Active Measurement: S1_HMR_01.itmx

<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra

Total Range | Total Area | All Intervals

Find: c7h7

C_3H_5+

m/z 41.0409

Dev. (ppm) 56.4

Area (cts) 368

Counts / Shot 0.0003

☐ Explained (%) 100.0

Resolution 2,149

Width (ns) 7.45

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

MassListPos (+)

This tutorial will cover the basics of data calibration. All data you recieve from the MAF will be calibrated, however it is always good to know how to calibrate your own data.

The default calibration set for positive ion data is:
CH3+, C2H3+, C3H5+

The default calibration set for negative ion data is:
CH-, OH-, C2H-

MassListPos

Mass Intervals

V	No.	m / z	Area / cts	Color	Peak Label	Description
☑	2	43.0569	248	🟥	43.06 u	C3H7
☑	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

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 the typically the middle peak in the next cluster of peaks.

Find: c7h7

MassListPos

Mass Intervals

V	No.	m / z	Area / cts	Color	Peak Label	Description
☑	2	43.0566	850449	🟥	43.06 u	C3H7
☑	3	45.0348	41872	🟦	45.03 u	PEG
☑	4	59.0138	42768	🟫	59.01 u	PMMA
☑	5	59.0512	25029	🟩	59.05 u	PEG
☑	6	69.0376	92774	⬜	69.04 u	PMMA
☑	7	69.0761	289533	🟥	69.08 u	
☑	8	73.0342	15305	⬛	73.03 u	PEG
☑	9	87.0477	5488	🟧	87.05 u	PEG
☑	10	89.0605	3641	🟪	89.06 u	PEG
☑	11	91.0587	586826	🟥	91.05 u	PS
☑	12	93.0731	40934	🟨	93.07 u	PMMA
☑	13	98.0765	65028	🟦	98.07 u	GTP
☑	14	101.0604	18365	🟩	101.06 u	PMMA
☑	15	103.0514	58432	🟩	103.05 u	PEG

Active Measurement: ThyroidLow_HMR_06.itmx

<No Sample Name> (ThyroidLow_HMR_06) - Measurement Explorer - Spectra

Total Range | Total Area | All Intervals | Find: c7h7

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 (+)

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

CH is typically the tallest peak in the first cluster of peaks.

OH is typically the second tall peak just after the C, CH, CH2 cluster.

C2H is the typically the middle peak in the next cluster of peaks.

MainNegList

V	No.	m / z	Area / cts	Color	Peak Label	Description
Special Intervals						
☐	1		832203974	🟥	total	total

To bring up the calibration dialogue select 'Mass Calibration...' from the 'Spectrum' menu, or press F3.

V	No.	m / z	Area / cts	Color	Peak Label	Description
☑	2	43.0569	248	🟥	43.06 u	C3H7
☑	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

Active Measurement: S1_HMR_01.itmx

Find: c7h7

C_3H_5+

m/z: 41.0409

Dev. (ppm): 56.4

Area (cts): 368

Counts / Shot: 0.0003

☐ Explained (%): 100.0

Resolution: 2,149

Width (ns): 7.45

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	
☑	2	43.0569	248	🟥	43.06 u	
☑	3	45.0333	5989	🟦	45.03 u	
☑	4	59.0125	945	🟫	59.01 u	
☑	5	59.0520	1168	🟩	59.05 u	
☑	6	69.0353	727	⬜	69.04 u	
☑	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

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

Ion : left click

☐ use selected channel

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

SF = 100000.000, K0 = 0.000, Positive

Find: c7h7

m/z 0.4415

Dev. (ppm)

Area (cts) 8,642

Counts / Shot 0.0073

☐ Explained (%) 0.0

Resolution 1,672

Width (ns) 0.99

Spectra

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

MassListPos (+)

Click on this peak.

MassListPos

Mass Intervals

V	No.	m / z	Area / cts			
☑	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 :

☐ use selected channel

Add

Delete All

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

SF = 100000.000, K0 = 0.000, Positive

Channel: 33222.80

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

<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra

Active Measurement: S1_HMR_01.itmx

Find: c7h7

m/z: 0.4415

Area (cts): 8,642

Counts / Shot: 0.0073

☐ Explained (%): 0.0

Resolution: 1,672

Width (ns): 0.99

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 (+)

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

Ion : H

☐ use selected channel

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

SF = 100000.000, K0 = 0.000, Positive

Channel: 33222.80

MassListPos — Mass Intervals

V	No.	m / z	Area / cts	Color	Peak Label	Descri
☑	2	43.0569	248	🟥	43.06 u	C3H7
☑	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

S1_HMR_01.itmx

<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra

Find: c7h7

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

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

MassListPos (+)

The next cluster of peaks might look familiar. The largest peak is CH3.

V	No.	m / z	Area / cts	Color	Peak Label	Description
☑	2	43.0569	248	🟥	43.06 u	C3H7
☑	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

Ion :
☐ 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

S1_HMR_01.itmx

<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra

Find: c7h7

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

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

MassListPos (+)

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

V	No.	m / z	Area / cts	Color	Peak Label	Descri
Mass Intervals						
☑	2	43.0569	248	🟥	43.06 u	C3H7
☑	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 : CH3 [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

Channel: 130763.33

Find: c7h7

m/z 6.8396

Explained (%) 0.0

Width (ns) 0.00

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 piont 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						
☑	2	43.0558	873874	🟥	43.06 u	C3H7
☑	3	45.0342	32389	🟦	45.03 u	PEG
☑	4	59.0121	53409	🟫	59.01 u	PMMA
☑	5	59.0496	37584	🟩	59.05 u	PEG
☑	6	69.0356	122335	⬜	69.04 u	PMMA
☑	7	69.0749	351368	🟥	69.08 u	
☑	8	73.0327	17312	⬛	73.03 u	PEG
☑	9	87.0455	5925	🟧	87.05 u	PEG
☑	10	89.0605	3378	🟪	89.06 u	PEG
☑	11	91.0539	236503	🟥	91.05 u	PS
☑	12	93.0705	56308	🟨	93.07 u	PMMA
☑	13	98.0732	73400	🟦	98.07 u	GTP
☑	14	101.0576	27812	🟩	101.06 u	PMMA
☑	15	103.0471	37193	🟩	103.05 u	PEG

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

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	🟥	43.06 u	C3H7
☑	3	45.0342	32389	🟦	45.03 u	PEG
☑	4	59.0121	53409	🟫	59.01 u	PMMA
☑	5	59.0496	37584	🟩	59.05 u	PEG
☑	6	69.0356	122335	⬜	69.04 u	PMMA
☑	7	69.0749	351368	🟥	69.08 u	
☑	8	73.0327	17312	⬜	73.03 u	PEG
☑	9	87.0455	5925	🟧	87.05 u	PEG
☑	10	89.0605	3378	🟪	89.06 u	PEG
☑	11	91.0539	236503	🟥	91.05 u	PS
☑	12	93.0705	56308	🟨	93.07 u	PMMA
☑	13	98.0732	73400	🟦	98.07 u	GTP
☑	14	101.0576	27812	🟩	101.06 u	PMMA
☑	15	103.0471	37193	🟩	103.05 u	PEG

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

Ion : BeH_2O+

☐ 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

Find: c7h7

BeH_2O+

m/z 27.0223

Dev. (ppm) 3.9

Area (cts) 352,554

Counts / Shot 0.2989

☐ Explained (%) 100.0

Resolution 5,572

Width (ns) 1.58

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	Des
Mass Intervals						
☑	2	43.0558	873874	🟥	43.06 u	C3H
☑	3	45.0342	32389	🟦	45.03 u	PEG
☑	4	59.0121	53409	🟫	59.01 u	PMMA
☑	5	59.0496	37584	🟩	59.05 u	PEG
☑	6	69.0356	122335	⬜	69.04 u	PMMA
☑	7	69.0749	351368	🟥	69.08 u	
☑	8	73.0327	17312	⬛	73.03 u	PEG
☑	9	87.0455	5925	🟧	87.05 u	PEG
☑	10	89.0605	3378	🟪	89.06 u	PEG
☑	11	91.0539	236503	🟥	91.05 u	PS
☑	12	93.0705	56308	🟨	93.07 u	PMMA
☑	13	98.0732	73400	🟦	98.07 u	GTP
☑	14	101.0576	27812	🟩	101.06 u	PMMA
☑	15	103.0471	37193	🟩	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

Ion : BeH_2O+

☐ 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

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

Active Measurement: S1_HMR_01.itmx

<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra

Total Range | Total Area | All Intervals

Find: c7h7

BeH_2O+

m/z: 27.0223

Dev. (ppm): 3.9

Area (cts): 352,554

Counts / Shot: 0.2989

☐ Explained (%): 100.0

Resolution: 5,572

Width (ns): 1.58

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						
☑	2	43.0558	873874	🟥	43.06 u	C3H7
☑	3	45.0342	32389	🟦	45.03 u	PEG
☑	4	59.0121	53409	■	59.01 u	PMMA
☑	5	59.0496	37584	🟩	59.05 u	PEG
☑	6	69.0356	122335	■	69.04 u	PMMA
☑	7	69.0749	351368	🟥	69.08 u	
☑	8	73.0327	17312	■	73.03 u	PEG
☑	9	87.0455	5925	🟧	87.05 u	PEG
☑	10	89.0605	3378	■	89.06 u	PEG
☑	11	91.0539	236503	🟥	91.05 u	PS
☑	12	93.0705	56308	🟨	93.07 u	PMMA
☑	13	98.0732	73400	🟦	98.07 u	GTP
☑	14	101.0576	27812	🟩	101.06 u	PMMA
☑	15	103.0471	37193	🟩	103.05 u	PEG

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

Ion : C2H3

☐ 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

Find: c7h7

C_3H_5+

m/z: 41.0401

Dev. (ppm): 38.3

Area (cts): 1,548,829

Counts / Shot: 1.3130

☐ Explained (%): 100.0

Resolution: 5,836

Width (ns): 1.86

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

You might recognize this third cluster of peaks. The middle peak is C3H5. Click on this peak.

MassListPos

V	No.	m / z	Area / cts	Color	Peak Label	Description
☑	2	43.0563	874524	🟥	43.06 u	C3H7
☑	3	45.0349	32640	🟦	45.03 u	PEG
☑	4	59.0131	52707	■	59.01 u	PMMA
☑	5	59.0506	37453	🟩	59.05 u	PEG
☑	6	69.0368	120075	■	69.04 u	PMMA
☑	7	69.0757	358653	🟥	69.08 u	
☑	8	73.0335	16832	■	73.03 u	PEG
☑	9	87.0468	6050	🟧	87.05 u	PEG
☑	10	89.0612	3651	■	89.06 u	PEG
☑	11	91.0555	238167	🟥	91.05 u	PS
☑	12	93.0719	55716	🟨	93.07 u	PMMA
☑	13	98.0749	71380	🟦	98.07 u	GTP
☑	14	101.0592	27408	🟩	101.06 u	PMMA
☑	15	103.0483	35923	🟩	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+

☐ 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

This time the software got it correct.

Find: c7h7

C_3H_5+

m/z: 41.0401

Dev. (ppm): 38.3

Area (cts): 1,548,829

Counts / Shot: 1.3130

☐ Explained (%): 100.0

Resolution: 5,836

Width (ns): 1.86

- 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
☑	2	43.0563	874524	🟥	43.06 u	C3H7
☑	3	45.0349	32640	🟦	45.03 u	PEG
☑	4	59.0131	52707	🟫	59.01 u	PMMA
☑	5	59.0506	37453	🟩	59.05 u	PEG
☑	6	69.0368	120075	⬜	69.04 u	PMMA
☑	7	69.0757	358653	🟥	69.08 u	
☑	8	73.0335	16832	⬛	73.03 u	PEG
☑	9	87.0468	6050	🟧	87.05 u	PEG
☑	10	89.0612	3651	🟪	89.06 u	PEG
☑	11	91.0555	238167	🟥	91.05 u	PS
☑	12	93.0719	55716	🟨	93.07 u	PMMA
☑	13	98.0749	71380	🟦	98.07 u	GTP
☑	14	101.0592	27408	🟩	101.06 u	PMMA
☑	15	103.0483	35923	🟩	103.05 u	PEG

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

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

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

<No Sample Name> (S1_HMR_01) * - Measurement Explorer - Spectra

Active Measurement: S1_HMR_01.itmx

Find: c7h7

C_3H_5+

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

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 – Mass Intervals

V	No.	m / z	Area / cts	Color	Peak Label	Descri
☑	2	43.0563	874524	🟥	43.06 u	C3H7
☑	3	45.0349	32640	🟦	45.03 u	PEG
☑	4	59.0131	52707	🟫	59.01 u	PMMA
☑	5	59.0506	37453	🟩	59.05 u	PEG
☑	6	69.0368	120075	⬜	69.04 u	PMMA
☑	7	69.0757	358653	🟥	69.08 u	
☑	8	73.0335	16832	⬜	73.03 u	PEG
☑	9	87.0468	6050	🟧	87.05 u	PEG
☑	10	89.0612	3651	🟪	89.06 u	PEG
☑	11	91.0555	238167	🟥	91.05 u	PS
☑	12	93.0719	55716	🟨	93.07 u	PMMA
☑	13	98.0749	71380	🟦	98.07 u	GTP
☑	14	101.0592	27408	🟩	101.06 u	PMMA
☑	15	103.0483	35923	🟩	103.05 u	PEG

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

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_3H_5+

m/z 41.0401

Dev. (ppm) 38.3

Area (cts) 1,548,829

Counts / Shot 1.3130

☐ Explained (%) 100.0

Resolution 5,836

Width (ns) 1.86

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
☑	2	43.0563	874524	🟥	43.06 u	C3H7
☑	3	45.0349	32640	🟦	45.03 u	PEG
☑	14	101.0592	27408	🟩	101.06 u	PMMA
☑	15	103.0483	35923	🟩	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

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.

Find: c7h7

C_3H_5+

m/z 41.0401

Dev. (ppm) 38.3

Area (cts) 1,548,829

Counts / Shot 1.3130

☐ Explained (%) 100.0

Resolution 5,836

Width (ns) 1.86

V	No.	m / z	Area / cts	Color	Peak Label	Description
☑	2	43.0563	874524	🟥	43.06 u	C3H7
☑	3	45.0349	32640	🟦	45.03 u	PEG
☑	4	59.0131	52707	🟫	59.01 u	PMMA
☑	5	59.0506	37453	🟩	59.05 u	PEG
☑	6	69.0368	120075	⬜	69.04 u	PMMA
☑	7	69.0757	358653	🟥	69.08 u	
☑	8	73.0335	16832	⬛	73.03 u	PEG
☑	9	87.0468	6050	🟧	87.05 u	PEG
☑	10	89.0612	3651	🟪	89.06 u	PEG
☑	11	91.0555	238167	🟥	91.05 u	PS
☑	12	93.0719	55716	🟨	93.07 u	PMMA
☑	13	98.0749	71380	🟦	98.07 u	GTP
☑	14	101.0592	27408	🟩	101.06 u	PMMA
☑	15	103.0483	35923	🟩	103.05 u	PEG

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

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

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

Peak Difference...

Mass Calibration Options

Maximum Counts Per Shot Accepted: 2

OK

Cancel

Change the 'Maximum Counts Per Shot Accepted:' to 2 and press 'OK'.

V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
☑	2	43.0563	874524	🟥	43.06 u	C3H7
☑	3	45.0349	32640	🟦	45.03 u	PEG
☑	4	59.0131	52707	🟫	59.01 u	PMMA
☑	5	59.0506	37453	🟩	59.05 u	PEG
☑	6	69.0368	120075	⬜	69.04 u	PMMA
☑	7	69.0757	358653	🟥	69.08 u	
☑	8	73.0335	16832	⬛	73.03 u	PEG
☑	9	87.0468	6050	🟧	87.05 u	PEG
☑	10	89.0612	3651	🟪	89.06 u	PEG
☑	11	91.0555	238167	🟥	91.05 u	PS
☑	12	93.0719	55716	🟨	93.07 u	PMMA
☑	13	98.0749	71380	🟦	98.07 u	GTP
☑	14	101.0592	27408	🟩	101.06 u	PMMA
☑	15	103.0483	35923	🟩	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

Add

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_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

Find: c7h7

C_3H_5+

m/z 41.0401

Dev. (ppm) 38.3

Area (cts) 1,548,829

Counts / Shot 1.3130

☐ Explained (%) 100.0

Resolution 5,836

Width (ns) 1.86

V	No.	m / z	Area / cts	Color	Peak Label	Description
☑	2	43.0563	874524	🟥	43.06 u	C3H7
☑	3	45.0349	32640	🟦	45.03 u	PEG
☑	4	59.0131	52707	🟫	59.01 u	PMMA
☑	5	59.0506	37453	🟩	59.05 u	PEG
☑	6	69.0368	120075	⬜	69.04 u	PMMA
☑	7	69.0757	358653	🟥	69.08 u	
☑	8	73.0335	16832	⬛	73.03 u	PEG
☑	9	87.0468	6050	🟧	87.05 u	PEG
☑	10	89.0612	3651	🟪	89.06 u	PEG
☑	11	91.0555	238167	🟥	91.05 u	PS
☑	12	93.0719	55716	🟨	93.07 u	PMMA
☑	13	98.0749	71380	🟦	98.07 u	GTP
☑	14	101.0592	27408	🟩	101.06 u	PMMA
☑	15	103.0483	35923	🟩	103.05 u	PEG

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

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

Find: c7h7

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

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
☑	2	43.0563	874524	🟥	43.06 u	C3H7
☑	3	45.0349	32640	🟦	45.03 u	PEG
☑	4	59.0131	52707	🟫	59.01 u	PMMA
☑	5	59.0506	37453	🟩	59.05 u	PEG
☑	6	69.0368	120075	⬜	69.04 u	PMMA
☑	7	69.0757	358653	🟥	69.08 u	
☑	8	73.0335	16832	⬛	73.03 u	PEG
☑	9	87.0468	6050	🟧	87.05 u	PEG
☑	10	89.0612	3651	🟪	89.06 u	PEG
☑	11	91.0555	238167	🟥	91.05 u	PS
☑	12	93.0719	55716	🟨	93.07 u	PMMA
☑	13	98.0749	71380	🟦	98.07 u	GTP
☑	14	101.0592	27408	🟩	101.06 u	PMMA
☑	15	103.0483	35923	🟩	103.05 u	PEG

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

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

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.

Find: c7h7

C_3H_3+
Check...
Add Peak
m/z 39.0228
Dev. (ppm) -3.5
Area (cts) 337,035
Counts / Shot 0.2857
☐ Explained (%) 100.0
Peak Difference...
Resolution 5,947
Width (ns) 1.78

Here I have selected C3H3. This is a peak that is also on most samples and is typically less intense than the C3H5.

V	No.	m / z	Area / cts	Color	Peak Label	Description
☑	2	43.0563	874524	🟥	43.06 u	C3H7
☑	3	45.0349	32640	🟦	45.03 u	PEG
☑	4	59.0131	52707	🟫	59.01 u	PMMA
☑	5	59.0506	37453	🟩	59.05 u	PEG
☑	6	69.0368	120075	⬜	69.04 u	PMMA
☑	7	69.0757	358653	🟥	69.08 u	
☑	8	73.0335	16832	⬛	73.03 u	PEG
☑	9	87.0468	6050	🟧	87.05 u	PEG
☑	10	89.0612	3651	🟪	89.06 u	PEG
☑	11	91.0555	238167	🟥	91.05 u	PS
☑	12	93.0719	55716	🟨	93.07 u	PMMA
☑	13	98.0749	71380	🟦	98.07 u	GTP
☑	14	101.0592	27408	🟩	101.06 u	PMMA
☑	15	103.0483	35923	🟩	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_3+
☐ use selected channel
Add
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_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

Channel: 211274.00

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

Find: c7h7

C_3H_3+

m/z 39.0228

Dev. (ppm) -3.5

Area (cts) 336,560

Counts / Shot 0.2853

☐ Explained (%) 100.0

Resolution 5,957

Width (ns) 1.78

V	No.	m / z	Area / cts	Color	Peak Label	Description
☑	2	43.0559	858049	🟥	43.06 u	C3H7
☑	3	45.0344	32551	🟦	45.03 u	PEG
☑	4	59.0124	53409	🟫	59.01 u	PMMA
☑	5	59.0499	37584	🟩	59.05 u	PEG
☑	6	69.0359	121654	⬜	69.04 u	PMMA
☑	7	69.0751	351368	🟥	69.08 u	
☑	8	73.0327	17157	⬛	73.03 u	PEG
☑	9	87.0457	5981	🟧	87.05 u	PEG
☑	10	89.0609	3378	🟪	89.06 u	PEG
☑	11	91.0542	237252	🟥	91.05 u	PS
☑	12	93.0708	56308	🟨	93.07 u	PMMA
☑	13	98.0735	72995	🟦	98.07 u	GTP
☑	14	101.0579	27710	🟩	101.06 u	PMMA
☑	15	103.0475	37193	🟩	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.

Ion :

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

Find: c7h7

C_3H_5+ m/z 41.0396 Dev. (ppm) 25.1

Area (cts) 1,548,829
Counts / Shot 1.3130

☐ Explained (%) 100.0

Resolution 5,836
Width (ns) 1.86

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
☑	2	43.0559	858049	🟥	43.06 u	C3H7
☑	3	45.0344	32551	🟦	45.03 u	PEG
☑	4	59.0124	53409	■	59.01 u	PMMA
☑	5	59.0499	37584	🟩	59.05 u	PEG
☑	6	69.0359	121654	■	69.04 u	PMMA
☑	7	69.0751	351368	🟥	69.08 u	
☑	8	73.0327	17157	■	73.03 u	PEG
☑	9	87.0457	5981	🟧	87.05 u	PEG
☑	10	89.0609	3378	■	89.06 u	PEG
☑	11	91.0542	237252	🟥	91.05 u	PS
☑	12	93.0708	56308	🟨	93.07 u	PMMA
☑	13	98.0735	72995	🟦	98.07 u	GTP
☑	14	101.0579	27710	🟩	101.06 u	PMMA
☑	15	103.0475	37193	🟩	103.05 u	PEG

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+	5	41...	25.1	1.0	1.31	✓

SF = 679

Channel: 216688.21

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

Find: c7h7

Ion: H+

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

V	No.	m / z	Area / cts	Color	Peak Label	Description
☑	2	43.0564	874524	🟥	43.06 u	C3H7
☑	3	45.0350	32640	🟦	45.03 u	PEG
☑	4	59.0132	52707	■	59.01 u	PMMA
☑	5	59.0507	37453	🟩	59.05 u	PEG
☑	6	69.0369	120075	■	69.04 u	PMMA
☑	7	69.0756	360124	🟥	69.08 u	
☑	8	73.0336	16832	■	73.03 u	PEG
☑	9	87.0470	6050	🟧	87.05 u	PEG
☑	10	89.0614	3651	■	89.06 u	PEG
☑	11	91.0557	238167	🟥	91.05 u	PS
☑	12	93.0721	55716	🟨	93.07 u	PMMA
☑	13	98.0751	71380	🟦	98.07 u	GTP
☑	14	101.0594	27408	🟩	101.06 u	PMMA
☑	15	103.0485	35923	🟩	103.05 u	PEG

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

Ion: H+ Deviation: -20.4 ppm

☐ use selected channel

Ion	+/-(mu)	Mass	Dev.(ppm)	Dev.(mu)	Counts/...	
H+	20	1	-20.4	-0.0	0.01	✓
CH_3+	[illegible]	[illegible]	14.8	0.2	0.04	✓
C_2H_	[illegible]	[illegible]	-5.2	-0.1	0.30	✓
C_3H_	[illegible]	[illegible]	-1.6	-0.1	0.29	✓

SF = 67916.906, K0 = -1717.263, Positive

Channel: 33222.80

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

Find: c7h7

H+

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

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

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

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

Once you have calibrated one spectrum you can apply the calibration to all the spectra of the same polarity by selecting the data you want calibrated...

Find: c7h7

H+

m/z 1.0071

Dev. (ppm) -147.6

Area (cts) 8,651

Counts / Shot 0.0073

Explained (%) 100.0

Resolution 1,711

Width (ns) 1.00

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						
☑	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

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

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

And then selecting 'Apply Mass Calibration To' -> 'Selected Spectra' from the 'Spectrum' menu.

Find: c7h7

ea (cts) 8,651
s / Shot 0.0073
☐ Explained (%) 100.0
Peak Difference...
Resolution 1,711
Width (ns) 1.00

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

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

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

Find: c7h7

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

If you double click on the second spectrum you can see that it has the same set of peaks in the calibration window now.

Mass Intervals

V	No.	m / z	Area / cts	Color	Peak Label	Description
☑	2	43.0566	850449	🟥	43.06 u	C3H7
☑	3	45.0348	41872	🟦	45.03 u	PEG
☑	4	59.0138	42768	■	59.01 u	PMMA
☑	5	59.0512	25029	🟩	59.05 u	PEG
☑	6	69.0376	92774	■	69.04 u	PMMA
☑	7	69.0761	289533	🟥	69.08 u	
☑	8	73.0342	15305	■	73.03 u	PEG
☑	9	87.0477	5488	🟧	87.05 u	PEG
☑	10	89.0605	3641	🟪	89.06 u	PEG
☑	11	91.0587	586826	🟥	91.05 u	PS
☑	12	93.0731	40934	🟨	93.07 u	PMMA
☑	13	98.0765	65028	🟦	98.07 u	GTP
☑	14	101.0604	18365	🟩	101.06 u	PMMA
☑	15	103.0514	58432	🟩	103.05 u	PEG

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

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

Active Measurement: S1_HMR_02.itmx

<No Sample Name> (S1_HMR_02) * - Measurement Explorer - Spectra

Find: c7h7

S1_HMR_0
<No Sample Name> (S1_HMR_01) *
S1_HMR_02_0 *
<No Sample Name> (S1_HMR_02) *

MassListPos (+)

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

MassListPos

V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
☑	2	43.0566	850449	🟥	43.06 u	C3H7
☑	3	45.0348	41872	🟦	45.03 u	PEG
☑	4	59.0138	42768	■	59.01 u	PMMA
☑	5	59.0512	25029	🟩	59.05 u	PEG
☑	6	69.0376	92774	■	69.04 u	PMMA
☑	7	69.0761	289533	🟥	69.08 u	
☑	8	73.0342	15305	■	73.03 u	PEG
☑	9	87.0477	5488	🟧	87.05 u	PEG
☑	10	89.0605	3641	■	89.06 u	PEG
☑	11	91.0587	586826	🟥	91.05 u	PS
☑	12	93.0731	40934	🟨	93.07 u	PMMA
☑	13	98.0765	65028	🟦	98.07 u	GTP
☑	14	101.0604	18365	🟩	101.06 u	PMMA
☑	15	103.0514	58432	🟩	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

Add
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

This will save the data with the new calibration.

V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
☑	2	43.0566	850449	🟥	43.06 u	C3H7
☑	3	45.0348	41872	🟦	45.03 u	PEG
☑	4	59.0138	42768	🟫	59.01 u	PMMA
☑	5	59.0512	25029	🟩	59.05 u	PEG
☑	6	69.0376	92774	⬜	69.04 u	PMMA
☑	7	69.0761	289533	🟥	69.08 u	
☑	8	73.0342	15305	⬛	73.03 u	PEG
☑	9	87.0477	5488	🟧	87.05 u	PEG
☑	10	89.0605	3641	🟪	89.06 u	PEG
☑	11	91.0587	586826	🟥	91.05 u	PS
☑	12	93.0731	40934	🟨	93.07 u	PMMA
☑	13	98.0765	65028	🟦	98.07 u	GTP
☑	14	101.0604	18365	🟩	101.06 u	PMMA
☑	15	103.0514	58432	🟩	103.05 u	PEG

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

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

V	No.	m / z	Area / cts	Color	Peak Label	Description
☑	2	43.0566	850449	🟥	43.06 u	C3H7
☑	3	45.0348	41872	🟦	45.03 u	PEG
☑	4	59.0138	42768	🟫	59.01 u	PMMA
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☑	6	69.0376	92774	⬜	69.04 u	PMMA
☑	7	69.0761	289533	🟥	69.08 u	
☑	8	73.0342	15305	⬛	73.03 u	PEG
☑	9	87.0477	5488	🟧	87.05 u	PEG
☑	10	89.0605	3641	🟪	89.06 u	PEG
☑	11	91.0587	586826	🟥	91.05 u	PS
☑	12	93.0731	40934	🟨	93.07 u	PMMA
☑	13	98.0765	65028	🟦	98.07 u	GTP
☑	14	101.0604	18365	🟩	101.06 u	PMMA
☑	15	103.0514	58432	🟩	103.05 u	PEG

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

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

Find: c7h7

That ends this tutorial on the basics of data calibration.

MassListPos

V	No.	m / z	Area / cts	Color	Peak Label	Description
Mass Intervals						
☑	2	43.0566	850449	🟥	43.06 u	C3H7
☑	3	45.0348	41872	🟦	45.03 u	PEG
☑	4	59.0138	42768	🟫	59.01 u	PMMA
☑	5	59.0512	25029	🟩	59.05 u	PEG
☑	6	69.0376	92774	⬜	69.04 u	PMMA
☑	7	69.0761	289533	🟥	69.08 u	
☑	8	73.0342	15305	⬛	73.03 u	PEG
☑	9	87.0477	5488	🟧	87.05 u	PEG
☑	10	89.0605	3641	🟪	89.06 u	PEG
☑	11	91.0587	586826	🟥	91.05 u	PS
☑	12	93.0731	40934	🟨	93.07 u	PMMA
☑	13	98.0765	65028	🟦	98.07 u	GTP
☑	14	101.0604	18365	🟩	101.06 u	PMMA
☑	15	103.0514	58432	🟩	103.05 u	PEG