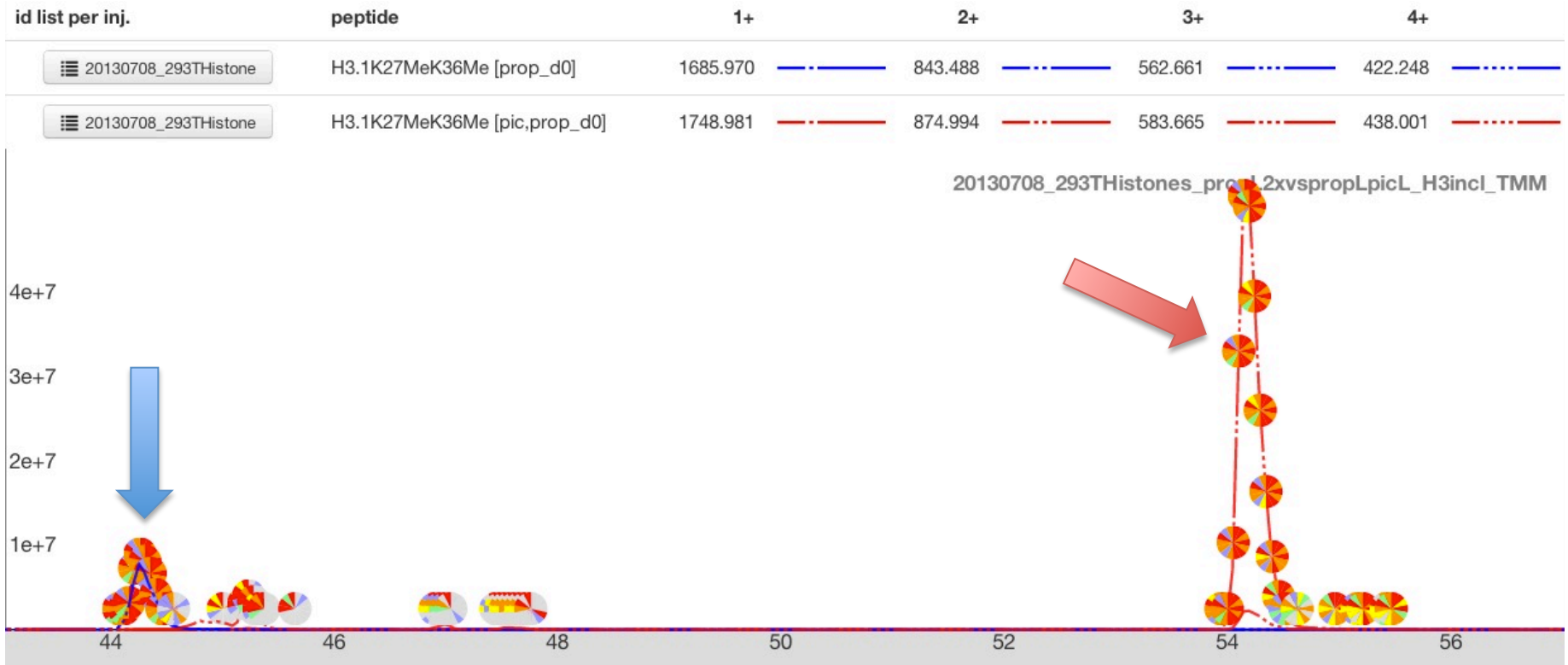


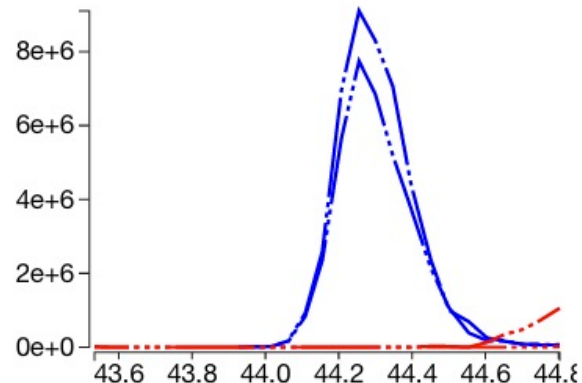
# H3.1\_K27-R40:

KMe1SAPATGGVKMe1KPHR



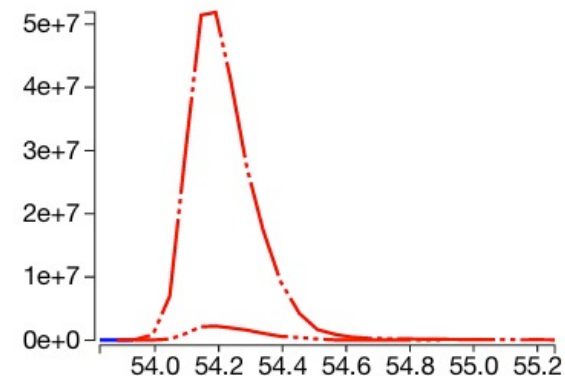
### Quanti event: 43.5-44.8min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me [prop_d0]	1	1685.9697	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me [pic,prop_d0]	1	1748.9806	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me [prop_d0]	2	843.4885	1.3e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me [pic,prop_d0]	2	874.9939	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me [prop_d0]	3	562.6614	1.1e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me [pic,prop_d0]	3	583.6651	6.8e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me [prop_d0]	4	422.2479	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me [pic,prop_d0]	4	438.0006	4.6e+4



### Quanti event: 53.8-55.3min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me [prop_d0]	1	1685.9697	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me [pic,prop_d0]	1	1748.9806	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me [prop_d0]	2	843.4885	1.3e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me [pic,prop_d0]	2	874.9939	7.2e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me [prop_d0]	3	562.6614	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me [pic,prop_d0]	3	583.6651	3.5e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me [prop_d0]	4	422.2479	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me [pic,prop_d0]	4	438.0006	0.0e+0



**Experimental spectrum**

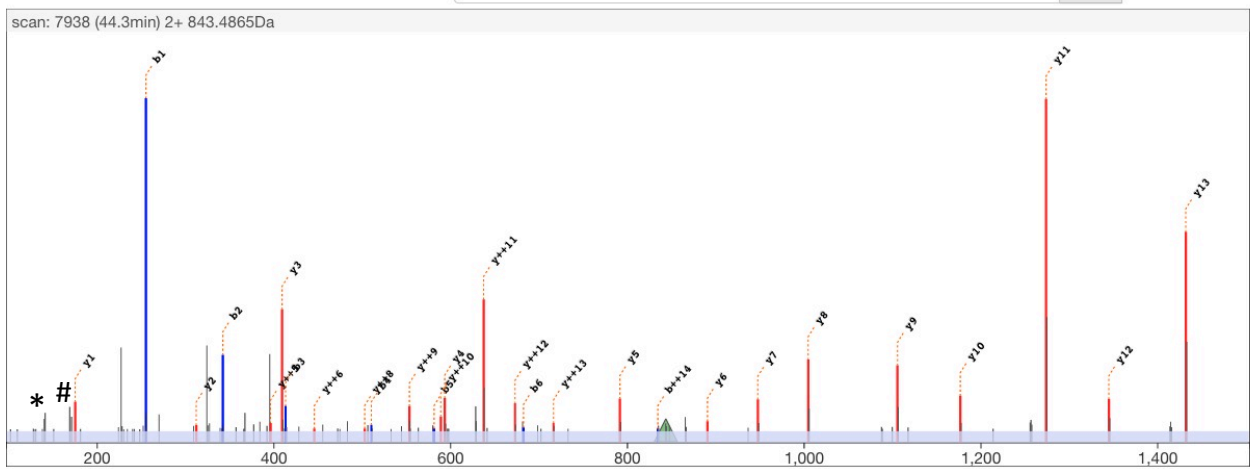
scan 7938  
 retention time 44.3min  
 precursor m/z 843.4865  
 precursor charge 2+

**Theoretical**

M H<sup>2+</sup> 843.4885  
 MH Δ<sub>mass</sub> Da -0.0041  
 MH Δ<sub>mass</sub> ppm -2.4

**edit peptide**

{Propionyl}K{Methyl,Propionyl}SAPATGGVK{Methyl,Propionyl}K{Propionyl}PHR align



	b++	b		y	y++	
			Propionyl	1629.94	815.48	14
1	128.09	255.17	Methyl(Propionyl)K	1431.81	716.41	13
2	171.60	342.20	S	1344.77	672.89	12
3	207.12	413.24	A	1273.74	637.37	11
4	255.65	510.29	P	1176.68	588.85	10
5	291.17	581.33	A	1105.65	553.33	9
6	341.69	682.38	T	1004.60	502.80	8
7	370.20	739.40	G	947.58	474.29	7
8	398.71	796.42	V	890.56	445.78	6
9	448.25	895.49	K	791.49	396.25	5
10	547.32	1093.63	Methyl(Propionyl)K	593.35	297.18	4
11	639.38	1277.75	Propionyl)K	409.23	205.12	3
12	687.90	1374.80	P	312.18	156.59	2
13	756.43	1511.86	H	175.12	88.06	1
14	834.48	1667.96	R			

\* = 140Da diagnostic ion  
 # = 171Da diagnostic ion

# H3.1\_K27-R40: PIC-KMe1SAPATGGVKMe1KPHR MS/MS

**Experimental spectrum**

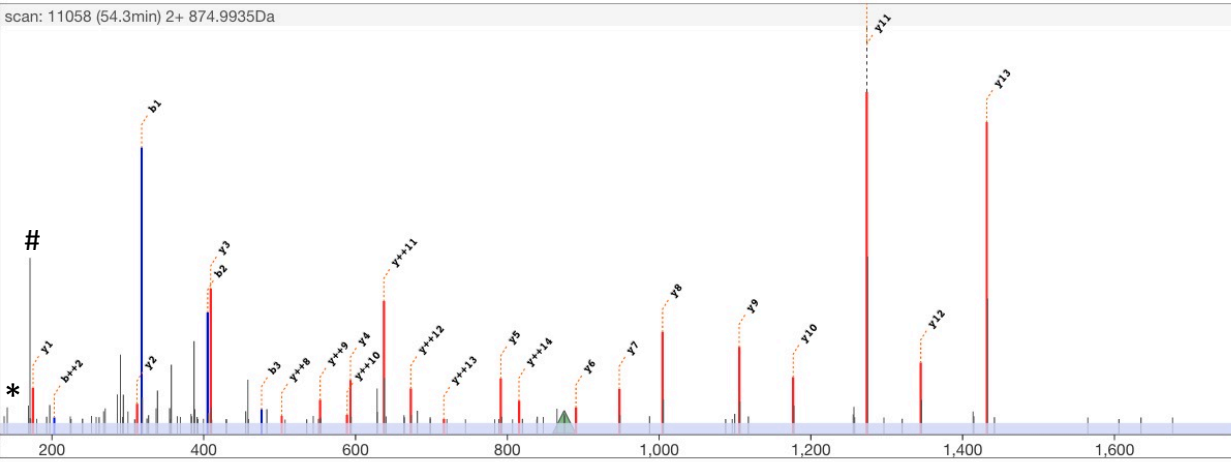
scan 11058  
 retention time 54.2min  
 precursor m/z 874.9935  
 precursor charge 2+

**Theoretical**

M H<sup>2+</sup> 874.9939  
 MH  $\Delta_{mass}$  Da -0.0008  
 MH  $\Delta_{mass}$  ppm -0.5

**edit peptide**

{PIC}K{Methyl,Propionyl}SAPATGGVK{Methyl,Propionyl}K{Propionyl}PHR align



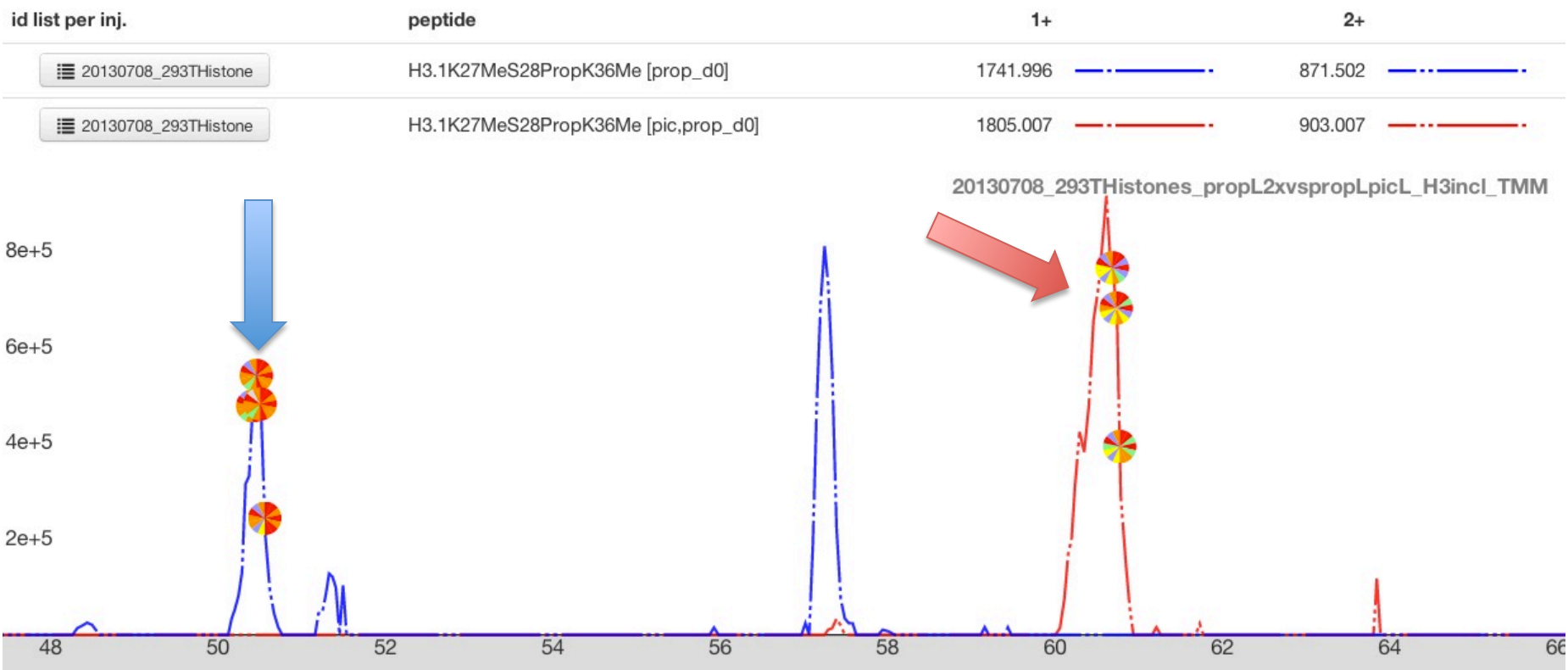
	b++	b		y	y++	
	60.53	120.04	PIC	1629.94	815.48	14
1	159.59	318.18	Methyl,Propionyl	1431.81	716.41	13
2	203.11	405.21	K	1344.77	672.89	12
3	238.63	476.25	S	1273.74	637.37	11
4	287.16	573.30	A	1176.68	588.85	10
5	322.67	644.34	P	1105.65	553.33	9
6	373.20	745.39	A	1004.60	502.80	8
7	401.71	802.41	T	947.58	474.29	7
8	430.22	859.43	G	890.56	445.78	6
9	479.75	958.50	V	791.49	396.25	5
10	578.82	1156.64	Methyl,Propionyl	593.35	297.18	4
11	670.88	1340.76	K	409.23	205.12	3
12	719.41	1437.81	Propionyl	312.18	156.59	2
13	787.94	1574.87	P	175.12	88.06	1
14	865.99	1730.97	H			
			R			

\* = 140Da diagnostic ion  
 # = 171Da diagnostic ion

# H3.1\_K27-R40:

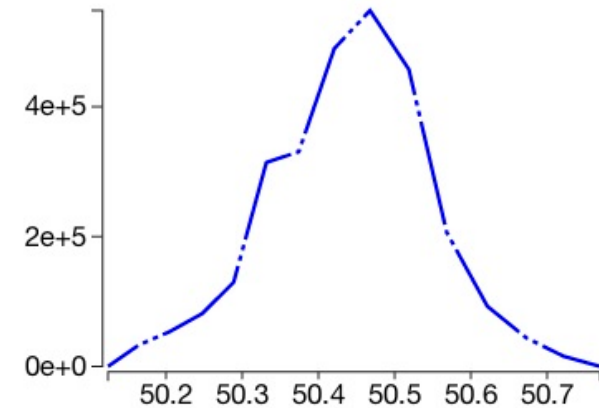
KMe1SProp?APATProp?GGVKMe1KPHR

Only S28-prop MS2 found for double peaks.



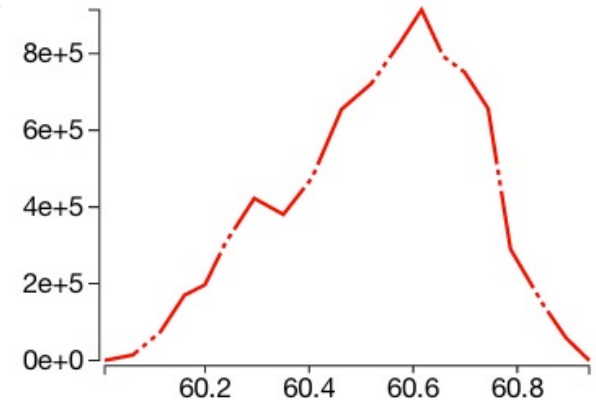
### Quanti event: 49.6-50.9min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me [prop_d0]	1	1741.9959	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me [pic,prop_d0]	1	1805.0068	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me [prop_d0]	2	871.5016	7.9e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me [pic,prop_d0]	2	903.0071	0.0e+0



### Quanti event: 59.7-61.1min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me [prop_d0]	1	1741.9959	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me [pic,prop_d0]	1	1805.0068	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me [prop_d0]	2	871.5016	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me [pic,prop_d0]	2	903.0071	2.3e+7



**Experimental spectrum**

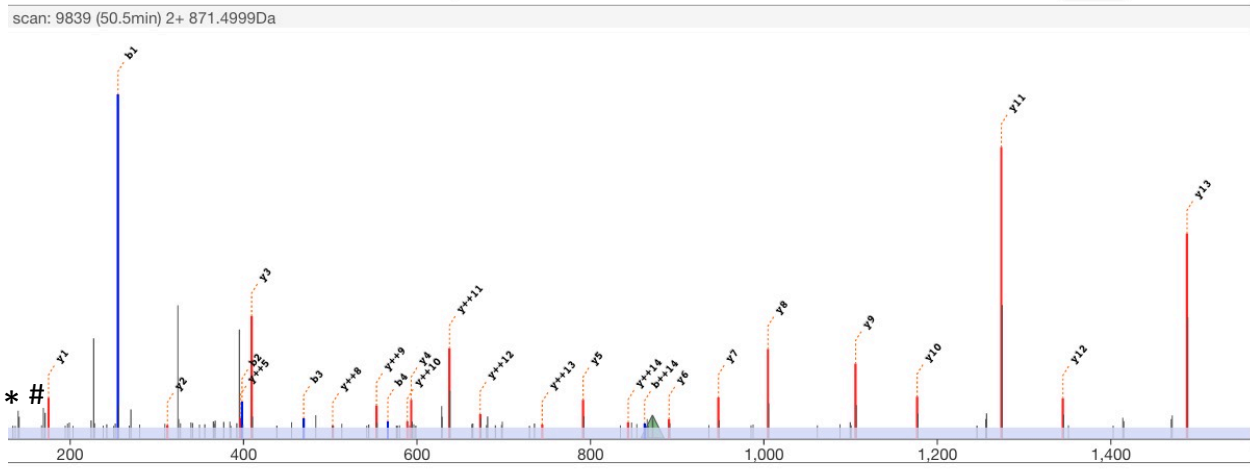
scan 9839  
 retention time 50.5min  
 precursor m/z 871.4999  
 precursor charge 2+

**Theoretical**

M H<sup>2+</sup> 871.5016  
 MH Δ<sub>mass</sub> Da -0.0035  
 MH Δ<sub>mass</sub> ppm -2.0

**edit peptide**

{Propionyl}K{(Methyl,Propionyl)S{Propionyl}APATGGVK{(Methyl,Propionyl)K{Propioi align



	b++	b	y	y++		
			Propionyl	1685.97	843.49	14
1	128.09	255.17	K	1487.83	744.42	13
			Methyl,Propionyl			
2	199.62	398.23	S	1344.77	672.89	12
			Propionyl			
3	235.14	469.27	A	1273.74	637.37	11
			P			
4	283.66	566.32	A	1176.68	588.85	10
			T			
5	319.18	637.36	A	1105.65	553.33	9
			T			
6	369.71	738.40	G	1004.60	502.80	8
			V			
7	398.22	795.42	G	947.58	474.29	7
			V			
8	426.73	852.45	K	890.56	445.78	6
			Methyl,Propionyl			
9	476.26	951.51	K	791.49	396.25	5
			Propionyl			
10	575.33	1149.65	K	593.35	297.18	4
			P			
11	667.39	1333.77	K	409.23	205.12	3
			H			
12	715.92	1430.83	R	312.18	156.59	2
13	784.45	1567.88		175.12	88.06	1
14	862.50	1723.99				

\* = 140Da diagnostic ion  
 # = 171Da diagnostic ion

**Experimental spectrum**

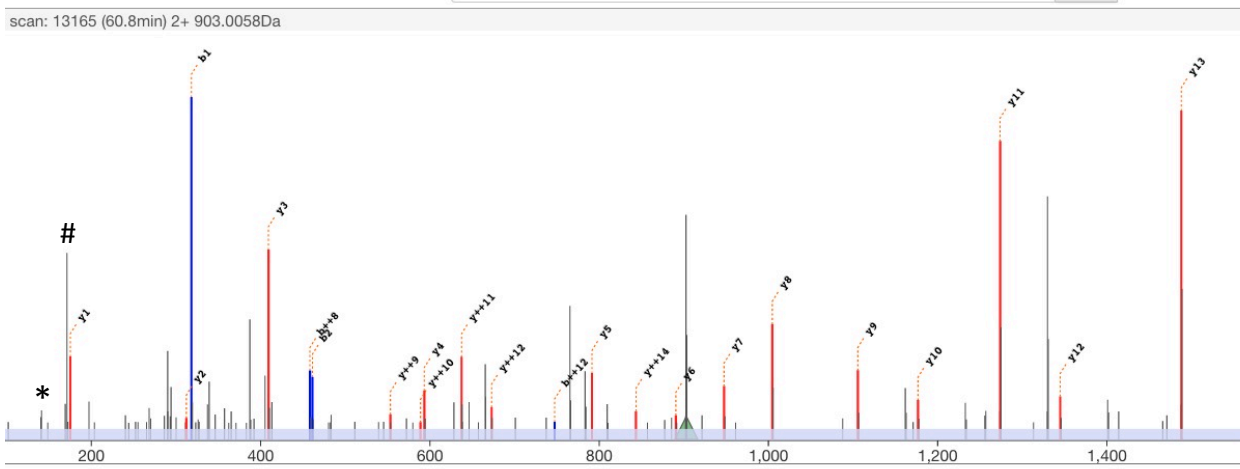
scan 13165  
 retention time 60.8min  
 precursor m/z 903.0058  
 precursor charge 2+

**Theoretical**

M H<sup>2+</sup> 903.0071  
 MH Δ<sub>mass</sub> Da -0.0025  
 MH Δ<sub>mass</sub> ppm -1.4

**edit peptide**

{PIC}K(Methyl,Propionyl)S(Propionyl)APATGGVK(Methyl,Propionyl)K(Propionyl)P- align



	b++	b		y	y++	
	60.53	120.04	PIC	1685.97	843.49	14
1	159.59	318.18	Methyl,Propionyl K	1487.83	744.42	13
2	231.12	461.24	S(Propionyl)	1344.77	672.89	12
3	266.64	532.28	A	1273.74	637.37	11
4	315.17	629.33	P	1176.68	588.85	10
5	350.69	700.37	A	1105.65	553.33	9
6	401.21	801.41	T	1004.60	502.80	8
7	429.72	858.44	G	947.58	474.29	7
8	458.23	915.46	V	890.56	445.78	6
9	507.77	1014.53	K	791.49	396.25	5
10	606.83	1212.66	Methyl,Propionyl K	593.35	297.18	4
11	698.90	1396.78	S(Propionyl) K	409.23	205.12	3
12	747.42	1493.84	P	312.18	156.59	2
13	815.95	1630.90	H	175.12	88.06	1
14	894.00	1787.00	R			

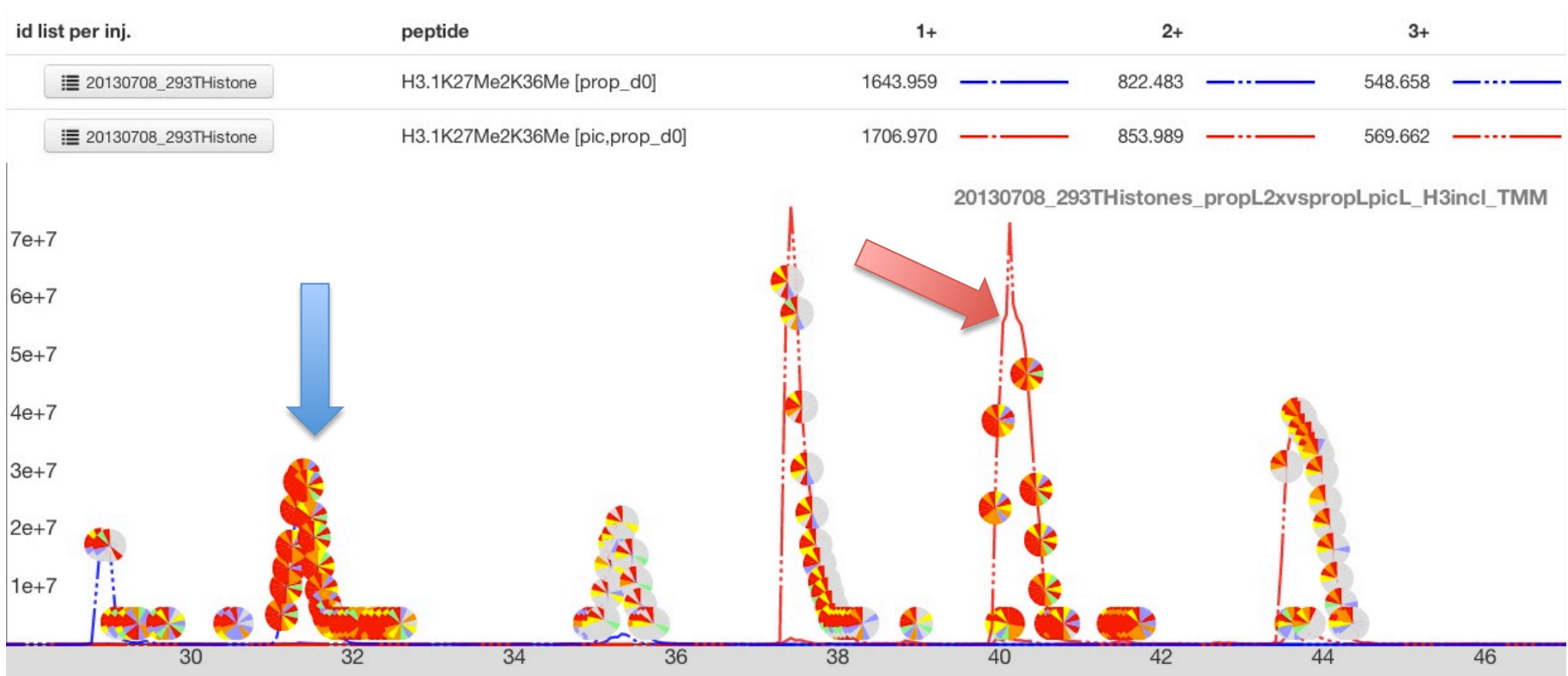
\* = 140Da diagnostic ion  
 # = 171Da diagnostic ion



# H3.1\_K27-R40:

KMe2SAPATGGVKMe1KPHR

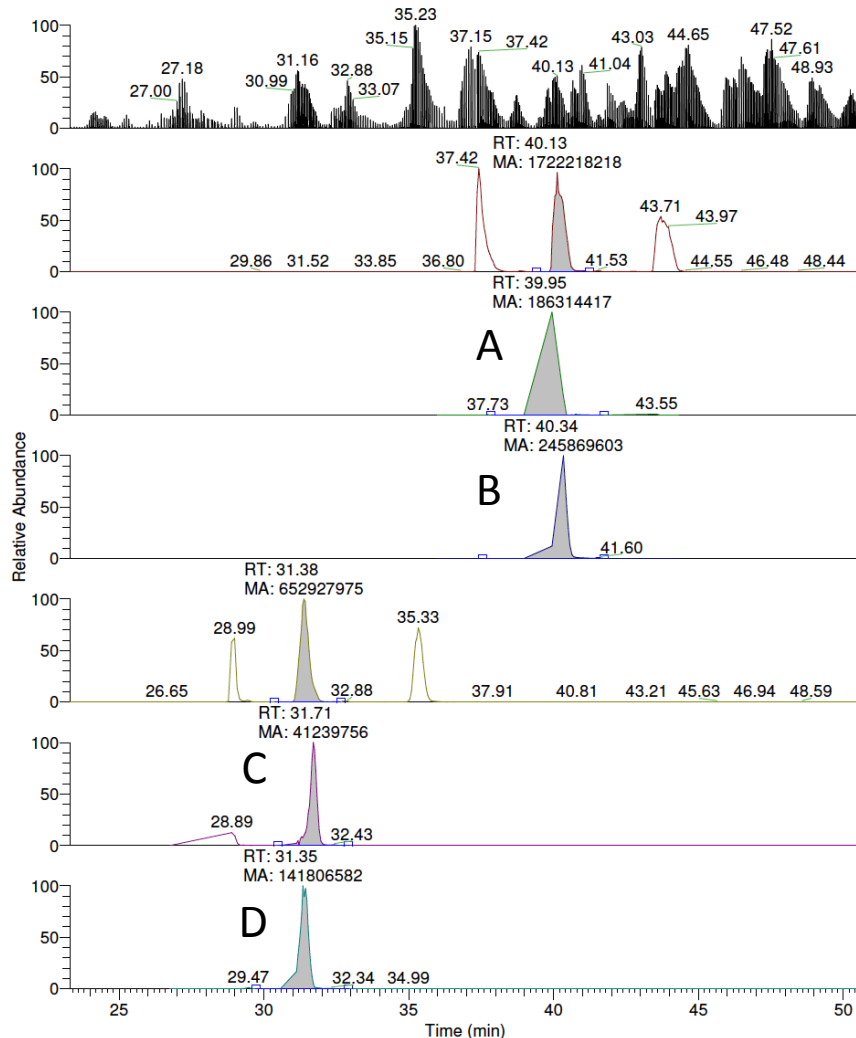
Overlaps with K27un,K36me3 (see page 243).



# H3.1\_K27-R40: KMe2SAPATGGVKMe1KPHR (Peak B & D)

20130708\_293THistones\_propL2xvpropLp... 7/8/2013 11:43:33 AM

6 of 10 ul, Histones RT: 23.31 - 50.59



AUC calculation on MS2 level:  
XIC-PIC 569.66 (3+)  
791.49, 817.42, 916.49, 1004.60  
XIC-Prop 548.658 (3+)  
371.23, 754.41, 791.49, 853.48,  
1004.60

- A = K36Me3-peak PIC
- B = K27Me2K36Me1-peak PIC
- C = K36Me3-peak Prop
- D = K27Me2K36Me1-peak Prop

**Experimental spectrum**

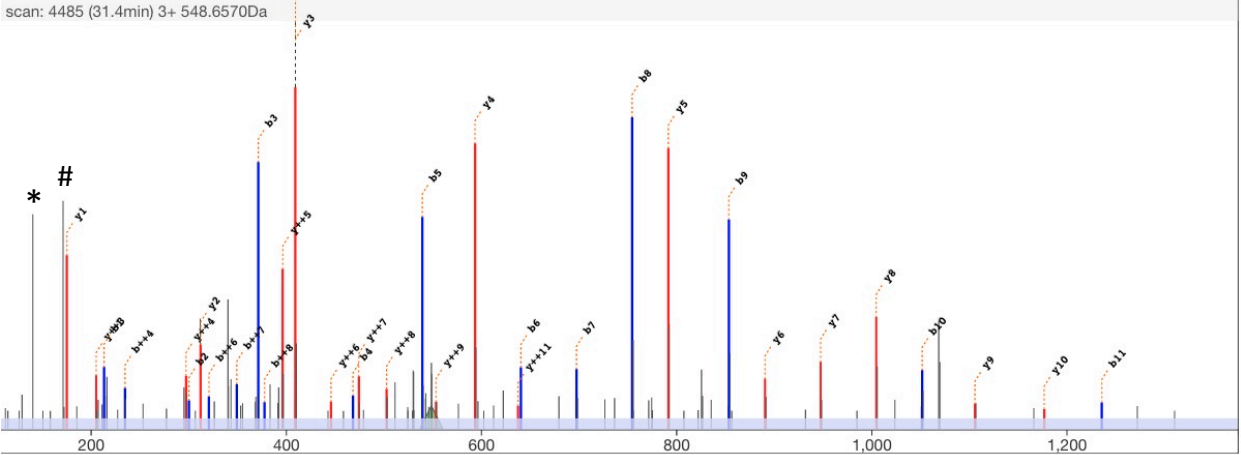
scan 4485  
 retention time 31.4min  
 precursor m/z 548.6570  
 precursor charge 3+

**Theoretical**

M H<sup>3+</sup> 548.6579  
 MH Δ<sub>mass</sub> Da -0.0026  
 MH Δ<sub>mass</sub> ppm -1.6

**edit peptide**

{Propionyl}K{Dimethyl}SAPATGGVK{Methyl,Propionyl}K{Propionyl}PHR align



	b++	b		y	y++	
			Propionyl	1587.93	794.47	14
1	107.08	213.16	K	1431.81	716.41	13
2	150.60	300.19	S	1344.77	672.89	12
3	186.12	371.23	A	1273.74	637.37	11
4	234.64	468.28	P	1176.68	588.85	10
5	270.16	539.32	A	1105.65	553.33	9
6	320.69	640.37	T	1004.60	502.80	8
7	349.20	697.39	G	947.58	474.29	7
8	377.71	754.41	V	890.56	445.78	6
9	427.24	853.48	K	791.49	396.25	5
10	526.31	1051.61	Methyl,Propionyl	593.35	297.18	4
11	618.37	1235.74	Propionyl	409.23	205.12	3
12	666.90	1332.79	K	312.18	156.59	2
13	735.43	1469.85	P	175.12	88.06	1
14	813.48	1625.95	H			

\* = 140Da diagnostic ion  
 # = 171Da diagnostic ion

**Experimental spectrum**

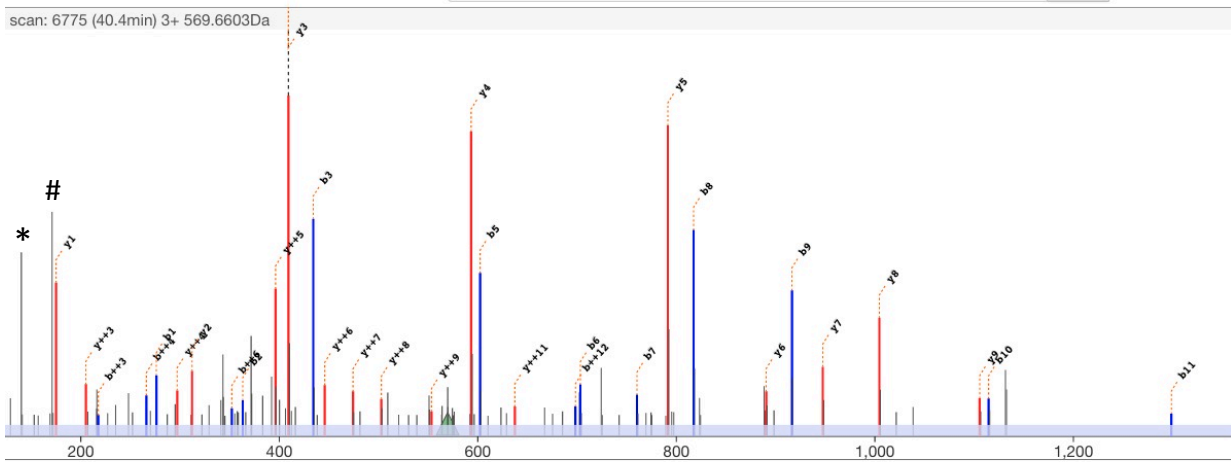
scan 6775  
 retention time 40.3min  
 precursor m/z 569.6603  
 precursor charge 3+

**Theoretical**

M H<sup>3+</sup> 569.6615  
 MH Δ<sub>mass</sub> Da -0.0036  
 MH Δ<sub>mass</sub> ppm -2.1

**edit peptide**

{PIC}K{Dimethyl}SAPATGGVK{Methyl,Propionyl}K{Propionyl}PHR

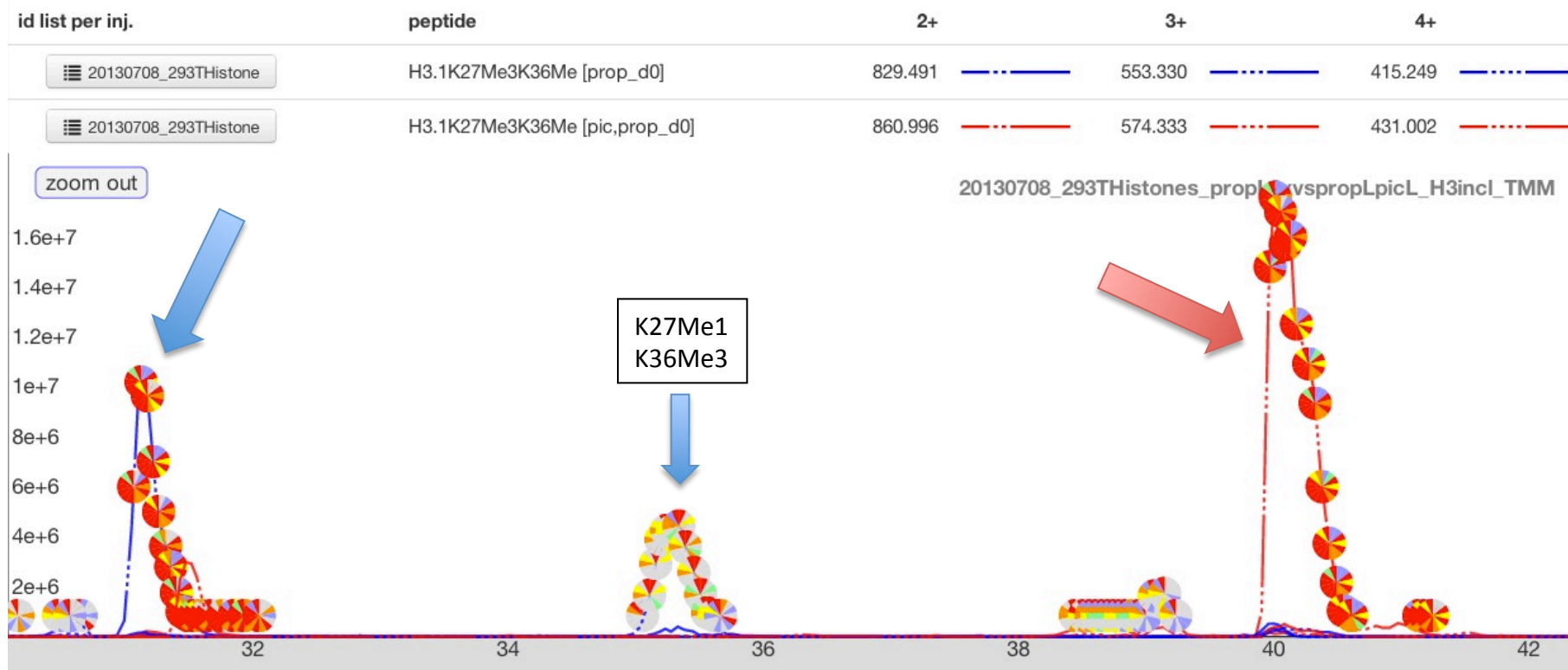


	b++	b		y	y++	
	60.53	120.04	PIC	1587.93	794.47	14
1	138.59	276.17	K	1431.81	716.41	13
			Dimethyl			
2	182.10	363.20	S	1344.77	672.89	12
3	217.62	434.24	A	1273.74	637.37	11
4	266.15	531.29	P	1176.68	588.85	10
5	301.67	602.33	A	1105.65	553.33	9
6	352.19	703.38	T	1004.60	502.80	8
7	380.70	760.40	G	947.58	474.29	7
8	409.21	817.42	V	890.56	445.78	6
9	458.75	916.49	K	791.49	396.25	5
10	557.82	1114.63	Methyl,Propionyl	593.35	297.18	4
			K			
11	649.88	1298.75	Propionyl	409.23	205.12	3
12	698.40	1395.80	P	312.18	156.59	2
13	766.93	1532.86	H	175.12	88.06	1
			R			
14	844.98	1688.96				

\* = 140Da diagnostic ion  
 # = 171Da diagnostic ion

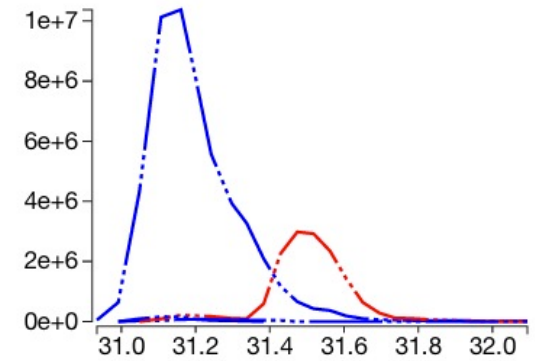
# H3.1\_K27-R40:

KMe3SAPATGGVKMe1KPHR



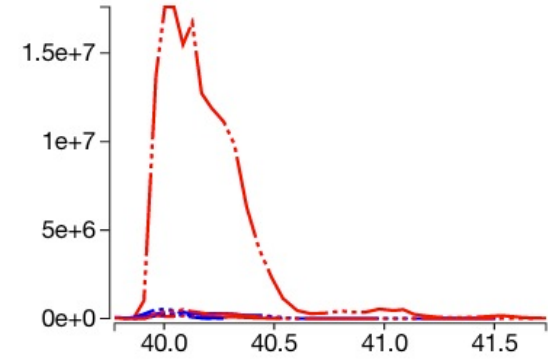
### Quanti event: 30.9-32.1min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me [prop_d0]	2	829.4910	8.1e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me [pic,prop_d0]	2	860.9965	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me [prop_d0]	3	553.3298	1.5e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me [pic,prop_d0]	3	574.3334	3.9e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me [prop_d0]	4	415.2492	2.2e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me [pic,prop_d0]	4	431.0019	0.0e+0



### Quanti event: 39.8-41.8min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me [prop_d0]	2	829.4910	3.2e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me [pic,prop_d0]	2	860.9965	3.4e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me [prop_d0]	3	553.3298	8.7e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me [pic,prop_d0]	3	574.3334	4.1e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me [prop_d0]	4	415.2492	6.0e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me [pic,prop_d0]	4	431.0019	9.1e+6



# H3.1\_K27-R40: Prop-KMe3SAPATGGVKMe1KPHR MS/MS

### Experimental spectrum

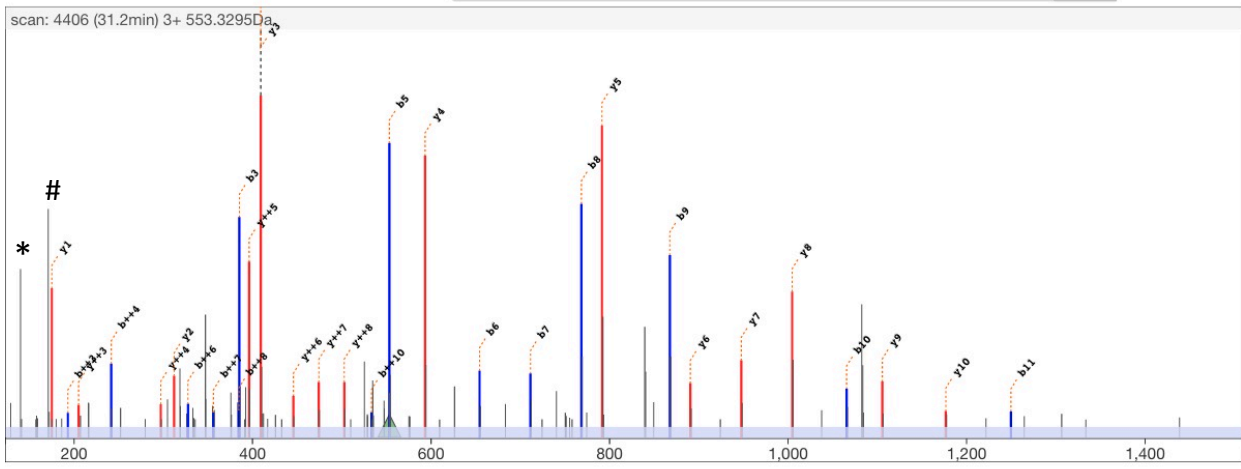
scan 4406  
 retention time 31.2min  
 precursor m/z 553.3295  
 precursor charge 3+

### Theoretical

M H<sup>3+</sup> 553.3298  
 MH Δ<sub>mass</sub> Da -0.0010  
 MH Δ<sub>mass</sub> ppm -0.6

### edit peptide

{Propionyl}K{Trimethyl}SAPATGGVK{Methyl,Propionyl}K{Propionyl}PHR



	b++	b		y	y++	
			Propionyl	1601.95	801.48	14
1	114.09	227.18	K	1431.81	716.41	13
			Trimethyl	1344.77	672.89	12
2	157.61	314.21	S	1273.74	637.37	11
3	193.13	385.24	A	1176.68	588.85	10
4	241.65	482.30	P	1105.65	553.33	9
5	277.17	553.33	A	1004.60	502.80	8
6	327.69	654.38	T	947.58	474.29	7
7	356.21	711.40	G	890.56	445.78	6
8	384.72	768.43	V	791.49	396.25	5
9	434.25	867.49	K	593.35	297.18	4
10	533.32	1065.63	Methyl/Propionyl	409.23	205.12	3
11	625.38	1249.75	K	312.18	156.59	2
12	673.91	1346.80	P	175.12	88.06	1
13	742.44	1483.86	H			
14	820.49	1639.96	R			

\* = 140Da diagnostic ion  
 # = 171Da diagnostic ion

# H3.1\_K27-R40: PIC-KMe3SAPATGGVKMe1KPHR MS/MS

**Experimental spectrum**

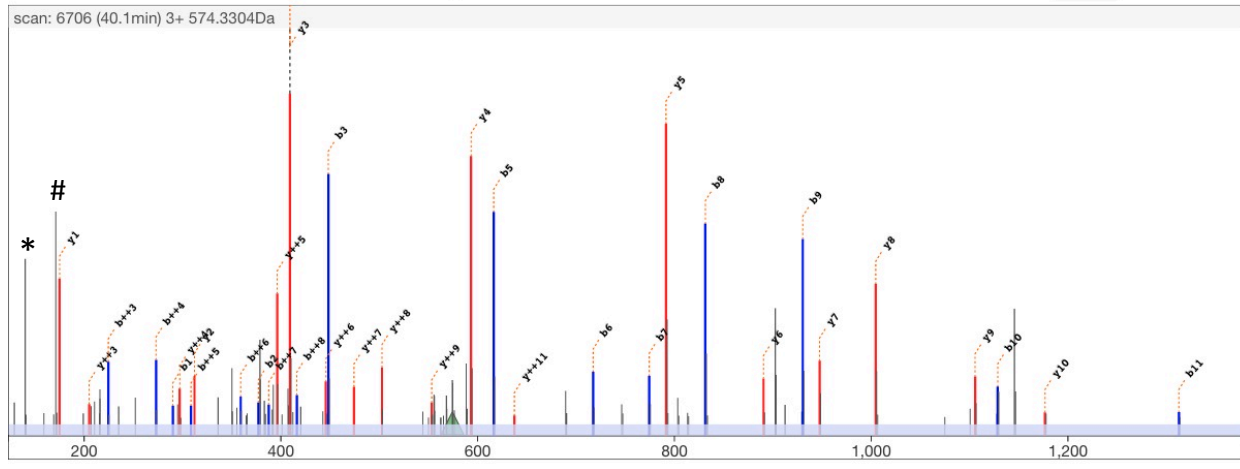
scan 6706  
 retention time 40.1min  
 precursor m/z 574.3304  
 precursor charge 3+

**Theoretical**

M H<sup>3+</sup> 574.3334  
 MH  $\Delta_{mass}$  Da -0.0089  
 MH  $\Delta_{mass}$  ppm -5.2

**edit peptide**

{PIC}K{Trimethyl}SAPATGGVK{Methyl,Propionyl}K{Propionyl}PHR align



	b++	b		y	y++	
	60.53	120.04	PIC	1601.95	801.48	14
1	145.60	290.19	K	1431.81	716.41	13
2	189.11	377.22	S	1344.77	672.89	12
3	224.63	448.26	A	1273.74	637.37	11
4	273.16	545.31	P	1176.68	588.85	10
5	308.68	616.35	A	1105.65	553.33	9
6	359.20	717.39	T	1004.60	502.80	8
7	387.71	774.41	G	947.58	474.29	7
8	416.22	831.44	G	890.56	445.78	6
9	465.76	930.50	V	791.49	396.25	5
10	564.82	1128.64	K	593.35	297.18	4
11	656.88	1312.76	K	409.23	205.12	3
12	705.41	1409.82	P	312.18	156.59	2
13	773.94	1546.87	H	175.12	88.06	1
14	851.99	1702.98	R			

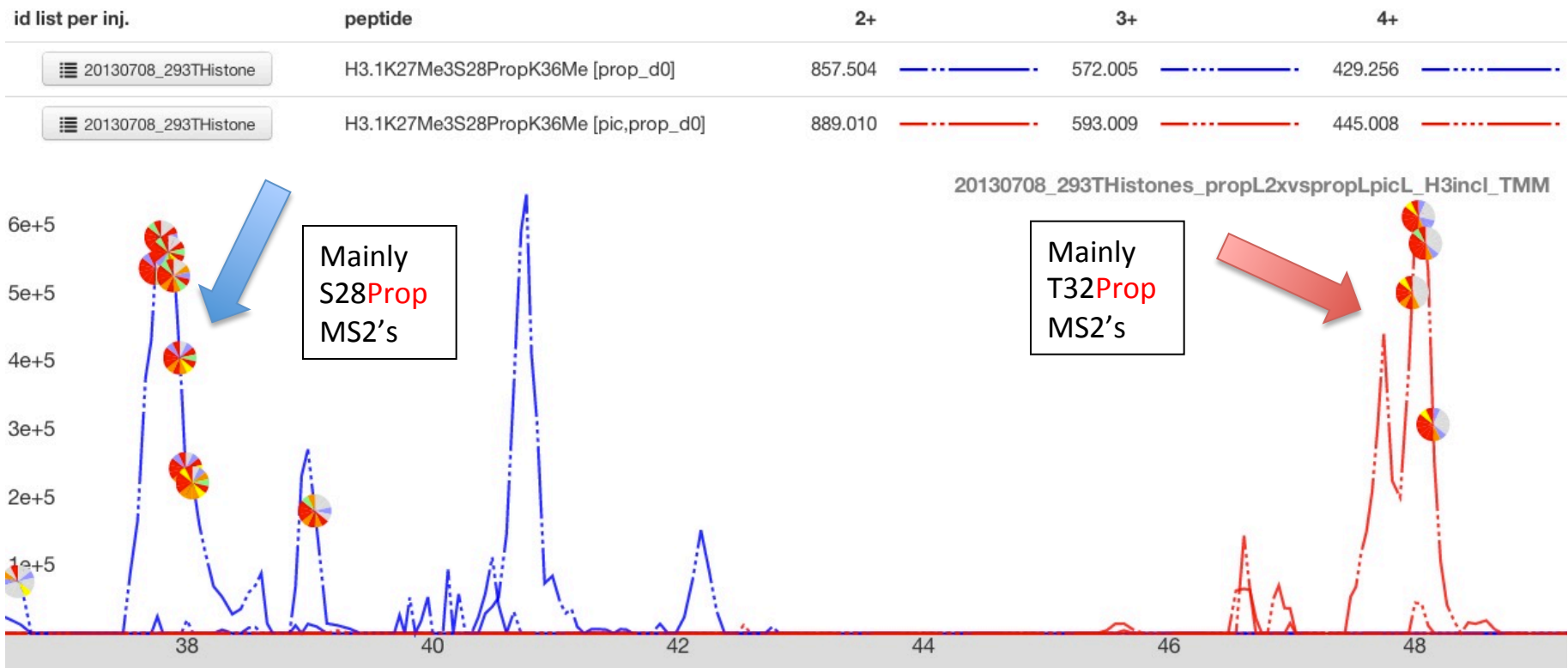
\* = 140Da diagnostic ion  
 # = 171Da diagnostic ion



# H3.1\_K27-R40:

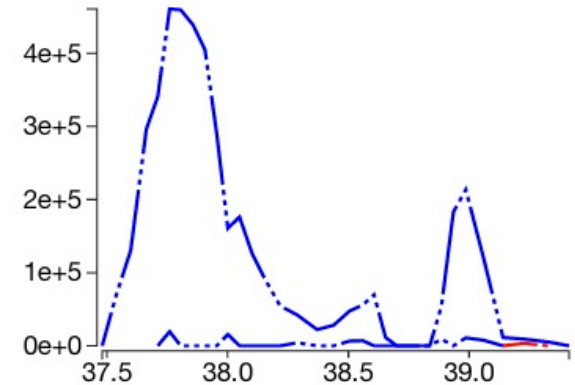
KMe3SProp?APATProp?GGVKMe1KPHR

Mainly T32-prop MS2 detected in PIC-labeling. T32-prop MS2 shown.



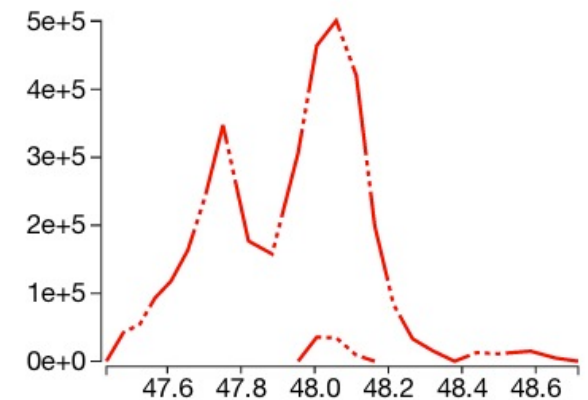
### Quanti event: 37.2-39.6min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me [prop_d0]	2	857.5041	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me [pic,prop_d0]	2	889.0096	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me [prop_d0]	3	572.0052	1.4e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me [pic,prop_d0]	3	593.0088	1.9e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me [prop_d0]	4	429.2557	2.7e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me [pic,prop_d0]	4	445.0084	0.0e+0



### Quanti event: 47.3-48.8min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me [prop_d0]	2	857.5041	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me [pic,prop_d0]	2	889.0096	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me [prop_d0]	3	572.0052	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me [pic,prop_d0]	3	593.0088	1.1e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me [prop_d0]	4	429.2557	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me [pic,prop_d0]	4	445.0084	2.5e+5



**Experimental spectrum**

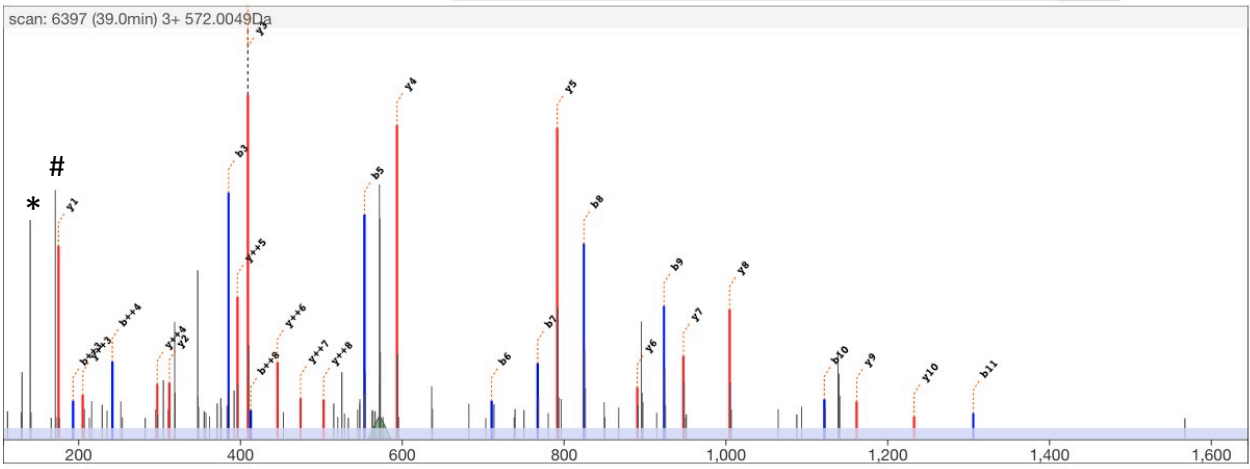
scan 6397  
 retention time 39.0min  
 precursor m/z 572.0049  
 precursor charge 3+

**Theoretical**

M H<sup>3+</sup> 572.0052  
 MH Δ<sub>mass</sub> Da -0.0007  
 MH Δ<sub>mass</sub> ppm -0.4

**edit peptide**

{Propionyl}K{Trimethyl}SAPAT{Propionyl}GGVK{Methyl,Propionyl}K{Propionyl}PHR align



	b++	b		y	y++	
			Propionyl	1657.97	829.49	14
1	114.09	227.18	K	1487.83	744.42	13
			Trimethyl	1400.80	700.90	12
2	157.61	314.21	S	1329.76	665.39	11
3	193.13	385.24	A	1232.71	616.86	10
4	241.65	482.30	P	1161.67	581.34	9
5	277.17	553.33	T	1004.60	502.80	8
6	355.71	710.41	Propionyl	947.58	474.29	7
7	384.22	767.43	G	890.56	445.78	6
8	412.73	824.45	V	824.45	445.78	6
9	462.26	923.52	G	791.49	396.25	5
10	561.33	1121.66	Methyl,Propionyl	593.35	297.18	4
11	653.39	1305.78	K	409.23	205.12	3
12	701.92	1402.83	Propionyl	312.18	156.59	2
13	770.45	1539.89	P	175.12	88.06	1
14	848.50	1695.99	H			
			R			

\* = 140Da diagnostic ion  
 # = 171Da diagnostic ion

**Experimental spectrum**

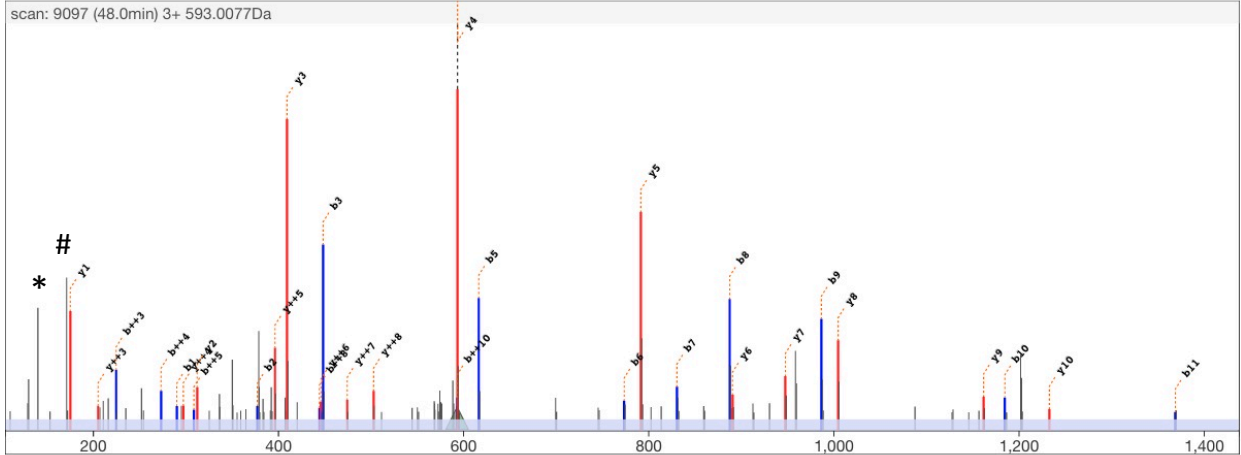
scan 9097  
 retention time 48.0min  
 precursor m/z 593.0077  
 precursor charge 3+

**Theoretical**

MH<sup>3+</sup> 593.0088  
 MH Δ<sub>mass</sub> Da -0.0034  
 MH Δ<sub>mass</sub> ppm -1.9

**edit peptide**

{PIC}K{Trimethyl}SAPAT{Propionyl}GGVK{Methyl,Propionyl}K{Propionyl}PHR align



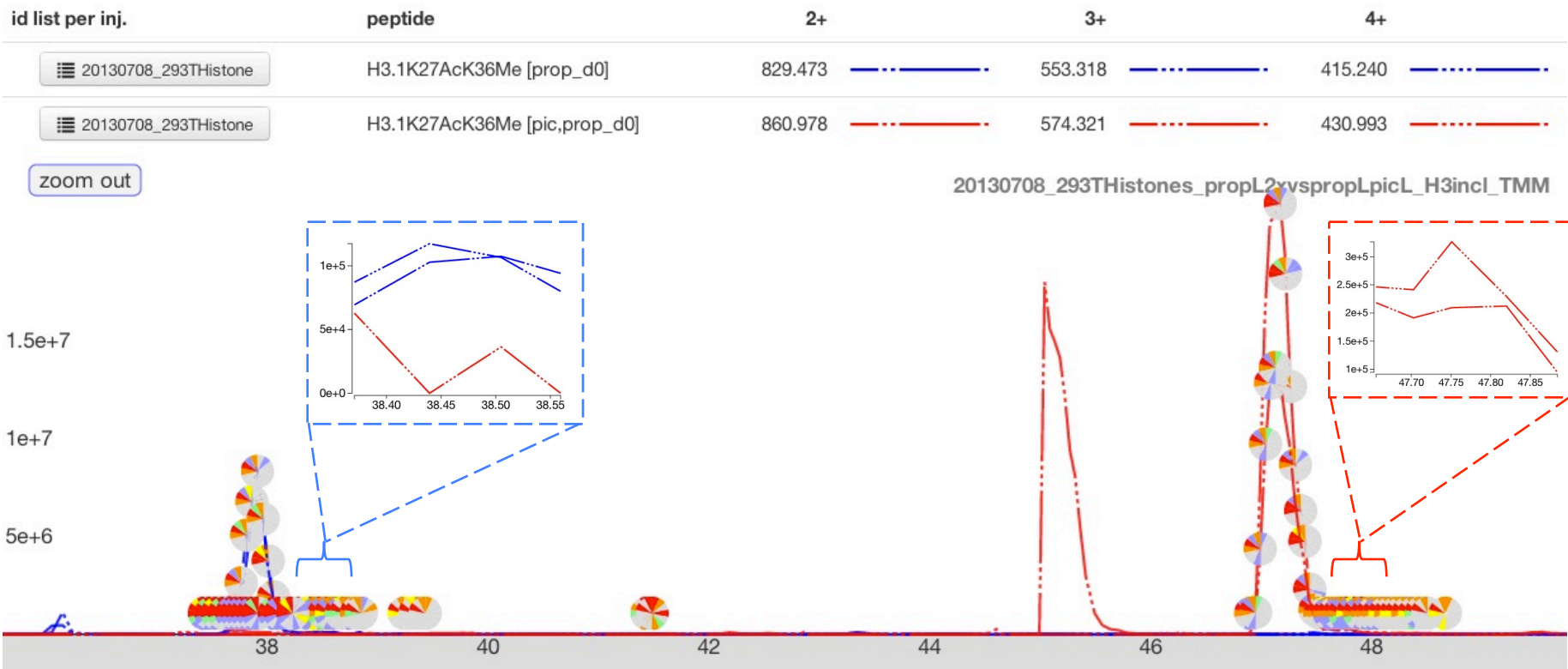
	b++	b		y	y++	
	60.53	120.04	PIC	1657.97	829.49	14
1	145.60	290.19	K	1487.83	744.42	13
2	189.11	377.22	S	1400.80	700.90	12
3	224.63	448.26	A	1329.76	665.39	11
4	273.16	545.31	P	1232.71	616.86	10
5	308.68	616.35	A	1161.67	581.34	9
6	387.21	773.42	T	1004.60	502.80	8
7	415.72	830.44	G	947.58	474.29	7
8	444.23	887.46	V	890.56	445.78	6
9	493.77	986.53	K	791.49	396.25	5
10	592.84	1184.67	K	593.35	297.18	4
11	684.90	1368.79	K	409.23	205.12	3
12	733.42	1465.84	P	312.18	156.59	2
13	801.95	1602.90	H	175.12	88.06	1
14	880.00	1759.00	R			

\* = 140Da diagnostic ion  
 # = 171Da diagnostic ion

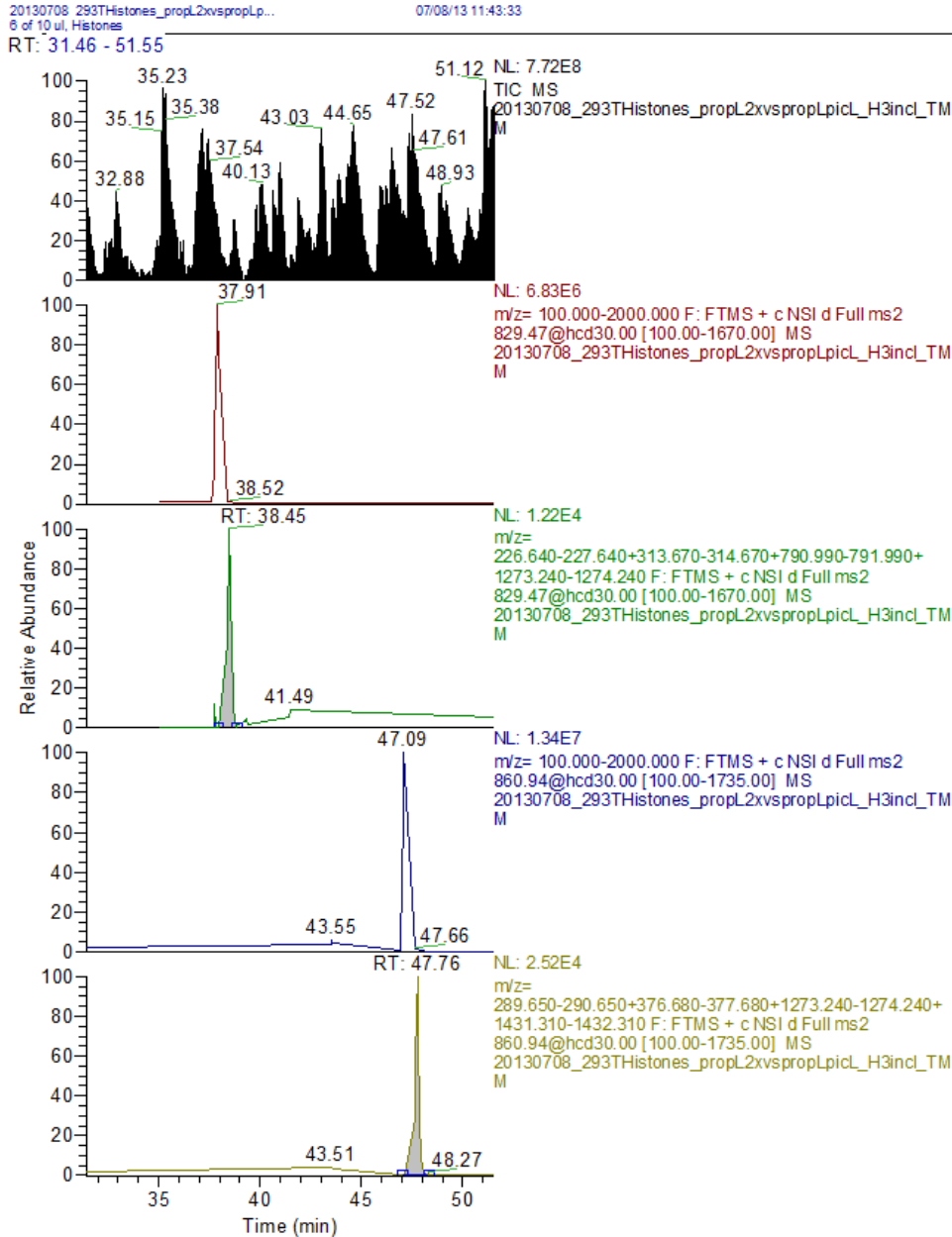
# H3.1\_K27-R40:

## KAcSAPATGGVKMe1KPHR

H3.1K27AcK36Me1 runs in end of peak for H3.1K27unmodified. Mixed MS2s, calculation via MS2 level.



# H3.1\_K27-R40: KAcSAPATGGVKMe1KPHR (Peak B & D)



AUC calculation on MS2 level:

XIC-PIC 829.472 (2+)

227.14, 314.17, 1273.74, 1431.81

XIC-Prop 860.976 (2+)

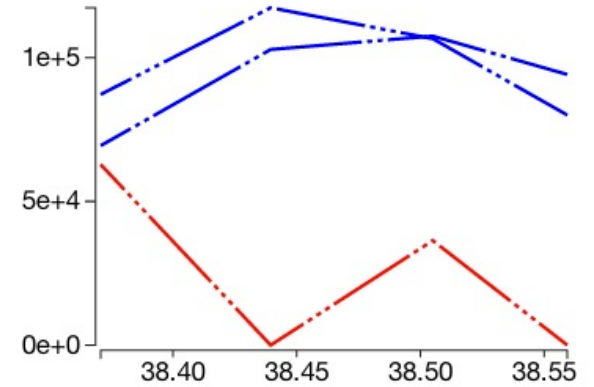
290.15, 377.18, 1273.74, 1431.81

A = K27AcK36Me1-peak Prop

B = K27AcK36Me1-peak PIC

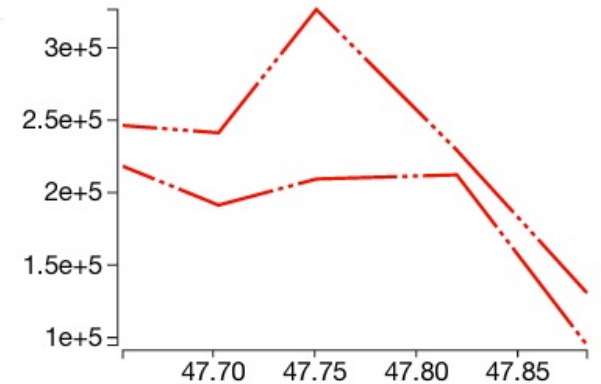
### Quanti event: 38.4-38.6min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27AcK36Me [prop_d0]	2	829.4728	1.1e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27AcK36Me [pic,prop_d0]	2	860.9783	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27AcK36Me [prop_d0]	3	553.3177	1.2e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27AcK36Me [pic,prop_d0]	3	574.3213	2.6e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27AcK36Me [prop_d0]	4	415.2401	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27AcK36Me [pic,prop_d0]	4	430.9928	0.0e+0



### Quanti event: 47.6-47.9min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27AcK36Me [prop_d0]	2	829.4728	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27AcK36Me [pic,prop_d0]	2	860.9783	2.6e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27AcK36Me [prop_d0]	3	553.3177	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27AcK36Me [pic,prop_d0]	3	574.3213	3.4e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27AcK36Me [prop_d0]	4	415.2401	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27AcK36Me [pic,prop_d0]	4	430.9928	0.0e+0



# H3.1\_K27-R40: Prop-KAcSAPATGGVKMe1KPHR MS/MS

**Experimental spectrum**

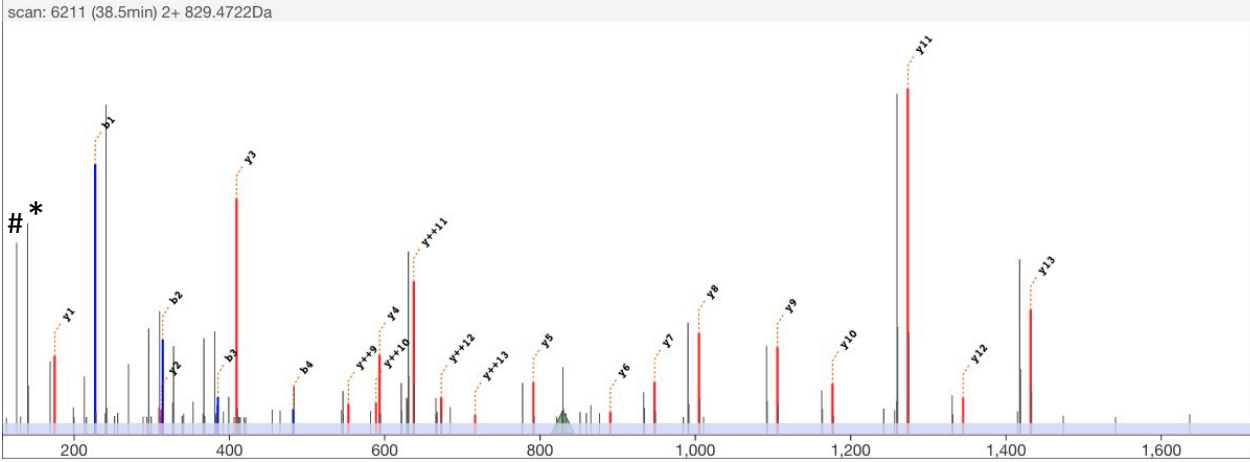
scan 6211  
 retention time 38.4min  
 precursor m/z 829.4722  
 precursor charge 2+

**Theoretical**

M H<sup>2+</sup> 829.4728  
 MH Δ<sub>mass</sub> Da -0.0014  
 MH Δ<sub>mass</sub> ppm -0.8

**edit peptide**

{Propionyl}K{Acetyl}SAPATGGVK{Methyl,Propionyl}K{Propionyl}PHR align



	b++	b	y	y++	
			1601.91	801.46	14
1	114.07	227.14	1431.81	716.41	13
2	157.59	314.17	1344.77	672.89	12
3	193.11	385.21	1273.74	637.37	11
4	241.63	482.26	1176.68	588.85	10
5	277.15	553.30	1105.65	553.33	9
6	327.68	654.35	1004.60	502.80	8
7	356.19	711.37	947.58	474.29	7
8	384.70	768.39	890.56	445.78	6
9	434.23	867.46	791.49	396.25	5
10	533.30	1065.59	593.35	297.18	4
11	625.36	1249.72	409.23	205.12	3
12	673.89	1346.77	312.18	156.59	2
13	742.42	1483.83	175.12	88.06	1
14	820.47	1639.93			

\* = 140Da diagnostic ion  
 # = 126Da diagnostic ion



# H3.1\_K27-R40: PIC-KAcSAPATGGVKMe1KPHR MS/MS

### Experimental spectrum

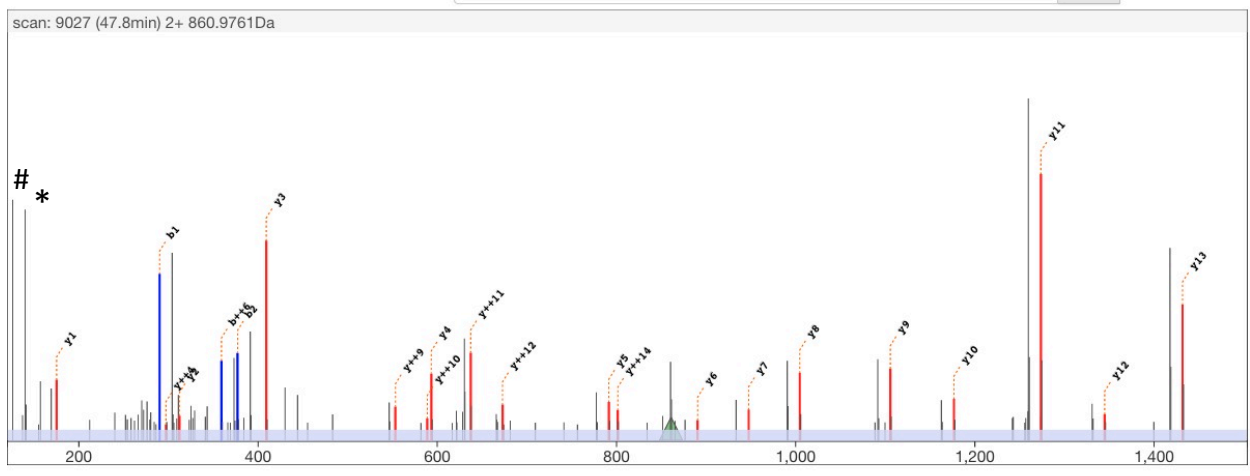
scan 9027  
 retention time 47.8min  
 precursor m/z 860.9761  
 precursor charge 2+

### Theoretical

M H<sup>2+</sup> 860.9783  
 MH Δ<sub>mass</sub> Da -0.0043  
 MH Δ<sub>mass</sub> ppm -2.5

### edit peptide

{PIC}K{Acetyl}SAPATGGVK{Methyl,Propionyl}K{Propionyl}PHR



	b++	b		y	y++	
	60.53	120.04	PIC	1601.91	801.46	14
1	145.58	290.15	K	1431.81	716.41	13
2	189.09	377.18	Acetyl	1344.77	672.89	12
3	224.61	448.22	S	1273.74	637.37	11
4	273.14	545.27	A	1176.68	588.85	10
5	308.66	616.31	P	1105.65	553.33	9
6	359.18	717.36	A	1004.60	502.80	8
7	387.69	774.38	T	947.58	474.29	7
8	416.20	831.40	G	890.56	445.78	6
9	465.74	930.47	V	791.49	396.25	5
10	564.81	1128.60	K	593.35	297.18	4
11	656.87	1312.73	Methyl,Propionyl	409.23	205.12	3
12	705.39	1409.78	Propionyl	312.18	156.59	2
13	773.92	1546.84	P	175.12	88.06	1
14	851.97	1702.94	H			
			R			

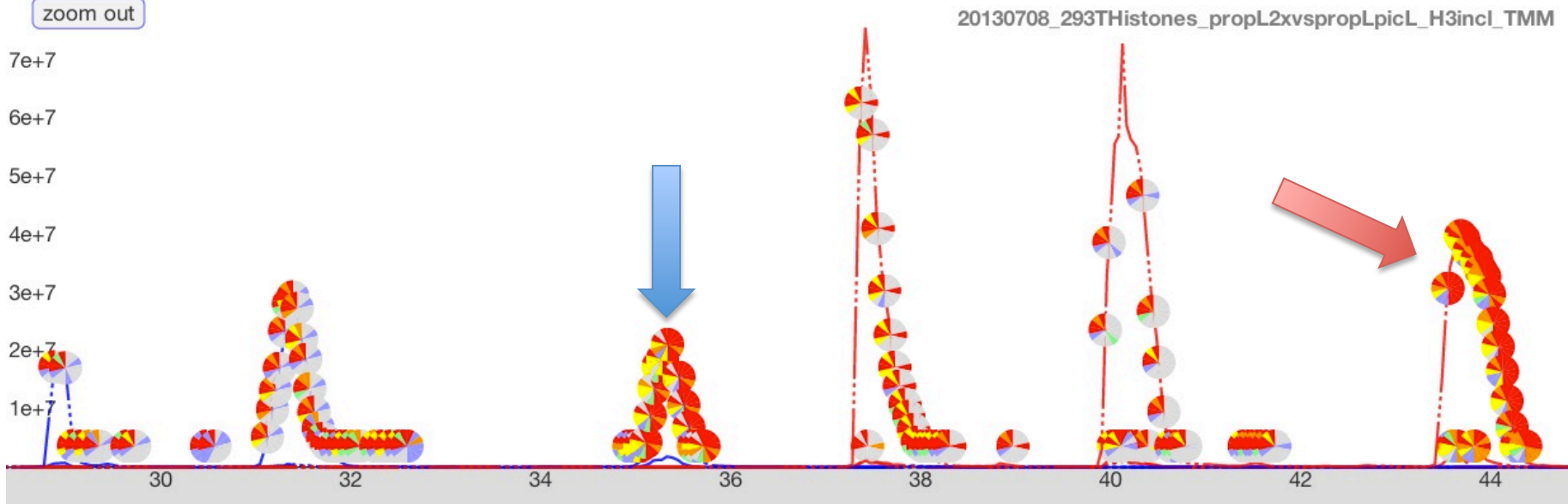
\* = 140Da diagnostic ion  
 # = 126Da diagnostic ion

# H3.1\_K27-R40:

## KMe1SAPATGGVKMe2KPHR

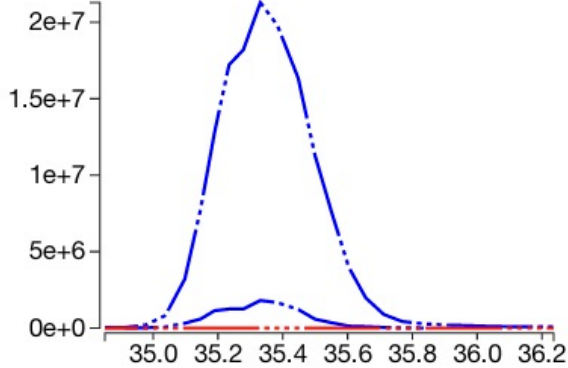
id list per inj.	peptide	2+	3+	4+
20130708_293THistone	H3.1K27MeK36Me2 [prop_d0]	822.483	548.658	411.745
20130708_293THistone	H3.1K27MeK36Me2 [pic,prop_d0]	853.989	569.662	427.498

zoom out



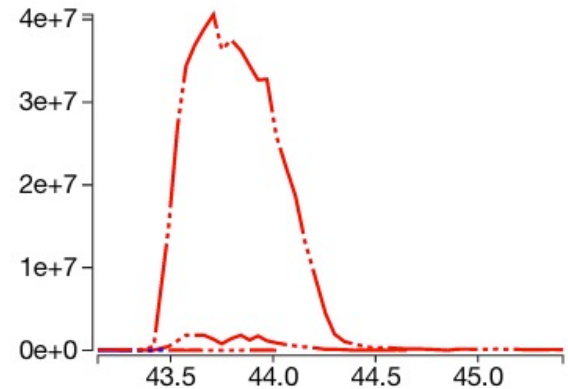
Quanti event: 34.8-36.3min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me2 [prop_d0]	2	822.4832	3.3e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me2 [pic,prop_d0]	2	853.9887	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me2 [prop_d0]	3	548.6579	4.5e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me2 [pic,prop_d0]	3	569.6615	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me2 [prop_d0]	4	411.7452	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me2 [pic,prop_d0]	4	427.4980	1.4e+5



Quanti event: 43.1-45.5min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me2 [prop_d0]	2	822.4832	5.4e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me2 [pic,prop_d0]	2	853.9887	5.3e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me2 [prop_d0]	3	548.6579	1.4e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me2 [pic,prop_d0]	3	569.6615	1.4e+9
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me2 [prop_d0]	4	411.7452	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me2 [pic,prop_d0]	4	427.4980	2.4e+5



# H3.1\_K27-R40: Prop-KMe1SAPATGGVKMe2KPHR MS/MS

### Experimental spectrum

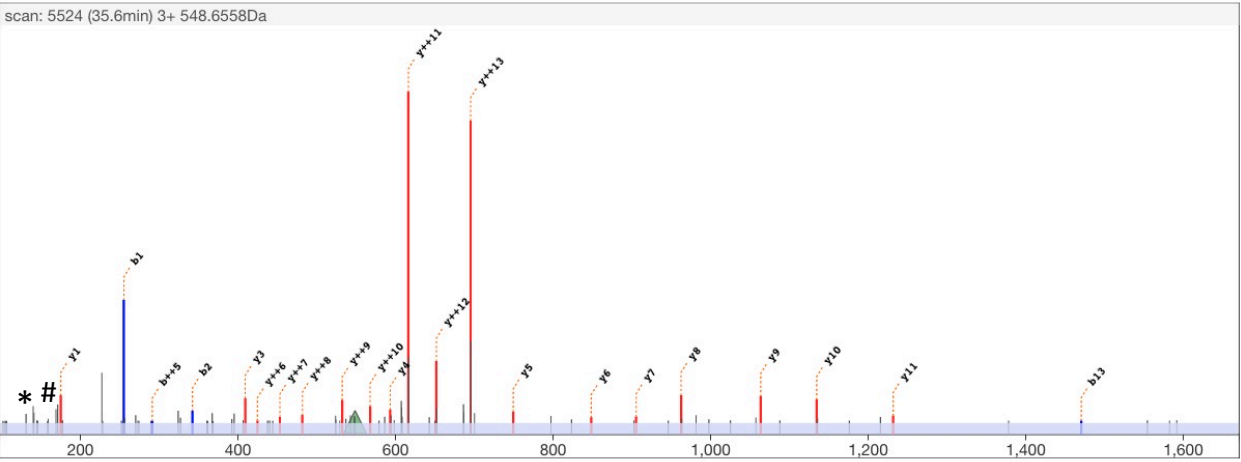
scan 5524  
 retention time 35.6min  
 precursor m/z 548.6558  
 precursor charge 3+

### Theoretical

M H<sup>3+</sup> 548.6579  
 MH Δ<sub>mass</sub> Da -0.0062  
 MH Δ<sub>mass</sub> ppm -3.8

### edit peptide

{Propionyl}K{Methyl,Propionyl}SAPATGGVK{Dimethyl}K{Propionyl}PHR align



	b++	b		y	y++	
			Propionyl	1587.93	794.47	14
1	128.09	255.17	K	1389.80	695.40	13
2	171.60	342.20	S	1302.76	651.89	12
3	207.12	413.24	A	1231.73	616.37	11
4	255.65	510.29	P	1134.67	567.84	10
5	291.17	581.33	A	1063.64	532.32	9
6	341.69	682.38	T	962.59	481.80	8
7	370.20	739.40	G	905.57	453.29	7
8	398.71	796.42	V	848.55	424.78	6
9	448.25	895.49	K	749.48	375.24	5
10	526.31	1051.61	Dimethyl	593.35	297.18	4
11	618.37	1235.74	Propionyl	409.23	205.12	3
12	666.90	1332.79	P	312.18	156.59	2
13	735.43	1469.85	H	175.12	88.06	1
14	813.48	1625.95	R			

\* = 140Da diagnostic ion  
 # = 171Da diagnostic ion

# H3.1\_K27-R40: PIC-KMe1SAPATGGVKMe2KPHR MS/MS

**Experimental spectrum**

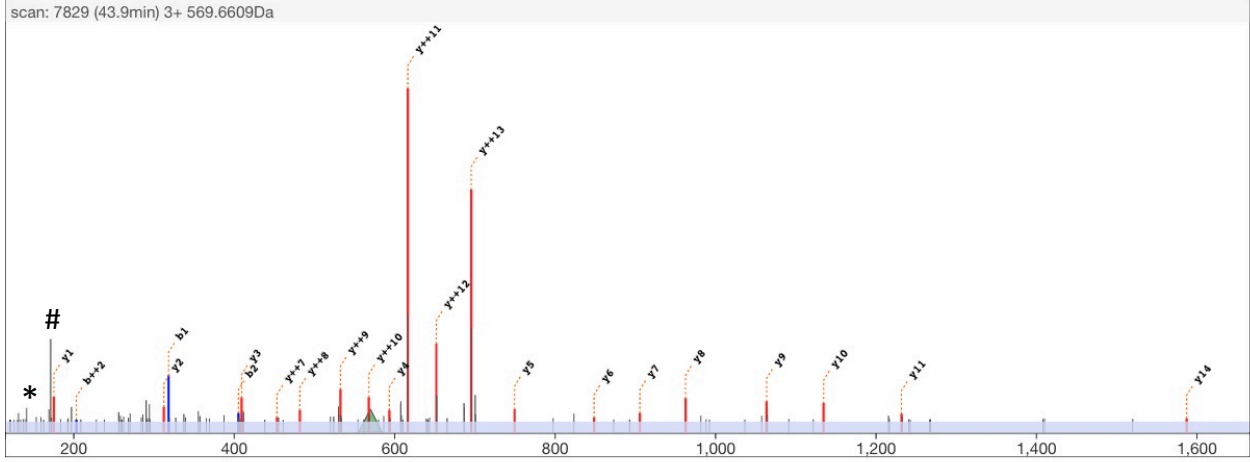
scan 7829  
 retention time 43.9min  
 precursor m/z 569.6609  
 precursor charge 3+

**Theoretical**

M H<sup>3+</sup> 569.6615  
 MH Δ<sub>mass</sub> Da -0.0018  
 MH Δ<sub>mass</sub> ppm -1.0

**edit peptide**

{PIC}K{Methyl,Propionyl}SAPATGGVK{Dimethyl}K{Propionyl}PHR



	b++	b		y	y++	
	60.53	120.04	PIC	1587.93	794.47	14
1	159.59	318.18	K	1389.80	695.40	13
2	203.11	405.21	Methyl,Propionyl	1302.76	651.89	12
3	238.63	476.25	S	1231.73	616.37	11
4	287.16	573.30	A	1134.67	567.84	10
5	322.67	644.34	P	1063.64	532.32	9
6	373.20	745.39	A	962.59	481.80	8
7	401.71	802.41	T	905.57	453.29	7
8	430.22	859.43	G	848.55	424.78	6
9	479.75	958.50	V	749.48	375.24	5
10	557.82	1114.63	K	593.35	297.18	4
11	649.88	1298.75	Dimethyl	409.23	205.12	3
12	698.40	1395.80	K	312.18	156.59	2
13	766.93	1532.86	Propionyl	175.12	88.06	1
14	844.98	1688.96	P			
			H			
			R			

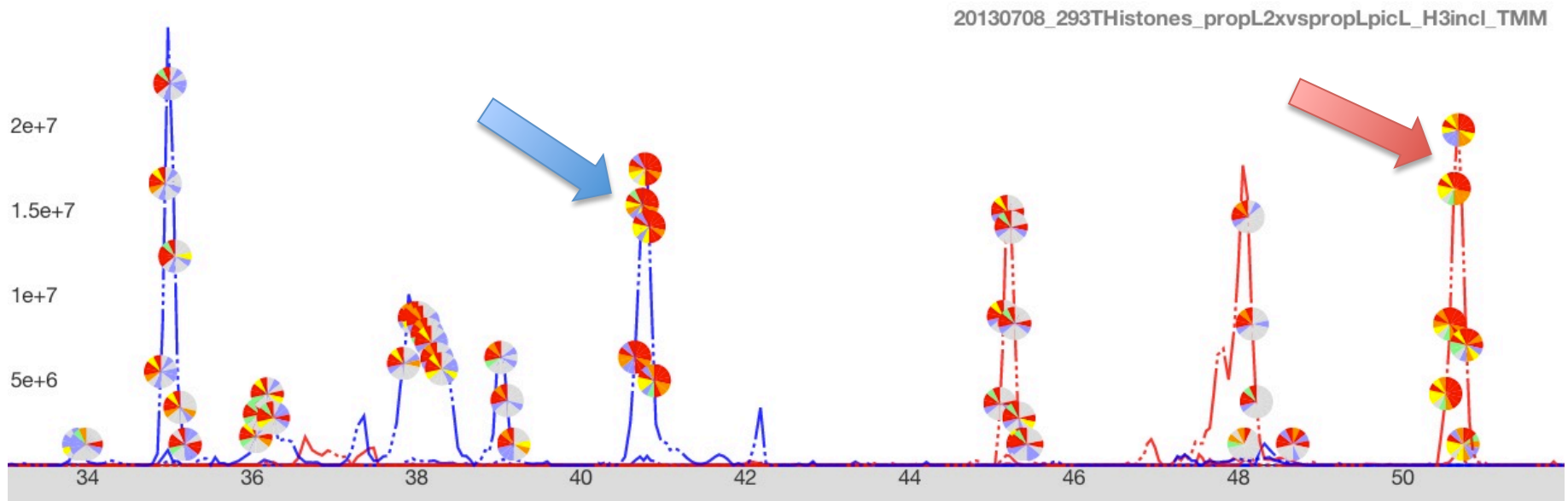
\* = 140Da diagnostic ion  
 # = 171Da diagnostic ion

# H3.1\_K27-R40:

KMe1SProp?APATProp?GGVKMe2KPHR

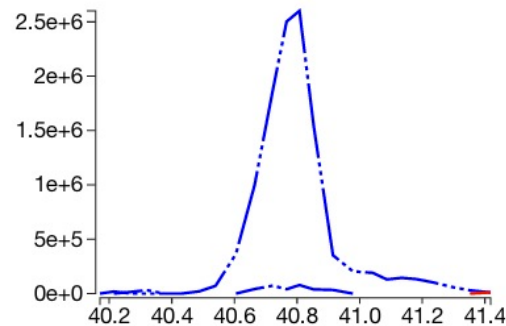
Mainly S28-prop MS2 detected in PIC-labeling. S28-prop MS2 shown.

id list per inj.	peptide	2+	3+	4+
20130708_293THistone	H3.1K27MeS28PropK36Me2 [prop_d0]	850.496	567.333	425.752
20130708_293THistone	H3.1K27MeS28PropK36Me2 [pic,prop_d0]	882.002	588.337	441.505



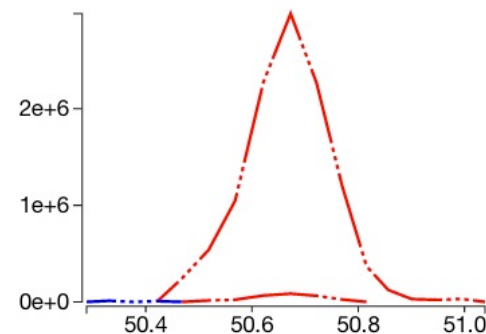
## Quanti event: 40.2-41.5min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me2 [prop_d0]	2	850.4963	9.2e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me2 [pic,prop_d0]	2	882.0018	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me2 [prop_d0]	3	567.3333	3.4e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me2 [pic,prop_d0]	3	588.3369	2.1e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me2 [prop_d0]	4	425.7518	1.5e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me2 [pic,prop_d0]	4	441.5045	0.0e+0



## Quanti event: 50.2-51.2min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me2 [prop_d0]	2	850.4963	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me2 [pic,prop_d0]	2	882.0018	8.3e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me2 [prop_d0]	3	567.3333	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me2 [pic,prop_d0]	3	588.3369	3.3e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me2 [prop_d0]	4	425.7518	5.2e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeS28PropK36Me2 [pic,prop_d0]	4	441.5045	0.0e+0



**Experimental spectrum**

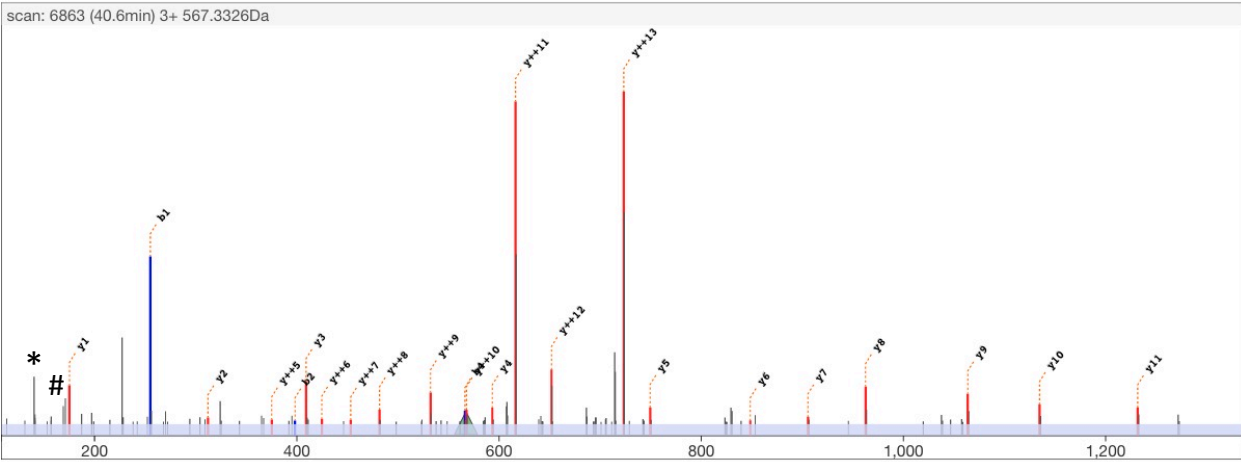
scan 6863  
 retention time 40.7min  
 precursor m/z 567.3326  
 precursor charge 3+

**Theoretical**

M H<sup>3+</sup> 567.3333  
 MH Δ<sub>mass</sub> Da -0.0022  
 MH Δ<sub>mass</sub> ppm -1.3

**edit peptide**

{Propionyl}K{(Methyl,Propionyl)S}{Propionyl}APATGGVK{(Dimethyl)K}{Propionyl}PHR align



	b++	b	y	y++		
			Propionyl	1643.96	822.48	14
1	128.09	255.17	K			13
			Methyl,Propionyl	1445.82	723.41	13
2	199.62	398.23	S			12
			Propionyl	1302.76	651.89	12
3	235.14	469.27	A			11
			Propionyl	1231.73	616.37	11
4	283.66	566.32	P			10
			Propionyl	1134.67	567.84	10
5	319.18	637.36	A			9
			Propionyl	1063.64	532.32	9
6	369.71	738.40	T			8
			Propionyl	962.59	481.80	8
7	398.22	795.42	G			7
			Propionyl	905.57	453.29	7
8	426.73	852.45	V			6
			Propionyl	848.55	424.78	6
9	476.26	951.51	K			5
			Propionyl	749.48	375.24	5
10	554.32	1107.64	K			4
			Dimethyl	593.35	297.18	4
11	646.38	1291.76	K			3
			Propionyl	409.23	205.12	3
12	694.91	1388.81	P			2
			Propionyl	312.18	156.59	2
13	763.44	1525.87	H			1
			Propionyl	175.12	88.06	1
14	841.49	1681.97	R			1

\* = 140Da diagnostic ion  
 # = 171Da diagnostic ion



**Experimental spectrum**

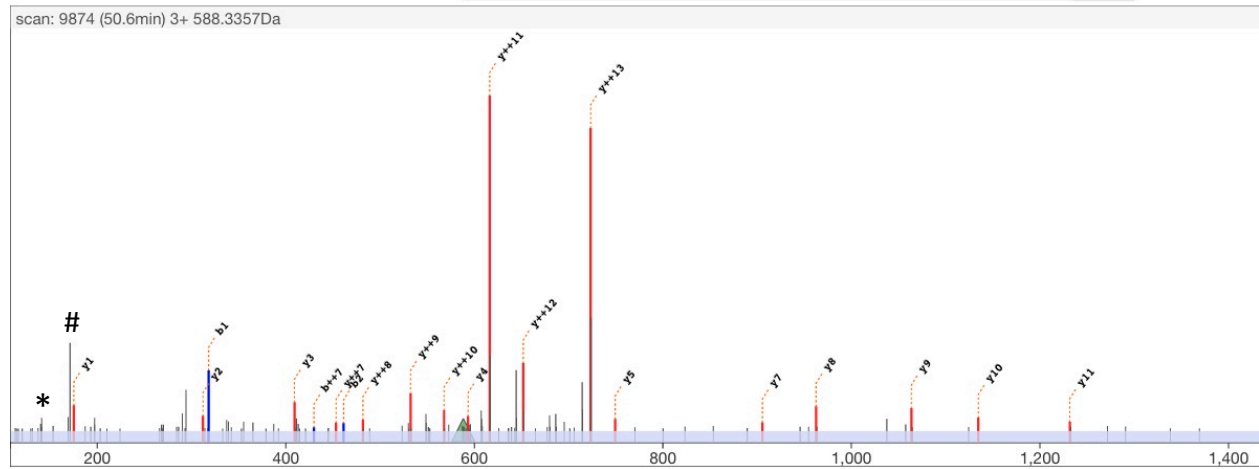
scan 9874  
 retention time 50.6min  
 precursor m/z 588.3357  
 precursor charge 3+

**Theoretical**

M H<sup>3+</sup> 588.3369  
 MH Δ<sub>mass</sub> Da -0.0037  
 MH Δ<sub>mass</sub> ppm -2.1

**edit peptide**

{PIC}K{Methyl,Propionyl}S{Propionyl}APATGGVK{Dimethyl}K{Propionyl}PHR align



	b++	b		y	y++	
	60.53	120.04	PIC	1643.96	822.48	14
1	159.59	318.18	K	1445.82	723.41	13
2	231.12	461.24	Methyl,Propionyl S	1302.76	651.89	12
3	266.64	532.28	Propionyl A	1231.73	616.37	11
4	315.17	629.33	P	1134.67	567.84	10
5	350.69	700.37	A	1063.64	532.32	9
6	401.21	801.41	T	962.59	481.80	8
7	429.72	858.44	G	905.57	453.29	7
8	458.23	915.46	V	848.55	424.78	6
9	507.77	1014.53	K	749.48	375.24	5
10	585.83	1170.65	Dimethyl K	593.35	297.18	4
11	677.89	1354.77	Propionyl K	409.23	205.12	3
12	726.42	1451.83	P	312.18	156.59	2
13	794.95	1588.88	H	175.12	88.06	1
14	873.00	1744.99	R			

\* = 140Da diagnostic ion  
 # = 171Da diagnostic ion

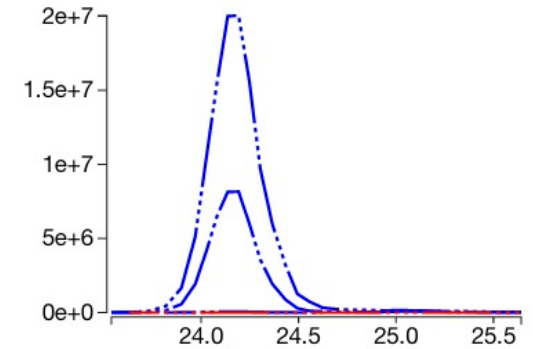
# H3.1\_K27-R40:

KMe2SAPATGGVKMe2KPHR



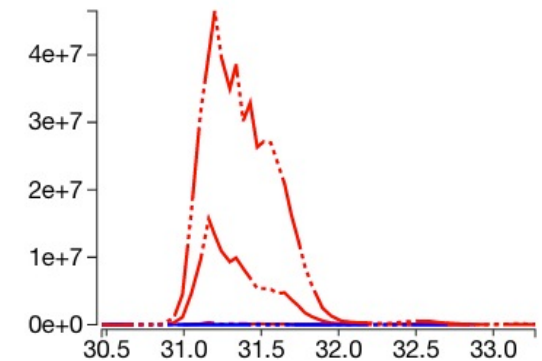
### Quanti event: 23.5-25.7min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me2 [prop_d0]	2	801.4779	1.1e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me2 [pic,prop_d0]	2	832.9834	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me2 [prop_d0]	3	534.6544	1.5e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me2 [pic,prop_d0]	3	555.6580	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me2 [prop_d0]	4	401.2426	3.9e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me2 [pic,prop_d0]	4	416.9953	1.7e+4



### Quanti event: 30.4-33.3min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me2 [prop_d0]	2	801.4779	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me2 [pic,prop_d0]	2	832.9834	5.3e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me2 [prop_d0]	3	534.6544	1.6e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me2 [pic,prop_d0]	3	555.6580	3.6e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me2 [prop_d0]	4	401.2426	2.8e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me2 [pic,prop_d0]	4	416.9953	1.4e+9



# H3.1\_K27-R40: Prop-KMe2SAPATGGVKMe2KPHR MS/MS

### Experimental spectrum

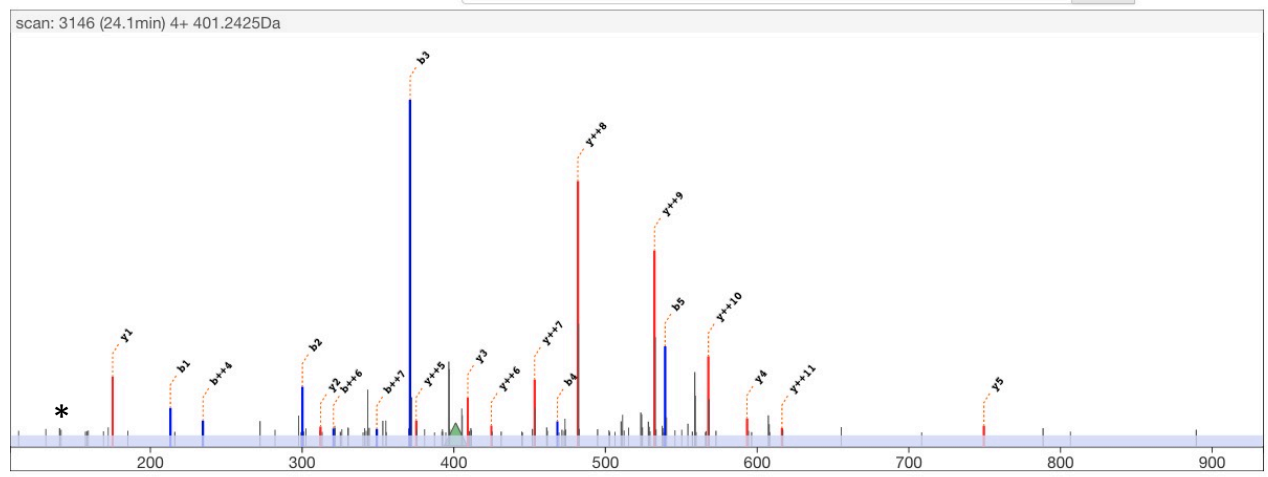
scan 3146  
 retention time 24.1min  
 precursor m/z 401.2425  
 precursor charge 4+

### Theoretical

M H<sup>4+</sup> 401.2426  
 MH Δ<sub>mass</sub> Da -0.0003  
 MH Δ<sub>mass</sub> ppm -0.2

### edit peptide

{Propionyl}K{Dimethyl}SAPATGGVK{Dimethyl}K{Propionyl}PHR align



	b++	b		y	y++	
			Propionyl	1545.92	773.46	14
1	107.08	213.16	K	1389.80	695.40	13
2	150.60	300.19	Dimethyl	1302.76	651.89	12
3	186.12	371.23	S	1231.73	616.37	11
4	234.64	468.28	A	1134.67	567.84	10
5	270.16	539.32	P	1063.64	532.32	9
6	320.69	640.37	A	962.59	481.80	8
7	349.20	697.39	T	905.57	453.29	7
8	377.71	754.41	G	848.55	424.78	6
9	427.24	853.48	V	749.48	375.24	5
10	505.31	1009.60	K	593.35	297.18	4
11	597.37	1193.73	Dimethyl	409.23	205.12	3
12	645.89	1290.78	K	312.18	156.59	2
13	714.42	1427.84	Propionyl	175.12	88.06	1
14	792.47	1583.94	P			
			H			
			R			

\* = 140Da diagnostic ion

# H3.1\_K27-R40: PIC-KMe2SAPATGGVKMe2KPHR MS/MS

### Experimental spectrum

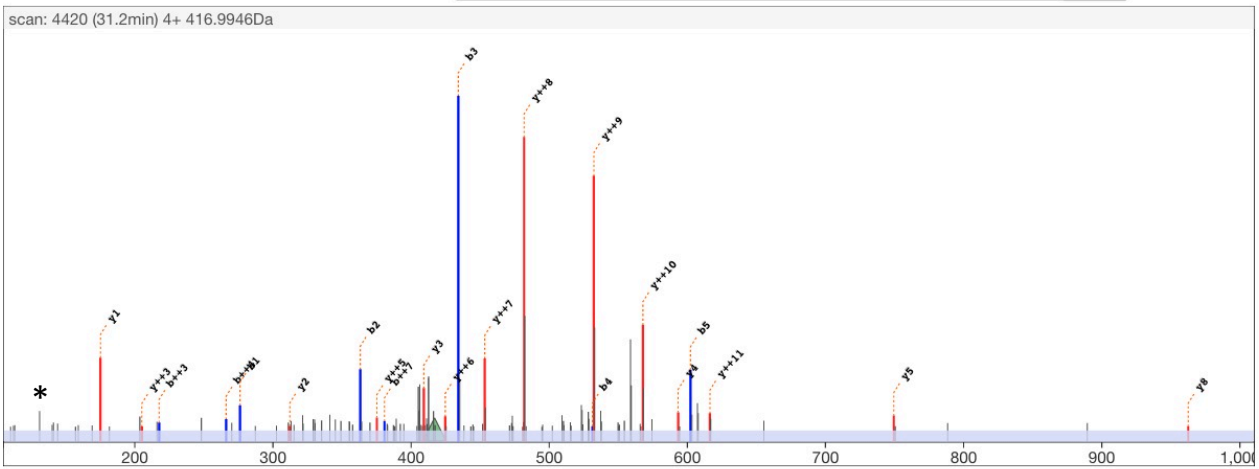
scan 4420  
 retention time 31.2min  
 precursor m/z 416.9946  
 precursor charge 4+

### Theoretical

M H<sup>4+</sup> 416.9953  
 MH Δ<sub>mass</sub> Da -0.0030  
 MH Δ<sub>mass</sub> ppm -1.8

### edit peptide

{PIC}K{Dimethyl}SAPATGGVK{Dimethyl}K{Propionyl}PHR



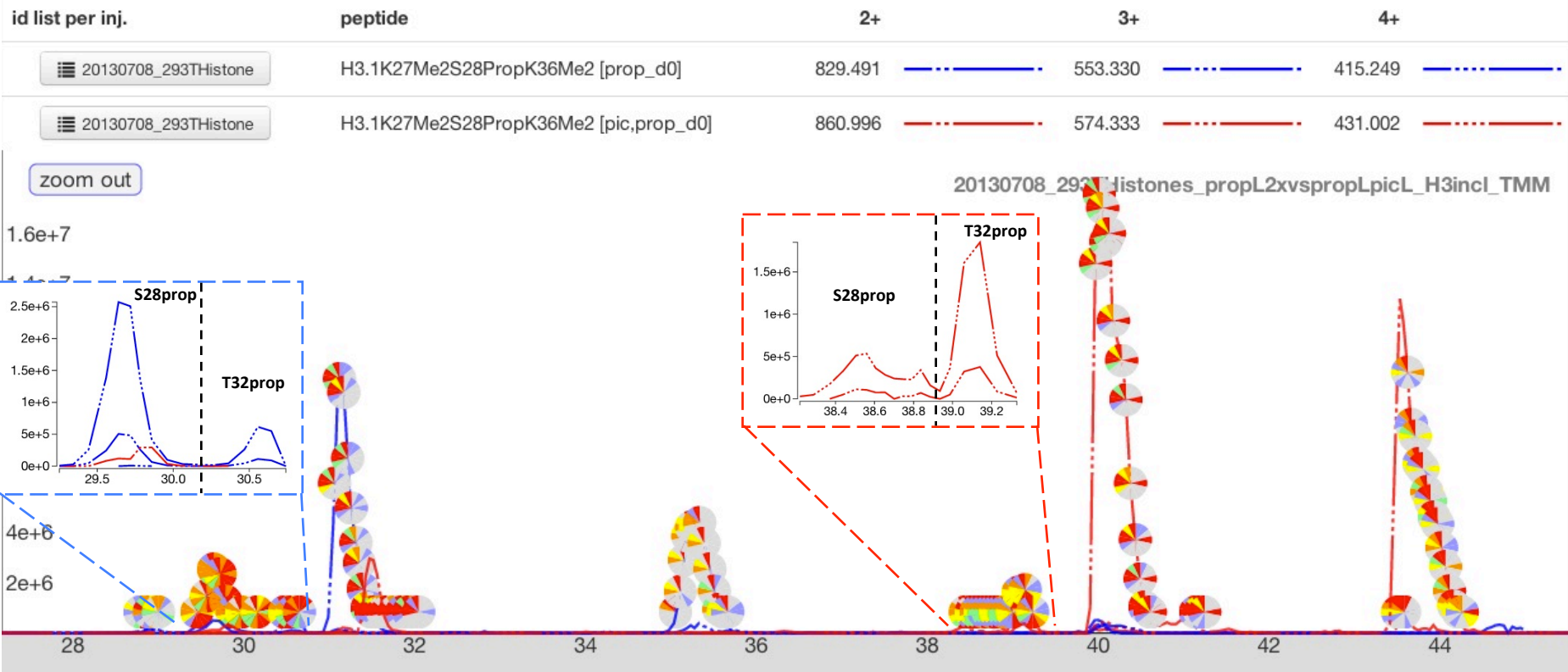
	b++	b		y	y++	
	60.53	120.04	PIC	1545.92	773.46	14
1	138.59	276.17	K	1389.80	695.40	13
2	182.10	363.20	S	1302.76	651.89	12
3	217.62	434.24	A	1231.73	616.37	11
4	266.15	531.29	P	1134.67	567.84	10
5	301.67	602.33	A	1063.64	532.32	9
6	352.19	703.38	T	962.59	481.80	8
7	380.70	760.40	G	905.57	453.29	7
8	409.21	817.42	V	848.55	424.78	6
9	458.75	916.49	K	749.48	375.24	5
10	536.81	1072.61	K	593.35	297.18	4
11	628.87	1256.74	K	409.23	205.12	3
12	677.40	1353.79	P	312.18	156.59	2
13	745.93	1490.85	H	175.12	88.06	1
14	823.98	1646.95	R			

\* = 140Da diagnostic ion

# H3.1\_K27-R40:

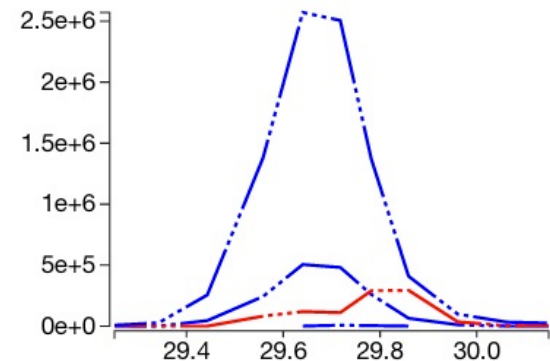
KMe2SPropAPATGGVKMe2KPHR

Two peaks, PIC-labeling shifts propionylation to T32.



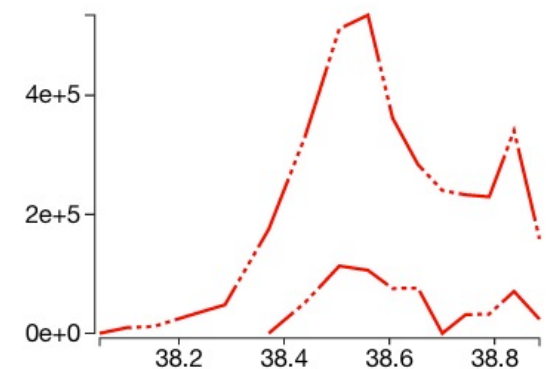
### Quanti event: 29.2-30.2min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me2 [prop_d0]	2	829.4910	5.0e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me2 [pic,prop_d0]	2	860.9965	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me2 [prop_d0]	3	553.3298	7.7e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me2 [pic,prop_d0]	3	574.3334	4.6e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me2 [prop_d0]	4	415.2492	4.2e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me2 [pic,prop_d0]	4	431.0019	0.0e+0



### Quanti event: 38.0-38.9min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me2 [prop_d0]	2	829.4910	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me2 [pic,prop_d0]	2	860.9965	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me2 [prop_d0]	3	553.3298	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me2 [pic,prop_d0]	3	574.3334	1.8e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me2 [prop_d0]	4	415.2492	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me2 [pic,prop_d0]	4	431.0019	1.1e+7



# H3.1\_K27-R40: Prop-KMe2SPropAPATGGVKMe2KPHR MS/MS

**Experimental spectrum**

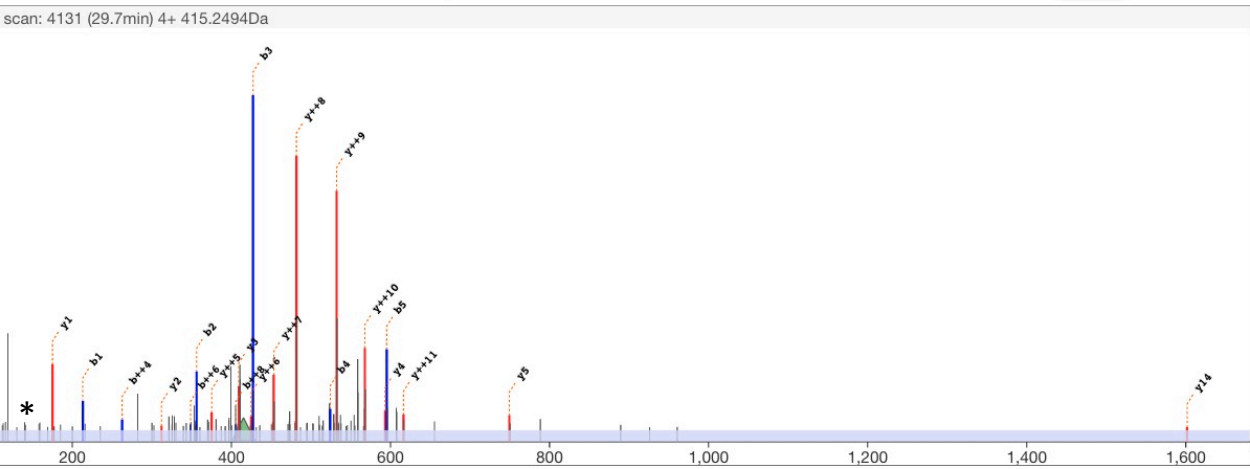
scan 4131  
 retention time 29.7min  
 precursor m/z 415.2494  
 precursor charge 4+

**Theoretical**

M H<sup>4+</sup> 415.2492  
 MH Δ<sub>mass</sub> Da 0.0009  
 MH Δ<sub>mass</sub> ppm 0.6

**edit peptide**

{Propionyl}K{Dimethyl}S{Propionyl}APATGGVK{Dimethyl}K{Propionyl}PHR align



	b++	b		y	y++	
			Propionyl	1601.95	801.48	14
1	107.08	213.16	K			
			Dimethyl	1445.82	723.41	13
2	178.61	356.22	S			
			Propionyl	1302.76	651.89	12
3	214.13	427.26	A			
4	262.66	524.31	P		616.37	11
5	298.18	595.34	A		567.84	10
6	348.70	696.39	T		532.32	9
7	377.21	753.41	G		481.80	8
8	405.72	810.44	V		453.29	7
9	455.26	909.50	K		424.78	6
			Propionyl	749.48	375.24	5
10	533.32	1065.63	K			
			Dimethyl	593.35	297.18	4
11	625.38	1249.75	K			
			Propionyl	409.23	205.12	3
12	673.91	1346.80	P			
13	742.44	1483.86	H		175.12	2
14	820.49	1639.96	R		88.06	1

\* = 140Da diagnostic ion



# H3.1\_K27-R40: PIC-KMe2SPropAPATGGVKMe2KPHR MS/MS

**Experimental spectrum**

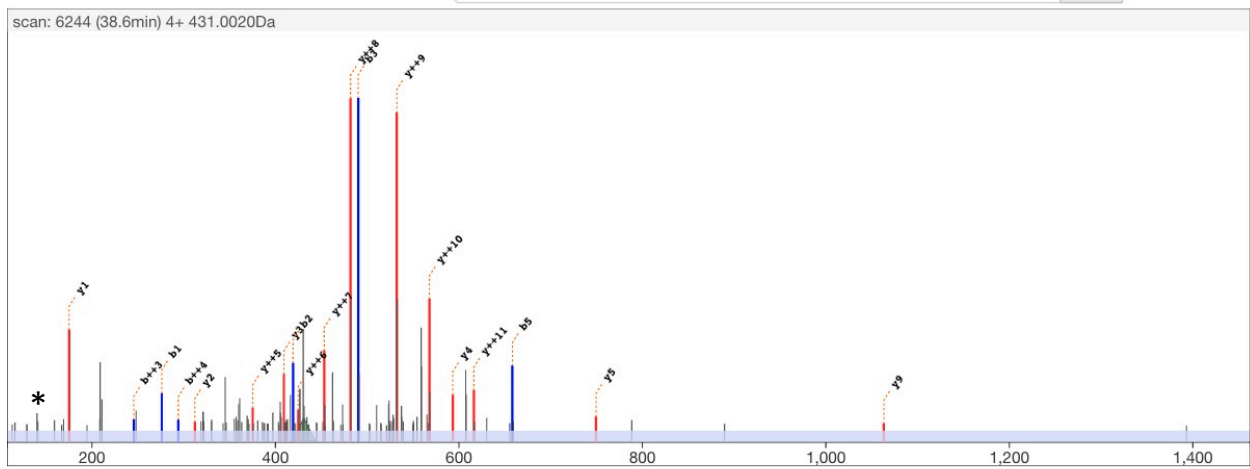
scan 6244  
 retention time 38.6min  
 precursor m/z 431.0020  
 precursor charge 4+

**Theoretical**

M H<sup>+</sup> 431.0019  
 MH Δ<sub>mass</sub> Da 0.0004  
 MH Δ<sub>mass</sub> ppm 0.2

**edit peptide**

{PIC}K{Dimethyl}S{Propionyl}APATGGVK{Dimethyl}K{Propionyl}PHR

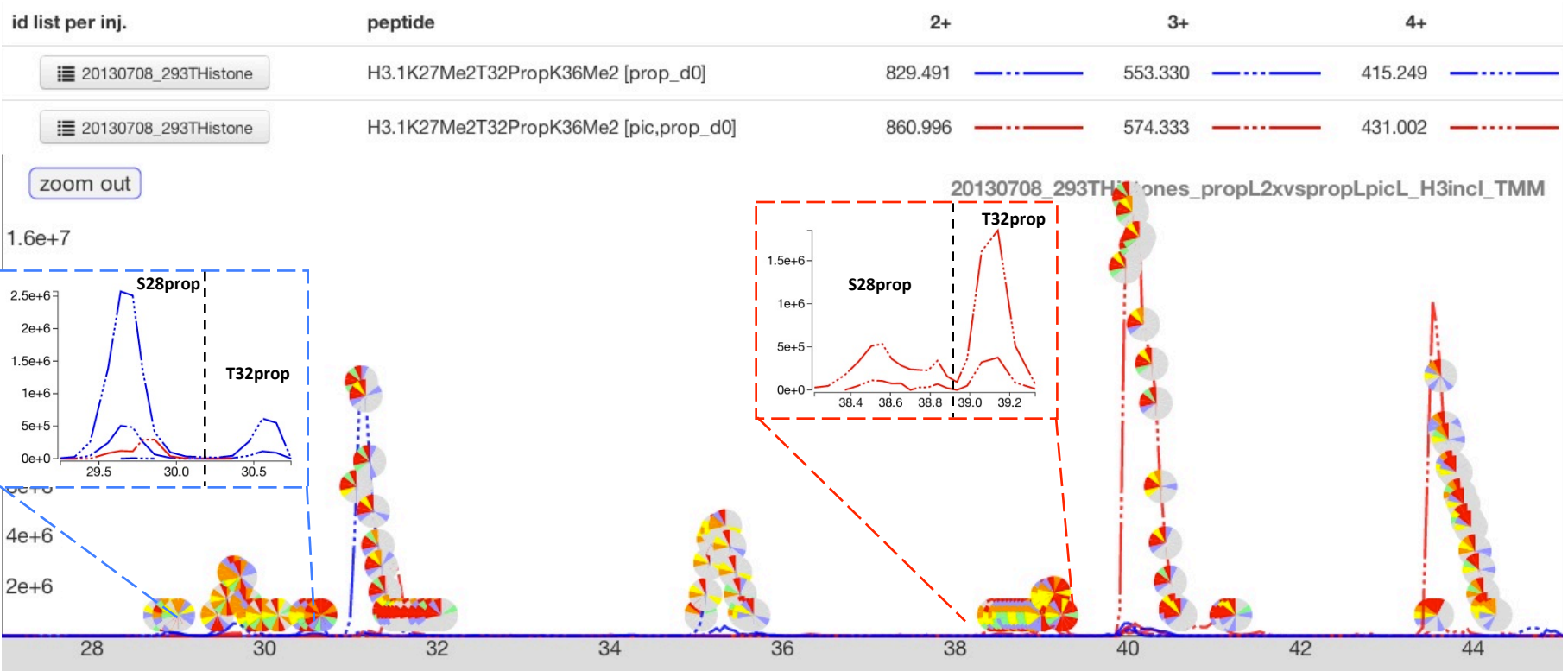


	b++	b		y	y++	
	60.53	120.04	PIC	1601.95	801.48	14
1	138.59	276.17	K	1445.82	723.41	13
2	210.12	419.23	S	1302.76	651.89	12
3	245.64	490.27	A	1231.73	616.37	11
4	294.16	587.32	P	1134.67	567.84	10
5	329.68	658.36	A	1063.64	532.32	9
6	380.21	759.40	T	962.59	481.80	8
7	408.72	816.43	G	905.57	453.29	7
8	437.23	873.45	V	848.55	424.78	6
9	486.76	972.51	K	749.48	375.24	5
10	564.82	1128.64	S	593.35	297.18	4
11	656.88	1312.76	K	409.23	205.12	3
12	705.41	1409.82	P	312.18	156.59	2
13	773.94	1546.87	H	175.12	88.06	1
14	851.99	1702.98	R			

\* = 140Da diagnostic ion

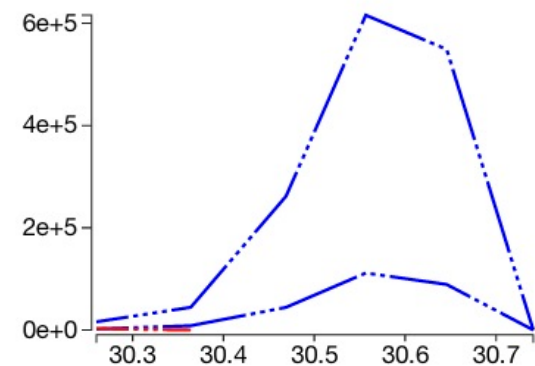
# H3.1\_K27-R40:

KMe2SAPATPropGGVKMe2KPHR



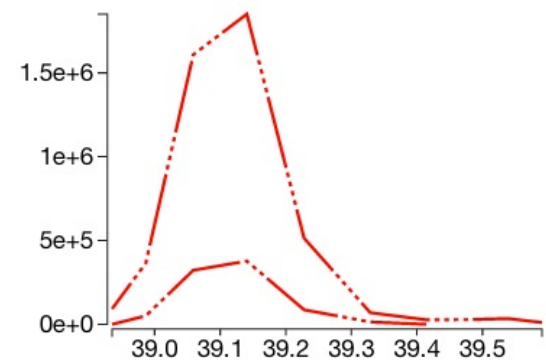
### Quanti event: 30.2-30.8min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me2 [prop_d0]	2	829.4910	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me2 [pic,prop_d0]	2	860.9965	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me2 [prop_d0]	3	553.3298	1.4e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me2 [pic,prop_d0]	3	574.3334	7.8e+3
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me2 [prop_d0]	4	415.2492	8.1e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me2 [pic,prop_d0]	4	431.0019	0.0e+0



### Quanti event: 38.9-39.6min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me2 [prop_d0]	2	829.4910	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me2 [pic,prop_d0]	2	860.9965	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me2 [prop_d0]	3	553.3298	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me2 [pic,prop_d0]	3	574.3334	4.2e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me2 [prop_d0]	4	415.2492	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me2 [pic,prop_d0]	4	431.0019	2.2e+7



# H3.1\_K27-R40: Prop-KMe2SAPATPropGGVKMe2KPHR MS/MS

### Experimental spectrum

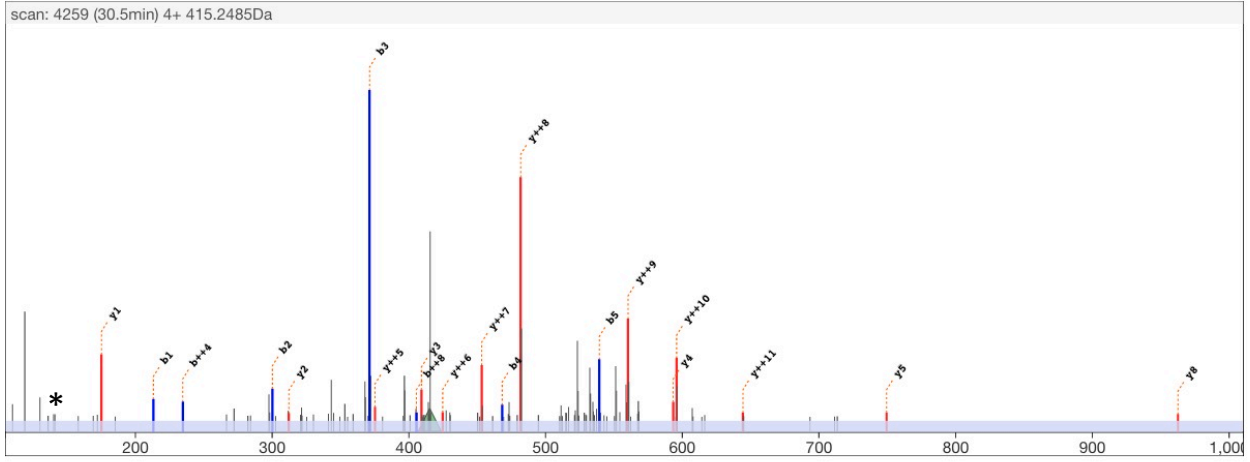
scan 4259  
 retention time 30.5min  
 precursor m/z 415.2485  
 precursor charge 4+

### Theoretical

M H<sup>4+</sup> 415.2492  
 MH Δ<sub>mass</sub> Da -0.0025  
 MH Δ<sub>mass</sub> ppm -1.5

### edit peptide

{Propionyl}K{Dimethyl}SAPAT{Propionyl}GGVK{Dimethyl}K{Propionyl}PHR



	b++	b		y	y++	
			Propionyl	1601.95	801.48	14
1	107.08	213.16	K			
			Dimethyl	1445.82	723.41	13
2	150.60	300.19	S			
			A	1358.79	679.90	12
3	186.12	371.23	P		644.38	11
4	234.64	468.28	A	1190.70	595.85	10
5	270.16	539.32	T	1119.66	560.34	9
6	348.70	696.39	Propionyl	962.59	481.80	8
7	377.21	753.41	G	905.57	453.29	7
8	405.72	810.44	V	848.55	424.78	6
9	455.26	909.50	K	749.48	375.24	5
10	533.32	1065.63	Dimethyl	593.35	297.18	4
11	625.38	1249.75	K	409.23	205.12	3
12	673.91	1346.80	P	312.18	156.59	2
13	742.44	1483.86	H	175.12	88.06	1
14	820.49	1639.96	R			

\* = 140Da diagnostic ion

# H3.1\_K27-R40: PIC-KMe2SAPATPropGGVKMe2KPHR MS/MS

**Experimental spectrum**

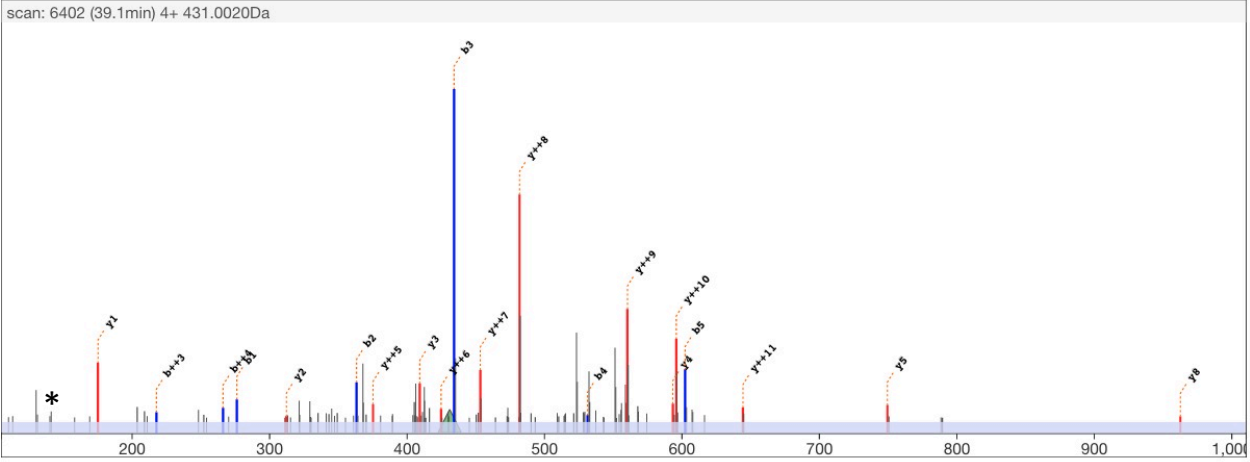
scan 6402  
 retention time 39.1min  
 precursor m/z 431.0020  
 precursor charge 4+

**Theoretical**

M H<sup>4+</sup> 431.0019  
 MH Δ<sub>mass</sub> Da 0.0003  
 MH Δ<sub>mass</sub> ppm 0.2

**edit peptide**

{PIC}K{Dimethyl}SAPAT{Propionyl}GGVK{Dimethyl}K{Propionyl}PHR align



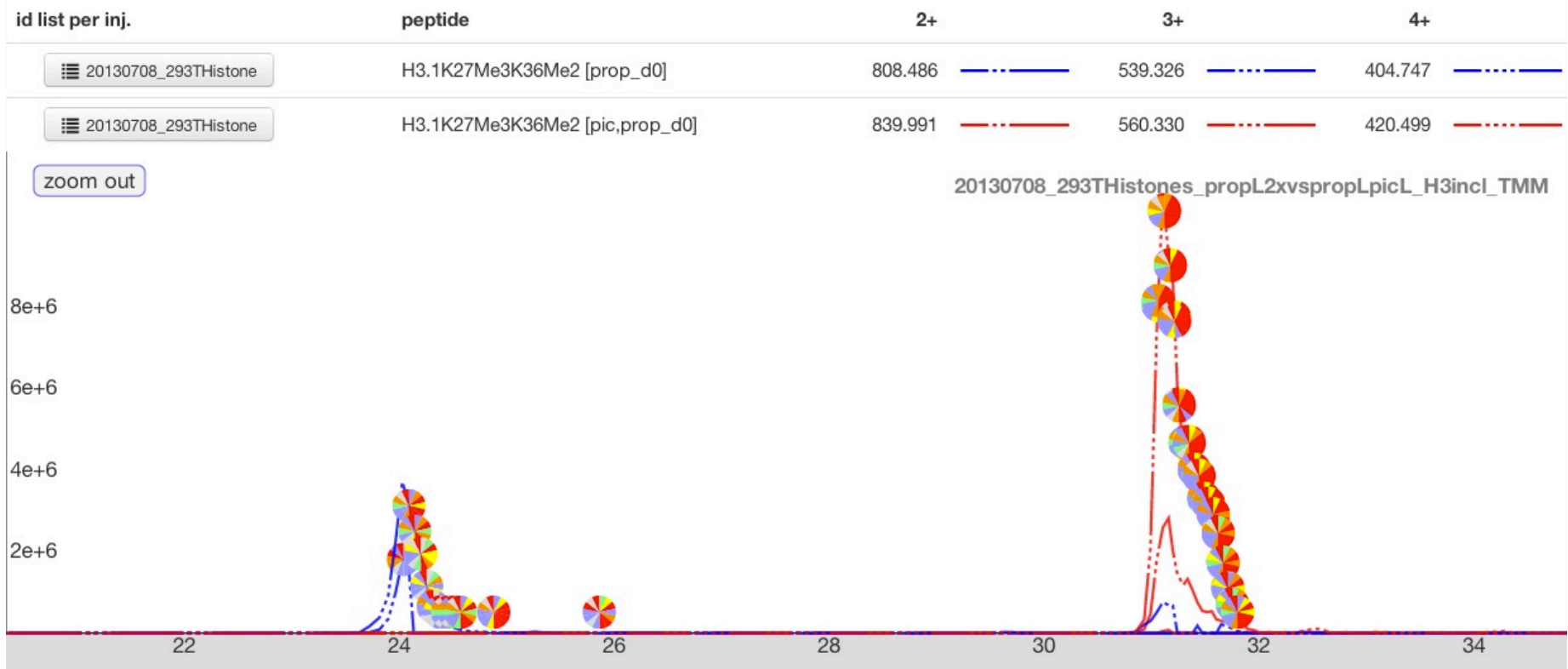
	b++	b		y	y++
	60.53	120.04	PIC	1601.95	801.48
1	138.59	276.17	K	1445.82	723.41
2	182.10	363.20	Dimethyl	1358.79	679.90
3	217.62	434.24	S	1287.75	644.38
4	266.15	531.29	A	1190.70	595.85
5	301.67	602.33	P	1119.66	560.34
6	380.21	759.40	T	962.59	481.80
7	408.72	816.43	Propionyl	905.57	453.29
8	437.23	873.45	G	848.55	424.78
9	486.76	972.51	V	749.48	375.24
10	564.82	1128.64	K	593.35	297.18
11	656.88	1312.76	Dimethyl	409.23	205.12
12	705.41	1409.82	K	312.18	156.59
13	773.94	1546.87	Propionyl	175.12	88.06
14	851.99	1702.98	K		
			P		
			H		
			R		

\* = 140Da diagnostic ion

# H3.1\_K27-R40:

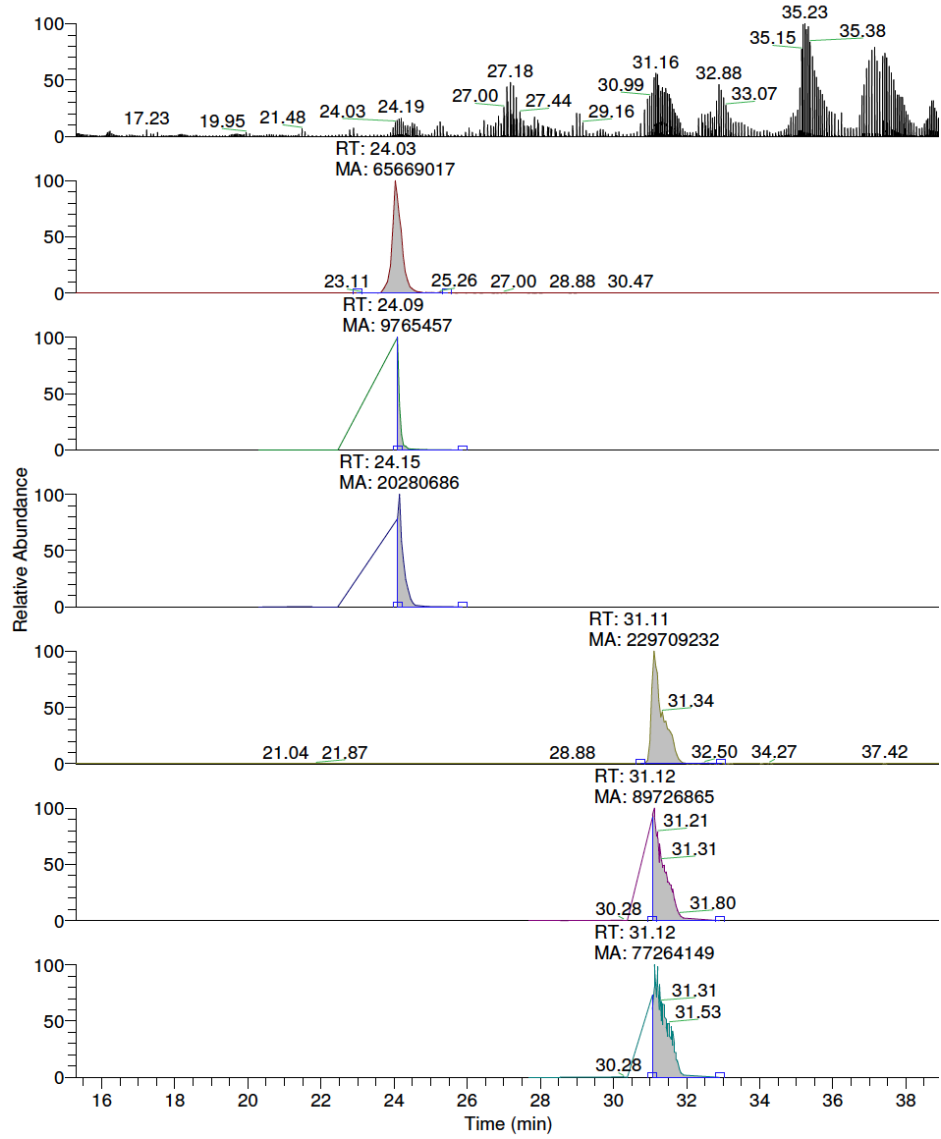
## KMe3SAPATGGVKMe2KPHR

Overlaps with K27Me2,K36me3 (see page 319). Calculation of AUC on MS2 level.



20130708 293THistones\_propL2xvspropLp... 7/8/2013 11:43:33 AM

6 of 10 ul. Histones  
RT: 15.31 - 38.94



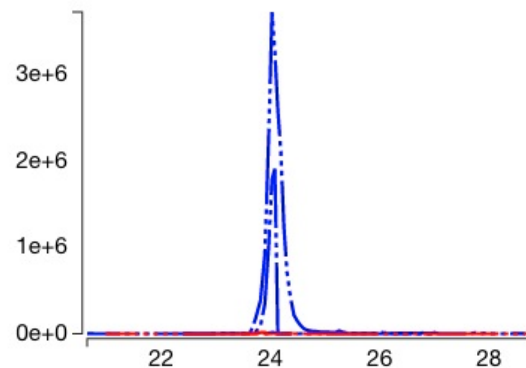
AUC calculation on MS2 level:

XIC-Prop 404.74 (4+)  
 227.18, 385.24, 481.80, 482.30,  
 532.32, 567.84, 749.48

XIC-PIC 420.499 (4+)  
 290.19, 377.22, 448.26, 481.80,  
 532.32, 567.84, 616.37

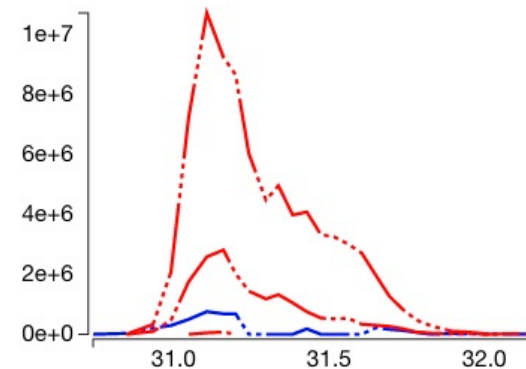
### Quanti event: 20.3-28.9min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me2 [prop_d0]	2	808.4858	1.4e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me2 [pic,prop_d0]	2	839.9912	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me2 [prop_d0]	3	539.3263	1.8e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me2 [pic,prop_d0]	3	560.3299	1.8e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me2 [prop_d0]	4	404.7465	6.7e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me2 [pic,prop_d0]	4	420.4992	1.2e+4



### Quanti event: 30.6-32.2min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me2 [prop_d0]	2	808.4858	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me2 [pic,prop_d0]	2	839.9912	3.7e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me2 [prop_d0]	3	539.3263	1.2e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me2 [pic,prop_d0]	3	560.3299	5.3e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me2 [prop_d0]	4	404.7465	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3K36Me2 [pic,prop_d0]	4	420.4992	2.3e+8





# H3.1\_K27-R40: Prop-KMe3SAPATGGVKMe2KPHR MS/MS

**Experimental spectrum**

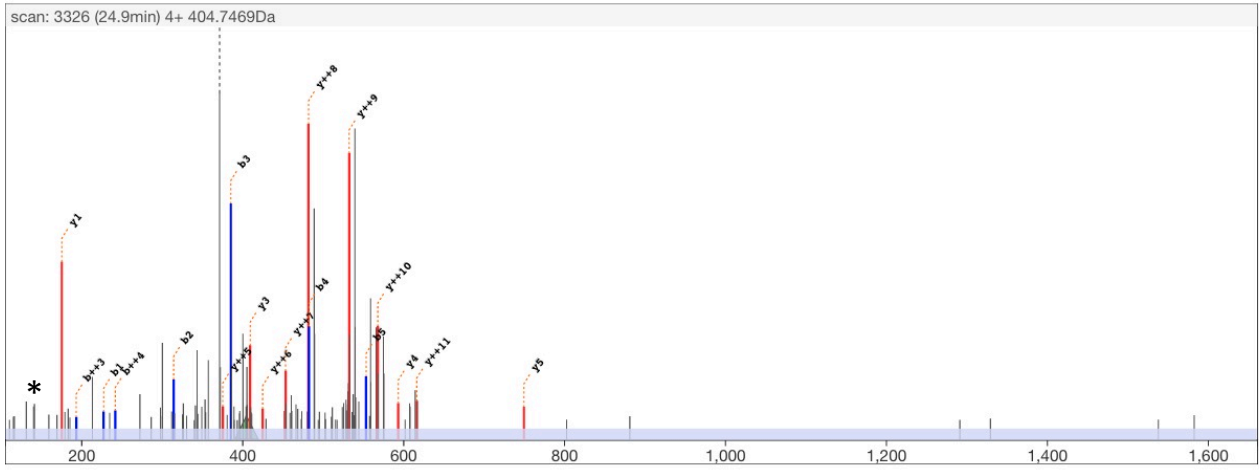
scan 3326  
 retention time 24.9min  
 precursor m/z 404.7469  
 precursor charge 4+

**Theoretical**

M H<sup>4+</sup> 404.7465  
 MH Δ<sub>mass</sub> Da 0.0017  
 MH Δ<sub>mass</sub> ppm 1.1

**edit peptide**

{Propionyl}K{Trimethyl}SAPATGGVK{Dimethyl}K{Propionyl}PHR align



	b++	b		y	y++
1	114.09	227.18	Propionyl K Trimethyl S A P A T G G V K K K Propionyl P H R	1559.94	780.47
2	157.61	314.21		1389.80	695.40
3	193.13	385.24		1302.76	651.89
4	241.65	482.30		1231.73	616.37
5	277.17	553.33		1134.67	567.84
6	327.69	654.38		1063.64	532.32
7	356.21	711.40		962.59	481.80
8	384.72	768.43		905.57	453.29
9	434.25	867.49		848.55	424.78
10	512.31	1023.62		749.48	375.24
11	604.37	1207.74		593.35	297.18
12	652.90	1304.79		409.23	205.12
13	721.43	1441.85		312.18	156.59
14	799.48	1597.95		175.12	88.06

\* = 140Da diagnostic ion

**Experimental spectrum**

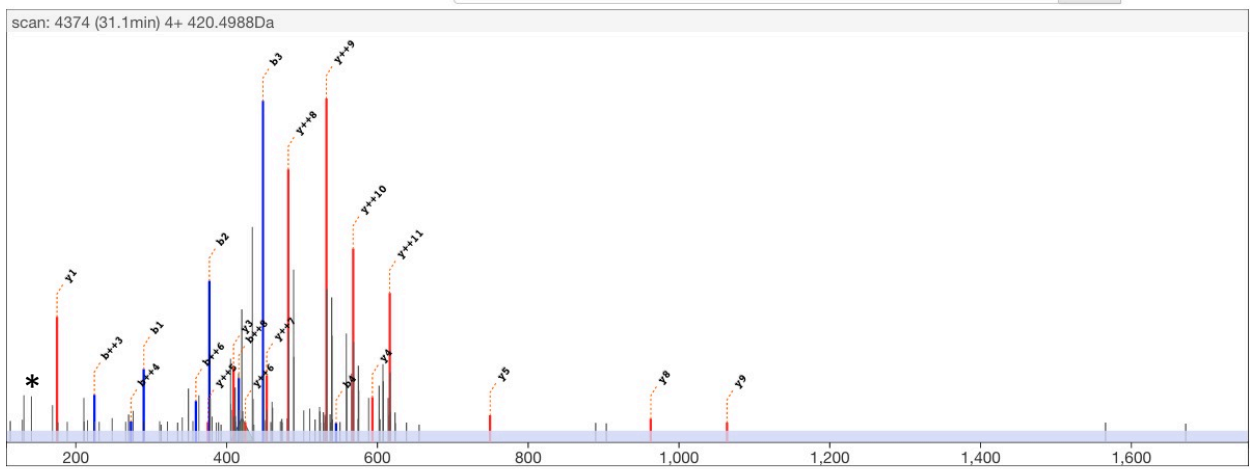
scan 4374  
 retention time 31.1min  
 precursor m/z 420.4988  
 precursor charge 4+

**Theoretical**

M H<sup>4+</sup> 420.4992  
 MH Δ<sub>mass</sub> Da -0.0018  
 MH Δ<sub>mass</sub> ppm -1.1

**edit peptide**

(PIC)K(Trimethyl)SAPATGGVK(Dimethyl)K(Propionyl)PHR



	b++	b		y	y++	
	60.53	120.04	PIC	1559.94	780.47	14
1	145.60	290.19	K	1389.80	695.40	13
2	189.11	377.22	S	1302.76	651.89	12
3	224.63	448.26	A	1231.73	616.37	11
4	273.16	545.31	P	1134.67	567.84	10
5	308.68	616.35	A	1063.64	532.32	9
6	359.20	717.39	T	962.59	481.80	8
7	387.71	774.41	G	905.57	453.29	7
8	416.22	831.44	V	848.55	424.78	6
9	465.76	930.50	K	749.48	375.24	5
10	543.82	1086.63	Dimethyl	593.35	297.18	4
11	635.88	1270.75	K	409.23	205.12	3
12	684.41	1367.80	Propionyl	312.18	156.59	2
13	752.94	1504.86	P	175.12	88.06	1
14	830.99	1660.96	H			
			R			

\* = 140Da diagnostic ion