkbox"/>	10	89.0617	3870	Blue	89.06 u	PEG
<input checked="" type="checkbox"/>	11	91.0566	238681	Red	91.05 u	PS
<input checked="" type="checkbox"/>	12	93.0730	55170	Yellow	93.07 u	PMMA
<input checked="" type="checkbox"/>	13	98.0763	70210	Blue	98.07 u	GTP
<input checked="" type="checkbox"/>	14	101.0605	26893	Green	101.06 u	PMMA
<input checked="" type="checkbox"/>	15	103.0490	34262	Light Green	103.05 u	PEG

After removing any peaks you should hit the 'Recalibrate' button to apply the calibration.

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: H+

use selected channel

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...
CH_3+	10	15...	3.5	0.1	0.04 ✓
C_2H_3+	5	27...	-6.0	-0.2	0.30 ✓
C_3H_3+	5	39...	2.8	0.1	0.29 ✓

SF = 67915.896, K0 = -1711.872, Positive

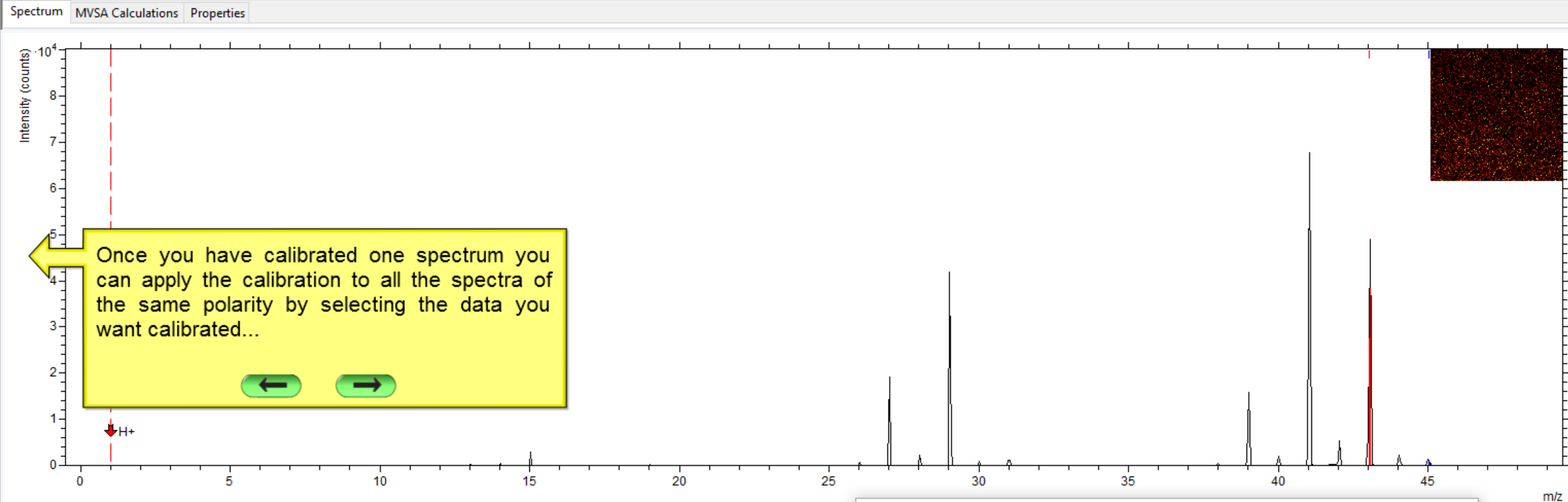
Channel: 33222.80

H+	m/z	1.0071	Area (cts)	8,651	Explained (%)	100.0	Resolution	1,711
Check...	Dev. (ppm)	-147.6	Counts / Shot	0.0073	Peak Difference...		Width (ns)	1.00

Compilations

Spectra

S1_HMR_01_0 *
 <No Sample Name> (S1_HMR_01) *
 S1_HMR_02_0
 <No Sample Name> (S1_HMR_02)



MassListPos

V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
<input checked="" type="checkbox"/>	2	43.0565	854832	Red	43.06 u	C3H7
<input checked="" type="checkbox"/>	3	45.0352	32713	Blue	45.03 u	PEG
<input checked="" type="checkbox"/>	4	59.0136	51836	Olive	59.01 u	PMMA
<input checked="" type="checkbox"/>	5	59.0511	37293	Green	59.05 u	PEG
<input checked="" type="checkbox"/>	6	69.0376	118182	Grey	69.04 u	PMMA
<input checked="" type="checkbox"/>	7	69.0762	360824	Red	69.08 u	
<input checked="" type="checkbox"/>	8	73.0342	16483	Grey	73.03 u	PEG
<input checked="" type="checkbox"/>	9	87.0478	6134	Orange	87.05 u	PEG
<input checked="" type="checkbox"/>	10	89.0617	3870	Blue	89.06 u	PEG
<input checked="" type="checkbox"/>	11	91.0566	238681	Red	91.05 u	PS
<input checked="" type="checkbox"/>	12	93.0730	55170	Yellow	93.07 u	PMMA
<input checked="" type="checkbox"/>	13	98.0763	70210	Blue	98.07 u	GTP
<input checked="" type="checkbox"/>	14	101.0605	26893	Green	101.06 u	PMMA
<input checked="" type="checkbox"/>	15	103.0490	34262	Light Green	103.05 u	PEG

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: H+ Add

use selected channel Delete All

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...
CH_3+	10	15...	3.5	0.1	0.04 ✓
C_2H_3+	5	27...	-6.0	-0.2	0.30 ✓
C_3H_3+	5	39...	2.8	0.1	0.29 ✓

SF = 67915.896, K0 = -1711.872, Positive

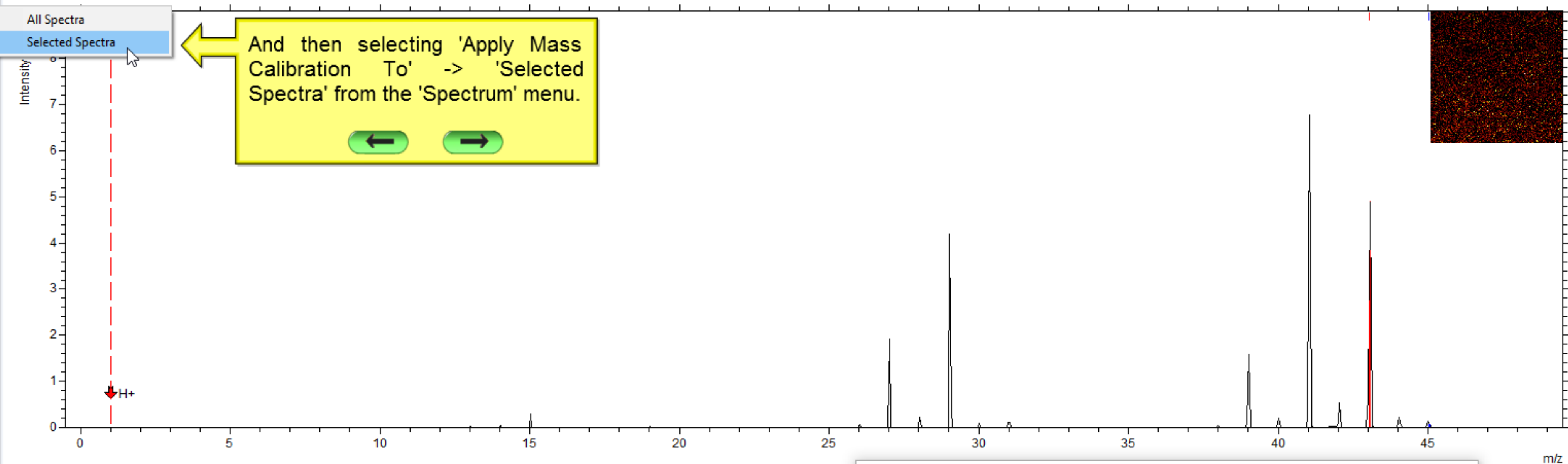
Channel: 33222.80

Options... Autocalibrate As Default... Revoke Recalibrate

Display Spectra As Line Spectra S
 Combine Line Spectra...
 Display Spectra as Overlay Z
 Spectra Overlay Options
 Mass Calibration ... F3
Apply Mass Calibration To
 Find Mass Ctrl+F
 Find Compound... Ctrl+G
 Add selected Peak Ctrl+A
 Add Background to selected Peak(s)
 Recalibrate Peak Searcher
 Search Peaks...
 Search Elements...
 Search Compounds...
 Mass Shift Correction...
 Add Lateral ROIs To
 Replace Lateral ROIs Of
 Copy z-ROIs To
 Add Interval Subsets To
 Replace Interval Subsets Of
 Show Analysis Peaklists
 Create G-SIMS Spectrum...
 Show G-SIMS Spectrum...
 Apply Smooth
 Smooth Properties...
 Element Information...
 Isotope Cluster Calculator...
 Spectra Library
 Add to Spectra Library
 Scale Spectra
 Scale Spectra by

Total Range Total Area All Intervals Find: c7h7
 Area (cts) 8,651 Explained (%) 100.0 Resolution 1,711
 Shots / Shot 0.0073 Peak Difference... Width (ns) 1.00

Spectrum MVSA Calculations Properties



V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
✓	2	43.0565	854832	Red	43.06 u	C3H7
✓	3	45.0352	32713	Blue	45.03 u	PEG
✓	4	59.0136	51836	Olive	59.01 u	PMMA
✓	5	59.0511	37293	Green	59.05 u	PEG
✓	6	69.0376	118182	Grey	69.04 u	PMMA
✓	7	69.0762	360824	Red	69.08 u	
✓	8	73.0342	16483	Grey	73.03 u	PEG
✓	9	87.0478	6134	Orange	87.05 u	PEG
✓	10	89.0617	3870	Blue	89.06 u	PEG
✓	11	91.0566	238681	Red	91.05 u	PS
✓	12	93.0730	55170	Yellow	93.07 u	PMMA
✓	13	98.0763	70210	Blue	98.07 u	GTP
✓	14	101.0605	26893	Green	101.06 u	PMMA
✓	15	103.0490	34262	Light Green	103.05 u	PEG

<No Sample Name> (S1_HMR_01) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

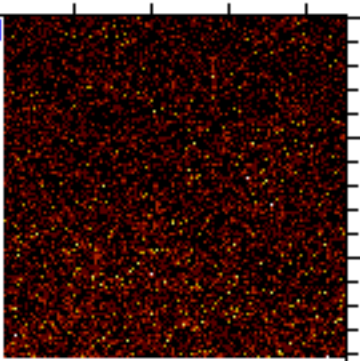
Ion: H+ Add
 use selected channel Delete All

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...
CH_3+	10	15...	3.5	0.1	0.04 ✓
C_2H_3+	5	27...	-6.0	-0.2	0.30 ✓
C_3H_3+	5	39...	2.8	0.1	0.29 ✓

SF = 67915.896, K0 = -1711.872, Positive

Channel: 33222.80

Options... Autocalibrate As Default... Revoke Recalibrate



1.016 m/z

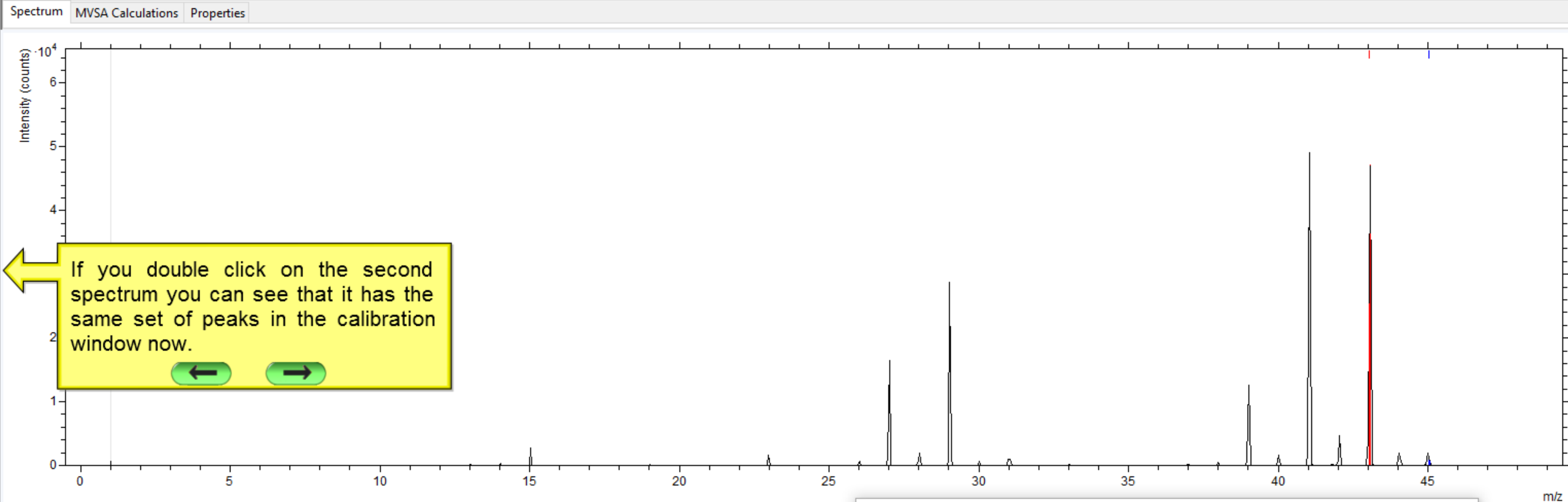
NUM

Explained (%)

Compilations

Spectra

- S1_HMR_01_0 *
<No Sample Name> (S1_HMR_01) *
- S1_HMR_02_0 *
<No Sample Name> (S1_HMR_02) *



V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
<input checked="" type="checkbox"/>	2	43.0566	850449	Red	43.06 u	C3H7
<input checked="" type="checkbox"/>	3	45.0348	41872	Blue	45.03 u	PEG
<input checked="" type="checkbox"/>	4	59.0138	42768	Olive	59.01 u	PMMA
<input checked="" type="checkbox"/>	5	59.0512	25029	Green	59.05 u	PEG
<input checked="" type="checkbox"/>	6	69.0376	92774	Grey	69.04 u	PMMA
<input checked="" type="checkbox"/>	7	69.0761	289533	Red	69.08 u	
<input checked="" type="checkbox"/>	8	73.0342	15305	Grey	73.03 u	PEG
<input checked="" type="checkbox"/>	9	87.0477	5488	Orange	87.05 u	PEG
<input checked="" type="checkbox"/>	10	89.0605	3641	Blue	89.06 u	PEG
<input checked="" type="checkbox"/>	11	91.0587	586826	Red	91.05 u	PS
<input checked="" type="checkbox"/>	12	93.0731	40934	Yellow	93.07 u	PMMA
<input checked="" type="checkbox"/>	13	98.0765	65028	Blue	98.07 u	GTP
<input checked="" type="checkbox"/>	14	101.0604	18365	Green	101.06 u	PMMA
<input checked="" type="checkbox"/>	15	103.0514	58432	Light Green	103.05 u	PEG

<No Sample Name> (S1_HMR_02) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: H+

use selected channel

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...
CH_3+	10	15...	4.7	0.1	0.04 ✓
C_2H_3+	5	27...	-7.9	-0.2	0.26 ✓
C_3H_3+	5	39...	3.7	0.1	0.23 ✓

SF = 67915.068, K0 = -1710.629, Positive

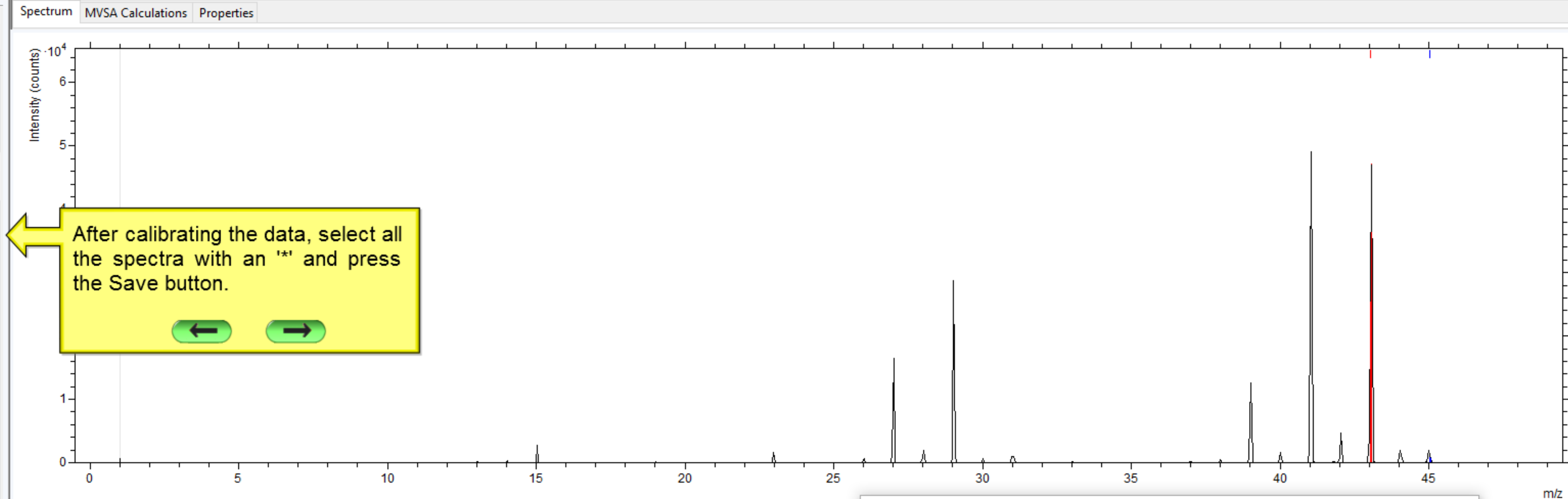
Channel: 33222.80

Check... Add Peak m/z Dev. (ppm) Area (cts) Counts / Shot Explained (%) Resolution Width (ns) Peak Difference...

Compilations

Spectra

- S1_HMR_02_0 * (Selected)
- <No Sample Name> (S1_HMR_01) *
- <No Sample Name> (S1_HMR_02) *



After calibrating the data, select all the spectra with an '*' and press the Save button.

Mass Interval Lists

MassListPos (+)

V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
<input checked="" type="checkbox"/>	2	43.0566	850449	Red	43.06 u	C3H7
<input checked="" type="checkbox"/>	3	45.0348	41872	Blue	45.03 u	PEG
<input checked="" type="checkbox"/>	4	59.0138	42768	Olive	59.01 u	PMMA
<input checked="" type="checkbox"/>	5	59.0512	25029	Green	59.05 u	PEG
<input checked="" type="checkbox"/>	6	69.0376	92774	Grey	69.04 u	PMMA
<input checked="" type="checkbox"/>	7	69.0761	289533	Red	69.08 u	
<input checked="" type="checkbox"/>	8	73.0342	15305	Grey	73.03 u	PEG
<input checked="" type="checkbox"/>	9	87.0477	5488	Orange	87.05 u	PEG
<input checked="" type="checkbox"/>	10	89.0605	3641	Blue	89.06 u	PEG
<input checked="" type="checkbox"/>	11	91.0587	586826	Red	91.05 u	PS
<input checked="" type="checkbox"/>	12	93.0731	40934	Yellow	93.07 u	PMMA
<input checked="" type="checkbox"/>	13	98.0765	65028	Blue	98.07 u	GTP
<input checked="" type="checkbox"/>	14	101.0604	18365	Green	101.06 u	PMMA
<input checked="" type="checkbox"/>	15	103.0514	58432	Light Green	103.05 u	PEG

<No Sample Name> (S1_HMR_02) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: H+ Add

use selected channel Delete All

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...
CH_3+	10	15...	4.7	0.1	0.04 ✓
C_2H_3+	5	27...	-7.9	-0.2	0.26 ✓
C_3H_3+	5	39...	3.7	0.1	0.23 ✓

SF = 67915.068, K0 = -1710.629, Positive

Channel: 33222.80

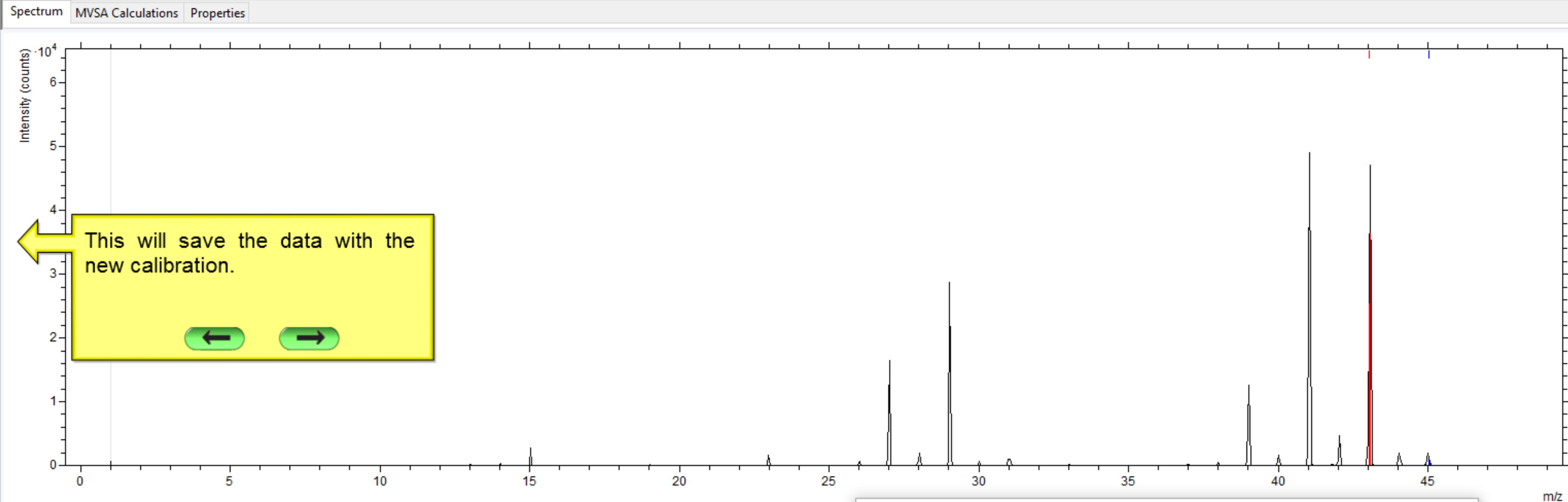
Options... Autocalibrate As Default... Revoke Recalibrate

Explained (%)

Compilations

Spectra

- S1_HMR_01_0
- <No Sample Name> (S1_HMR_01)
- S1_HMR_02_0
- <No Sample Name> (S1_HMR_02)



V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
<input checked="" type="checkbox"/>	2	43.0566	850449	Red	43.06 u	C3H7
<input checked="" type="checkbox"/>	3	45.0348	41872	Blue	45.03 u	PEG
<input checked="" type="checkbox"/>	4	59.0138	42768	Olive	59.01 u	PMMA
<input checked="" type="checkbox"/>	5	59.0512	25029	Green	59.05 u	PEG
<input checked="" type="checkbox"/>	6	69.0376	92774	Grey	69.04 u	PMMA
<input checked="" type="checkbox"/>	7	69.0761	289533	Red	69.08 u	
<input checked="" type="checkbox"/>	8	73.0342	15305	Grey	73.03 u	PEG
<input checked="" type="checkbox"/>	9	87.0477	5488	Orange	87.05 u	PEG
<input checked="" type="checkbox"/>	10	89.0605	3641	Blue	89.06 u	PEG
<input checked="" type="checkbox"/>	11	91.0587	586826	Red	91.05 u	PS
<input checked="" type="checkbox"/>	12	93.0731	40934	Yellow	93.07 u	PMMA
<input checked="" type="checkbox"/>	13	98.0765	65028	Blue	98.07 u	GTP
<input checked="" type="checkbox"/>	14	101.0604	18365	Green	101.06 u	PMMA
<input checked="" type="checkbox"/>	15	103.0514	58432	Light Green	103.05 u	PEG

<No Sample Name> (S1_HMR_02) * - Mass Calibration

Calibration Points List 1 List 2 List 3 List 4 List 5

Ion: H+

use selected channel

Ion	+/- (mu)	Mass	Dev. (ppm)	Dev. (mu)	Counts/...
CH_3+	10	15...	4.7	0.1	0.04 ✓
C_2H_3+	5	27...	-7.9	-0.2	0.26 ✓
C_3H_3+	5	39...	3.7	0.1	0.23 ✓

SF = 67915.068, K0 = -1710.629, Positive

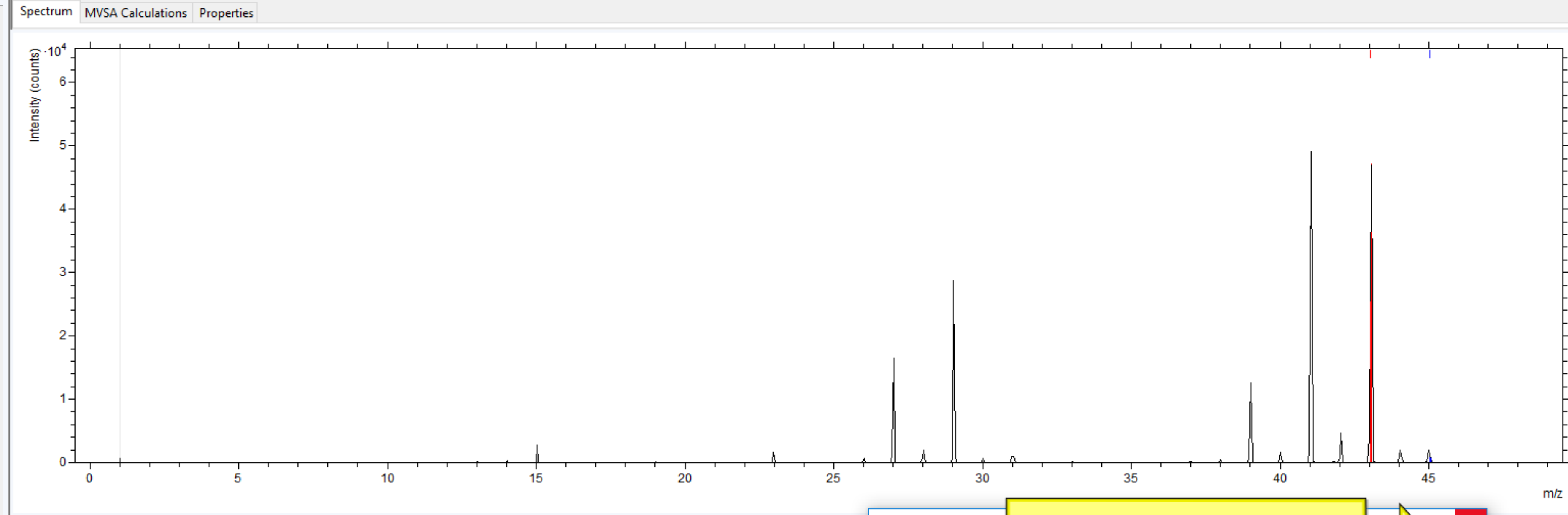
Channel: 33222.80

m/z Area (cts) Explained (%) Resolution
 Dev. (ppm) Counts / Shot Peak Difference... Width (ns)

Compilations

Spectra

- S1_HMR_01_0
<No Sample Name> (S1_HMR_01) +
- S1_HMR_02_0
<No Sample Name> (S1_HMR_02) +



V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
<input checked="" type="checkbox"/>	2	43.0566	850449	Red	43.06 u	C3H7
<input checked="" type="checkbox"/>	3	45.0348	41872	Blue	45.03 u	PEG
<input checked="" type="checkbox"/>	4	59.0138	42768	Olive	59.01 u	PMMA
<input checked="" type="checkbox"/>	5	59.0512	25029	Green	59.05 u	PEG
<input checked="" type="checkbox"/>	6	69.0376	92774	Grey	69.04 u	PMMA
<input checked="" type="checkbox"/>	7	69.0761	289533	Red	69.08 u	
<input checked="" type="checkbox"/>	8	73.0342	15305	Grey	73.03 u	PEG
<input checked="" type="checkbox"/>	9	87.0477	5488	Orange	87.05 u	PEG
<input checked="" type="checkbox"/>	10	89.0605	3641	Blue	89.06 u	PEG
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<input checked="" type="checkbox"/>	13	98.0765	65028	Blue	98.07 u	GTP
<input checked="" type="checkbox"/>	14	101.0604	18365	Green	101.06 u	PMMA
<input checked="" type="checkbox"/>	15	103.0514	58432	Light Green	103.05 u	PEG

<No Sample Name> (S1_HMR_02) * - Calibration Points

Ion: left click

use selected calibration points

Ion	+/(m/z)	Mass	Dev.(ppm)	Dev.(m/z)	Counts/...	
CH_3+	10	15...	4.7	0.1	0.04	✓
C_2H_3+	5	27...	-7.9	-0.2	0.26	✓
C_3H_3+	5	39...	3.7	0.1	0.23	✓

SF = 67915.068, K0 = -1710.629, Positive

Buttons: Add, Delete All

You can now close the calibration dialog by pressing the red X.

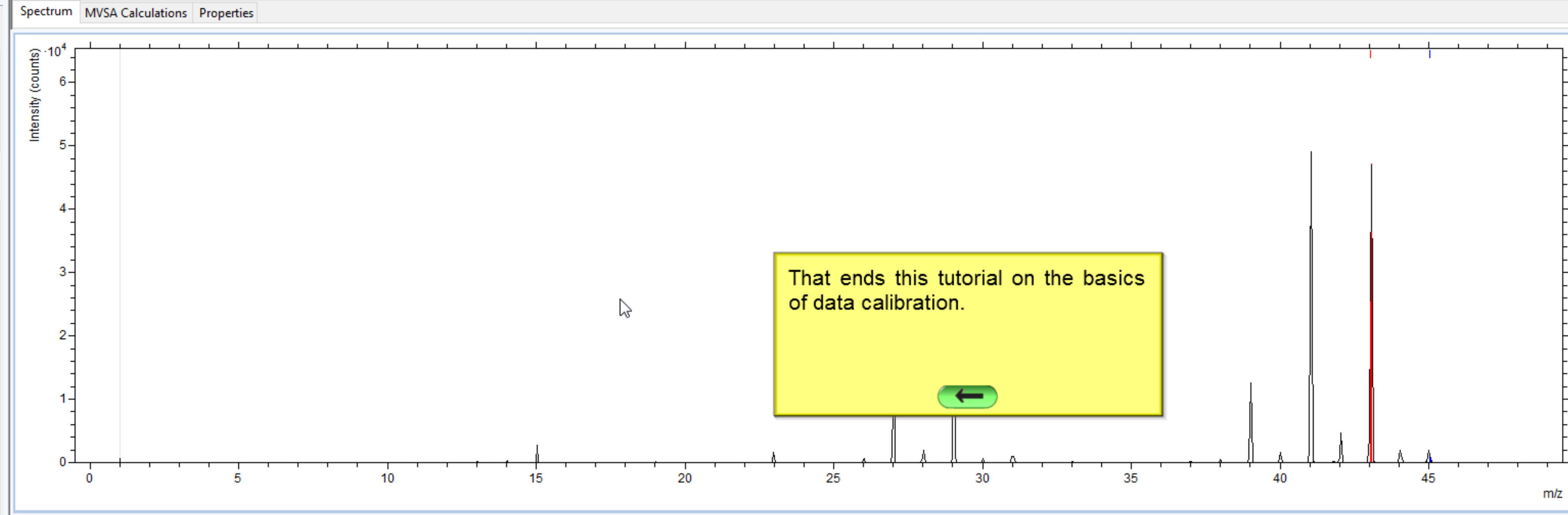
m/z Area (cts) Explained (%) Resolution
 Dev. (ppm) Counts / Shot Peak Difference... Width (ns)

Compilations

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 (+)

V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
<input checked="" type="checkbox"/>	2	43.0566	850449	Red	43.06 u	C3H7
<input checked="" type="checkbox"/>	3	45.0348	41872	Blue	45.03 u	PEG
<input checked="" type="checkbox"/>	4	59.0138	42768	Olive	59.01 u	PMMA
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<input checked="" type="checkbox"/>	14	101.0604	18365	Green	101.06 u	PMMA
<input checked="" type="checkbox"/>	15	103.0514	58432	Light Green	103.05 u	PEG

