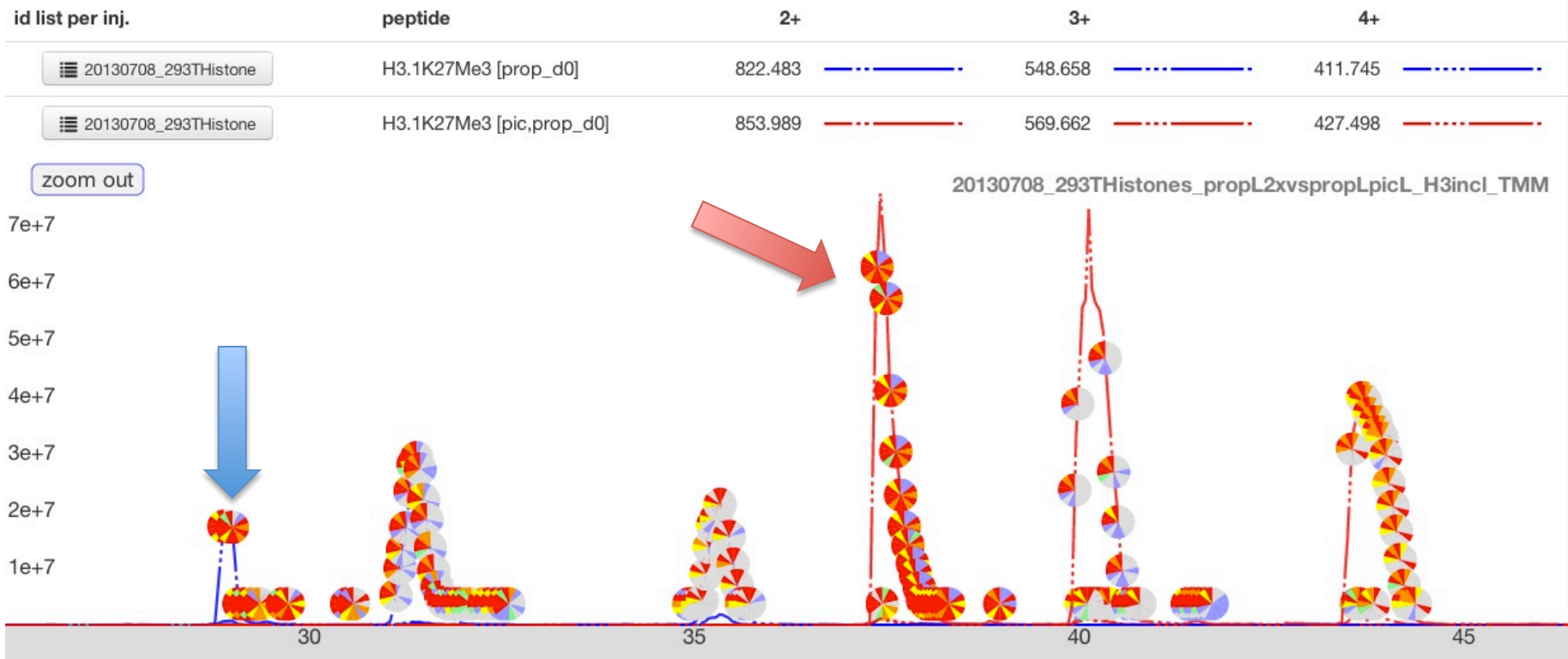


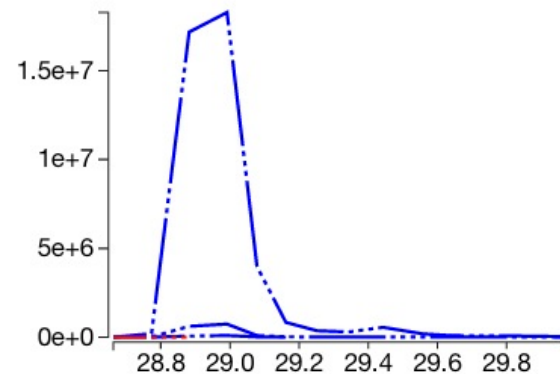
H3.1_K27-R40:

KMe3SAPATGGVKKPHR



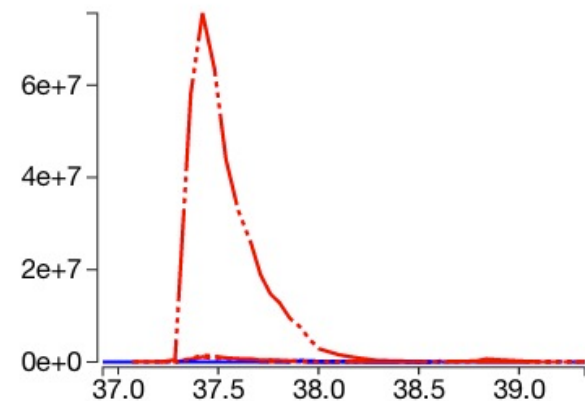
Quanti event: 28.6-30.0min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3 [prop_d0]	2	822.4832	1.0e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3 [pic,prop_d0]	2	853.9887	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3 [prop_d0]	3	548.6579	2.6e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3 [pic,prop_d0]	3	569.6615	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3 [prop_d0]	4	411.7452	9.5e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3 [pic,prop_d0]	4	427.4980	1.1e+4



Quanti event: 36.9-39.3min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3 [prop_d0]	2	822.4832	3.9e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3 [pic,prop_d0]	2	853.9887	1.6e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3 [prop_d0]	3	548.6579	2.2e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3 [pic,prop_d0]	3	569.6615	1.3e+9
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3 [prop_d0]	4	411.7452	4.3e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3 [pic,prop_d0]	4	427.4980	2.7e+7



H3.1_K27-R40: Prop-KMe3SAPATGGVKKPHR MS/MS

Experimental spectrum

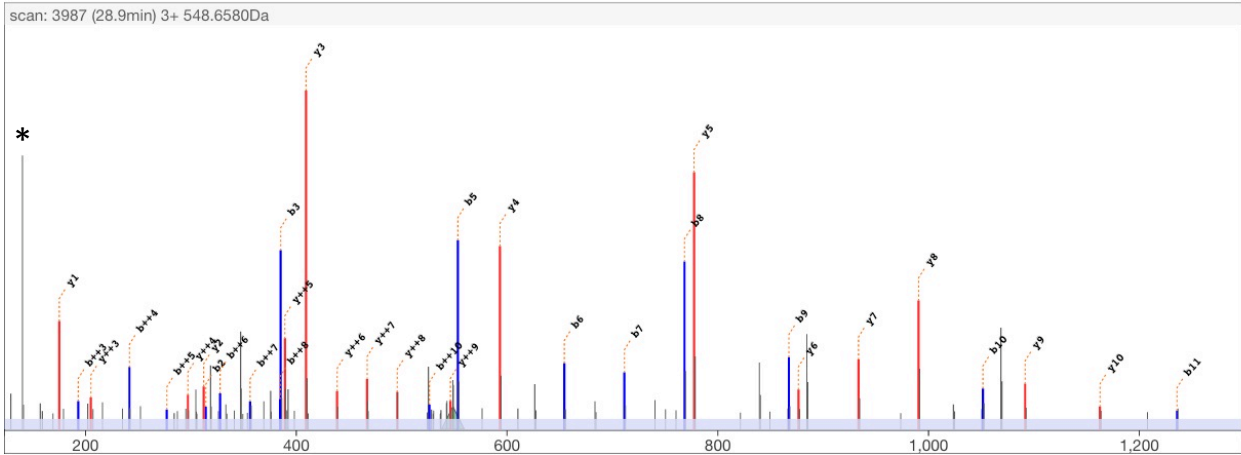
scan 3987
 retention time 28.9min
 precursor m/z 548.6580
 precursor charge 3+

Theoretical

M H³⁺ 548.6579
 MH Δ_{mass} Da 0.0002
 MH Δ_{mass} ppm 0.1

edit peptide

{Propionyl}K{Trimethyl}SAPATGGV{Propionyl}K{Propionyl}PHR



	b++	b		y	y++	
			Propionyl	1587.93	794.47	14
1	114.09	227.18	K	1417.79	709.40	13
2	157.61	314.21	S	1330.76	665.88	12
3	193.13	385.24	A	1259.72	630.36	11
4	241.65	482.30	P	1162.67	581.84	10
5	277.17	553.33	A	1091.63	546.32	9
6	327.69	654.38	T	990.58	495.80	8
7	356.21	711.40	G	933.56	467.29	7
8	384.72	768.43	V	876.54	438.77	6
9	434.25	867.49	K	777.47	389.24	5
10	526.31	1051.61	Propionyl	593.35	297.18	4
11	618.37	1235.74	K	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

H3.1_K27-R40: PIC-KMe3SAPATGGVKKPHR MS/MS

Experimental spectrum

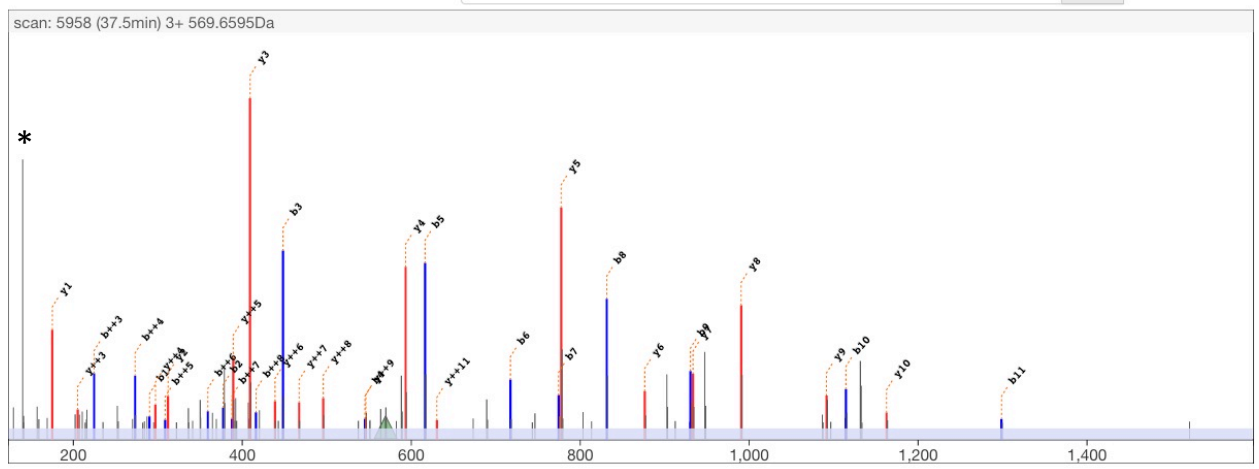
scan 5958
 retention time 37.6min
 precursor m/z 569.6595
 precursor charge 3+

Theoretical

M H³⁺ 569.6615
 MH Δ_{mass} Da -0.0062
 MH Δ_{mass} ppm -3.6

edit peptide

{PIC}K{Trimethyl}SAPATGGV{Propionyl}K{Propionyl}PHR

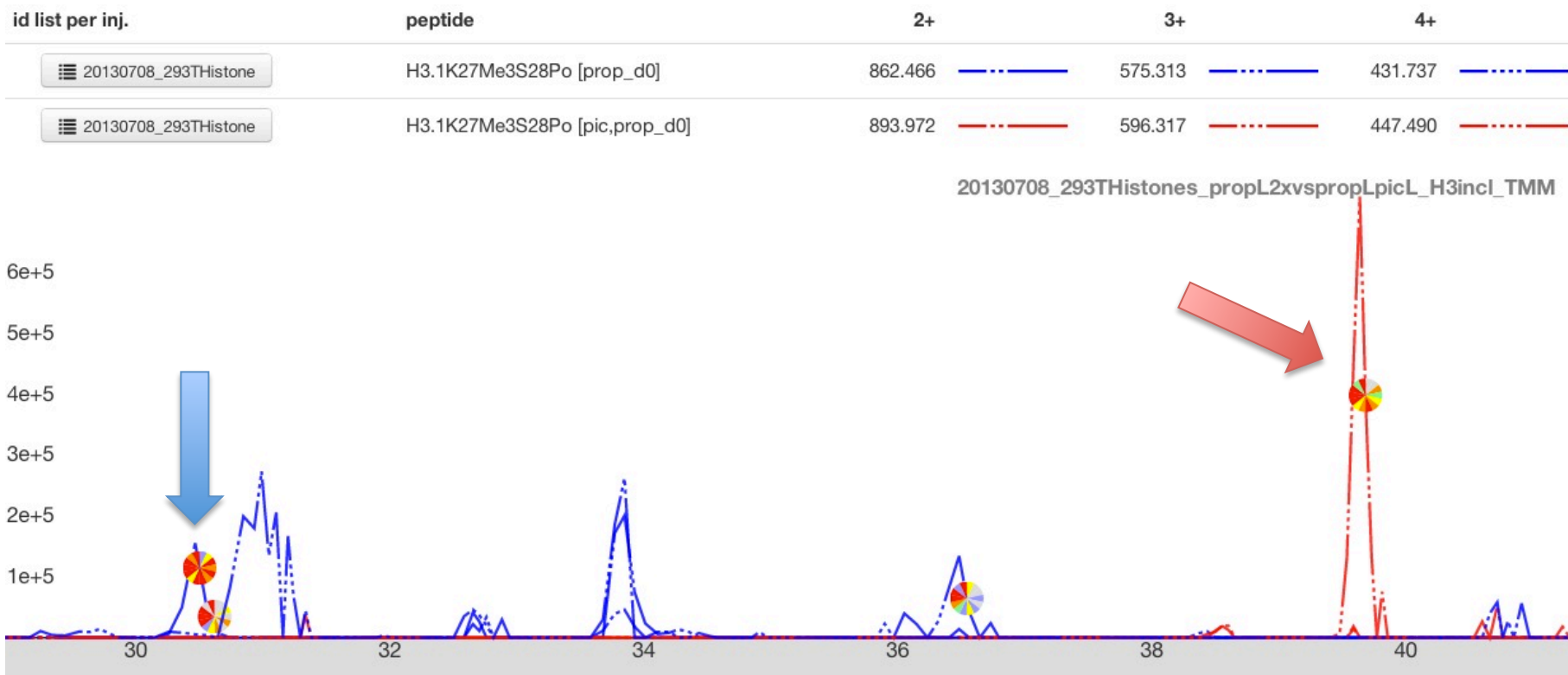


	b++	b		y	y++	
	60.53	120.04	PIC	1587.93	794.47	14
1	145.60	290.19	K	1417.79	709.40	13
2	189.11	377.22	S	1330.76	665.88	12
3	224.63	448.26	A	1259.72	630.36	11
4	273.16	545.31	P	1162.67	581.84	10
5	308.68	616.35	A	1091.63	546.32	9
6	359.20	717.39	T	990.58	495.80	8
7	387.71	774.41	G	933.56	467.29	7
8	416.22	831.44	V	876.54	438.77	6
9	465.76	930.50	K	777.47	389.24	5
10	557.82	1114.63	Propionyl	593.35	297.18	4
11	649.88	1298.75	K	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
14	844.98	1688.96	R			

* = 140Da diagnostic ion

H3.1_K27-R40:

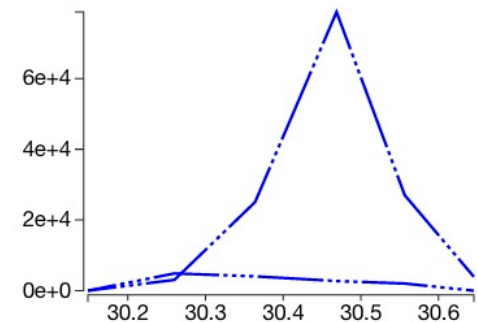
KMe3SPoAPATGGVKKPHR



Quanti event: 30.1-30.7min



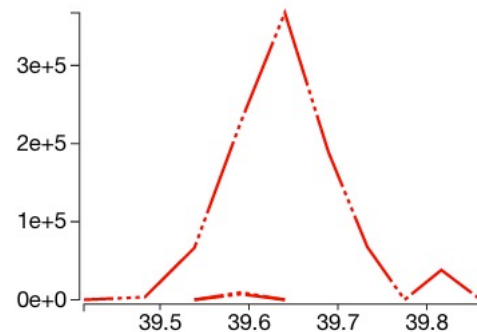
injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Po [prop_d0]	2	862.4664	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Po [pic,prop_d0]	2	893.9718	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Po [prop_d0]	3	575.3133	7.9e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Po [pic,prop_d0]	3	596.3170	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Po [prop_d0]	4	431.7368	8.3e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Po [pic,prop_d0]	4	447.4896	0.0e+0



Quanti event: 39.3-40.1min



injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Po [prop_d0]	2	862.4664	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Po [pic,prop_d0]	2	893.9718	2.2e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Po [prop_d0]	3	575.3133	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Po [pic,prop_d0]	3	596.3170	2.8e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Po [prop_d0]	4	431.7368	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Po [pic,prop_d0]	4	447.4896	2.9e+4



Experimental spectrum

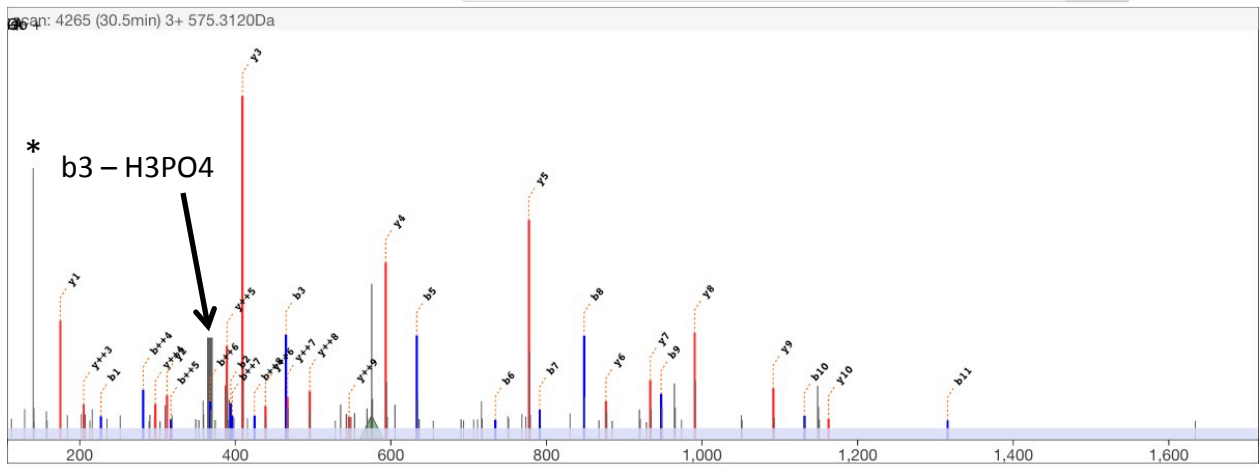
scan 4265
 retention time 30.5min
 precursor m/z 575.3120
 precursor charge 3+

Theoretical

M H³⁺ 575.3133
 MH Δ_{mass} Da -0.0042
 MH Δ_{mass} ppm -2.4

edit peptide

{Propionyl}K{Trimethyl}S{Phospho}APATGGV{Propionyl}K{Propionyl}PHR



Anchor	Current
click on peak	mouse over peak
m/z 465.2105	m/z 367.2333
intensity 2022	intensity 1956
int. rank 6	int. rank 9

Explanation?
 delta mass could be...
 Δ_{m/z} -97.97714

Tune the seq
 Align anchor peak

	b++	b		y	y++	
			Propionyl	1667.90	834.45	14
1	114.09	227.18	K	1497.76	749.38	13
			Trimethyl			
2	197.59	394.17	S	1330.76	665.88	12
			Phospho			
3	233.11	465.21	A	1259.72	630.36	11
4	281.64	562.26	P	1162.67	581.84	10
5	317.15	633.30	A	1091.63	546.32	9
6	367.68	734.35	T	990.58	495.80	8
7	396.19	791.37	G	933.56	467.29	7
8	424.70	848.39	V	876.54	438.77	6
9	474.23	947.46	K	777.47	389.24	5
10	566.29	1131.58	Propionyl	593.35	297.18	4
11	658.35	1315.70	K	409.23	205.12	3
12	706.88	1412.75	P	312.18	156.59	2
13	775.41	1549.81	H	175.12	88.06	1
14	853.46	1705.91	R			

* = 140Da diagnostic ion

Phospho-loss also on b5 and b8 ions.

Experimental spectrum

scan 6544
 retention time 39.7min
 precursor m/z 596.3169
 precursor charge 3+

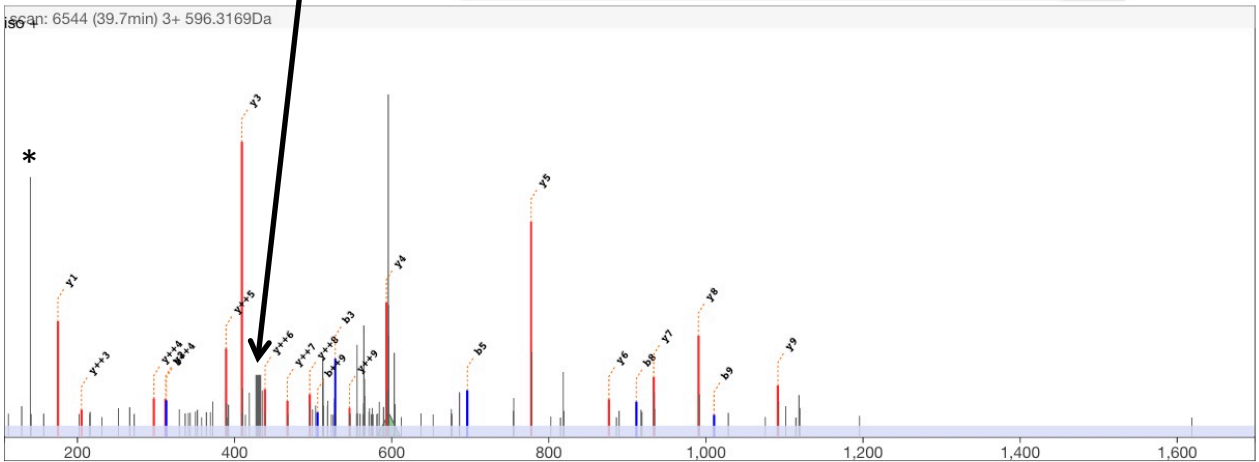
Theoretical

M H³⁺ 596.3170
 MH Δ_{mass} Da -0.0003
 MH Δ_{mass} ppm -0.1

edit peptide

(PIC)K(Trimethyl)S(Phospho)APATGGV(K)(Propionyl)PHR

b3 - H3PO4



Anchor	Current
click on peak	mouse over peak
m/z 528.2213	m/z 430.2456
intensity 4575	intensity 3476
int. rank 13	int. rank 16

Explanation?
 delta mass could be...
 $\Delta_{m/z}$ -97.97568

Tune the seq
 Align anchor peak

	b++	b		y	y++	
	60.53	120.04	PIC	1667.90	834.45	14
1	145.60	290.19	K	1497.76	749.38	13
2	229.10	457.18	S	1330.76	665.88	12
3	264.61	528.22	Phospho	1259.72	630.36	11
4	313.14	625.27	A	1162.67	581.84	10
5	348.66	696.31	P	1091.63	546.32	9
6	399.18	797.36	T	990.58	495.80	8
7	427.69	854.38	G	933.56	467.29	7
8	456.20	911.40	V	876.54	438.77	6
9	505.74	1010.47	K	777.47	389.24	5
10	597.80	1194.59	Propionyl	593.35	297.18	4
11	689.86	1378.71	K	409.23	205.12	3
12	738.39	1475.77	Propionyl	312.18	156.59	2
13	806.92	1612.82	P	175.12	88.06	1
14	884.97	1768.93	H			
			R			

* = 140Da diagnostic ion

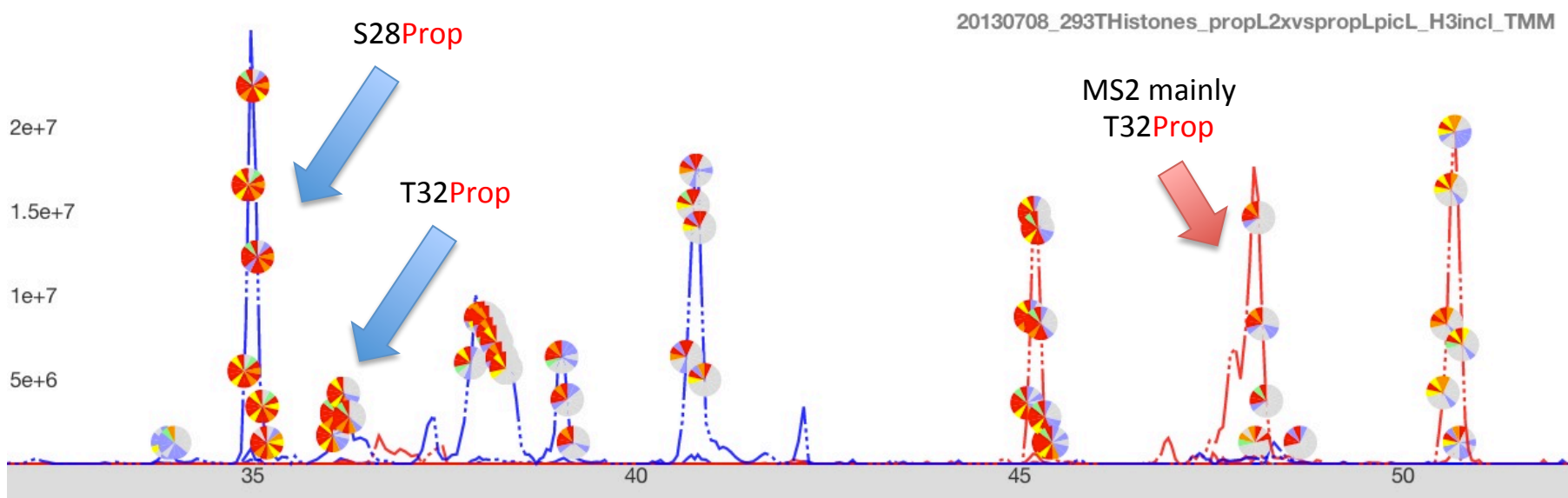
Phospho-loss also on b5 and b8 ions.

H3.1_K27-R40:

KMe3SProp?APATProp?GGVKKPHR

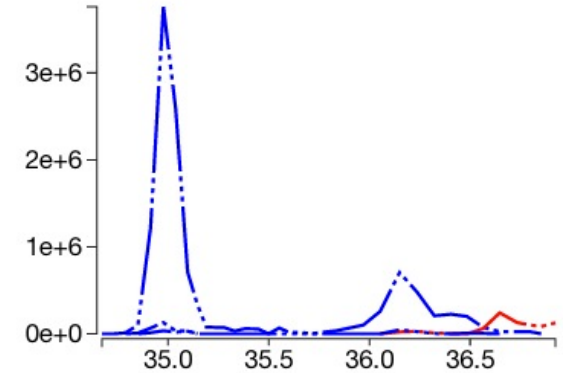
Earlier eluting peak is S28-prop. Double-peak for Prop-labeling and merged peak for PIC-labeling. Combined AUCs for both PTMs. T32-MS2s shown.

id list per inj.	peptide	2+	3+	4+
20130708_293THistone	H3.1K27Me3S28Prop [prop_d0]	850.496	567.333	425.752
20130708_293THistone	H3.1K27Me3S28Prop [pic,prop_d0]	882.002	588.337	441.505



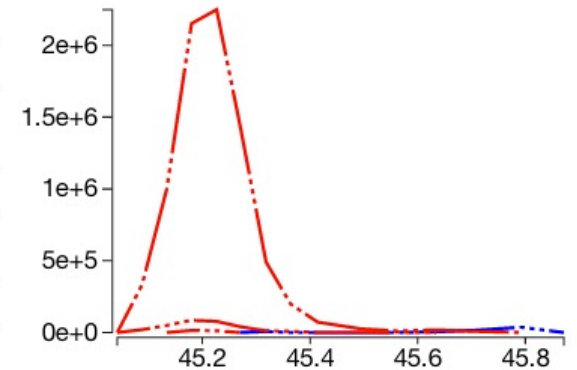
Quanti event: 34.7-37.0min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Prop [prop_d0]	2	850.4963	3.5e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Prop [pic,prop_d0]	2	882.0018	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Prop [prop_d0]	3	567.3333	4.6e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Prop [pic,prop_d0]	3	588.3369	3.4e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Prop [prop_d0]	4	425.7518	1.5e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Prop [pic,prop_d0]	4	441.5045	0.0e+0



Quanti event: 45.0-46.0min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Prop [prop_d0]	2	850.4963	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Prop [pic,prop_d0]	2	882.0018	7.3e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Prop [prop_d0]	3	567.3333	3.0e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Prop [pic,prop_d0]	3	588.3369	2.2e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Prop [prop_d0]	4	425.7518	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28Prop [pic,prop_d0]	4	441.5045	8.2e+5



H3.1_K27-R40: Prop-KMe3SAPATPropGGVKKPHR MS/MS

Experimental spectrum

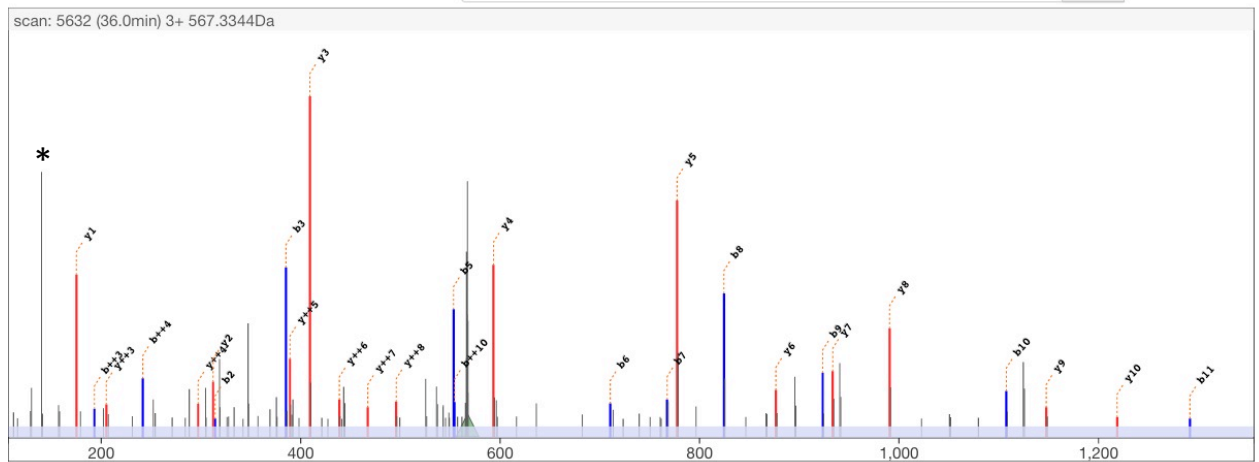
scan 5632
 retention time 36.0min
 precursor m/z 567.3344
 precursor charge 3+

Theoretical

M H³⁺ 567.3333
 MH Δ_{mass} Da 0.0033
 MH Δ_{mass} ppm 1.9

edit peptide

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



	b++	b		y	y++	
			Propionyl	1643.96	822.48	14
1	114.09	227.18	K	1473.82	737.41	13
			Trimethyl			
2	157.61	314.21	S	1386.79	693.90	12
			A	1315.75	658.38	11
3	193.13	385.24	P	1218.70	609.85	10
			A	1147.66	574.33	9
4	241.65	482.30	T	990.58	495.80	8
5	277.17	553.33	G	933.56	467.29	7
6	355.71	710.41	V	876.54	438.77	6
7	384.22	767.43	G	777.47	389.24	5
8	412.73	824.45	V	593.35	297.18	4
9	462.26	923.52	K	409.23	205.12	3
10	554.32	1107.64	K	312.18	156.59	2
11	646.38	1291.76	P	175.12	88.06	1
12	694.91	1388.81	H			
13	763.44	1525.87	R			
14	841.49	1681.97				

* = 140Da diagnostic ion

H3.1_K27-R40: PIC-KMe3SAPATPropGGVKKPHR MS/MS

Experimental spectrum

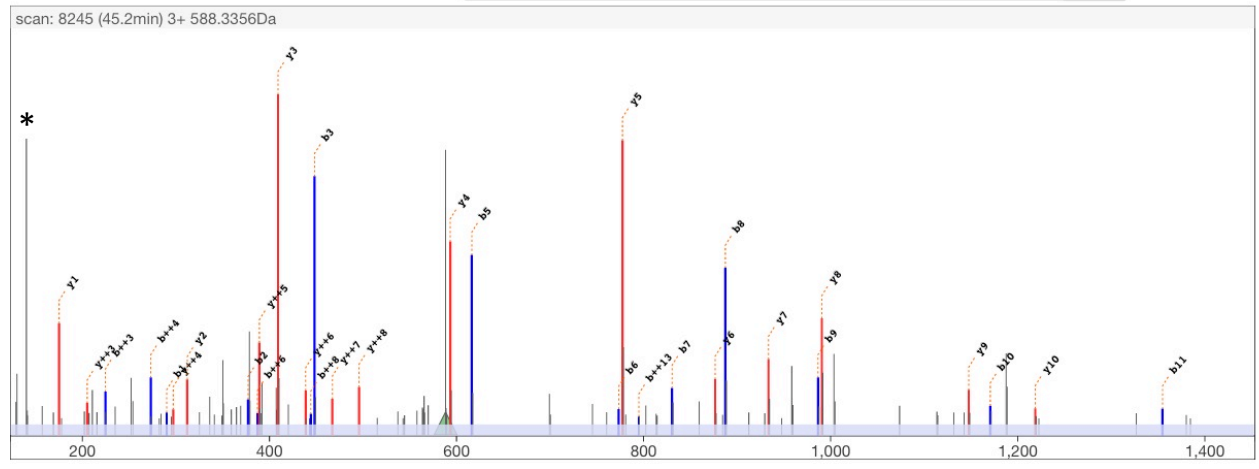
scan 8245
 retention time 45.2min
 precursor m/z 588.3356
 precursor charge 3+

Theoretical

M H³⁺ 588.3369
 MH Δ_{mass} Da -0.0041
 MH Δ_{mass} ppm -2.3

edit peptide

{PIC}K{Trimethyl}SAPAT{Propionyl}GGVK{Propionyl}K{Propionyl}PHR



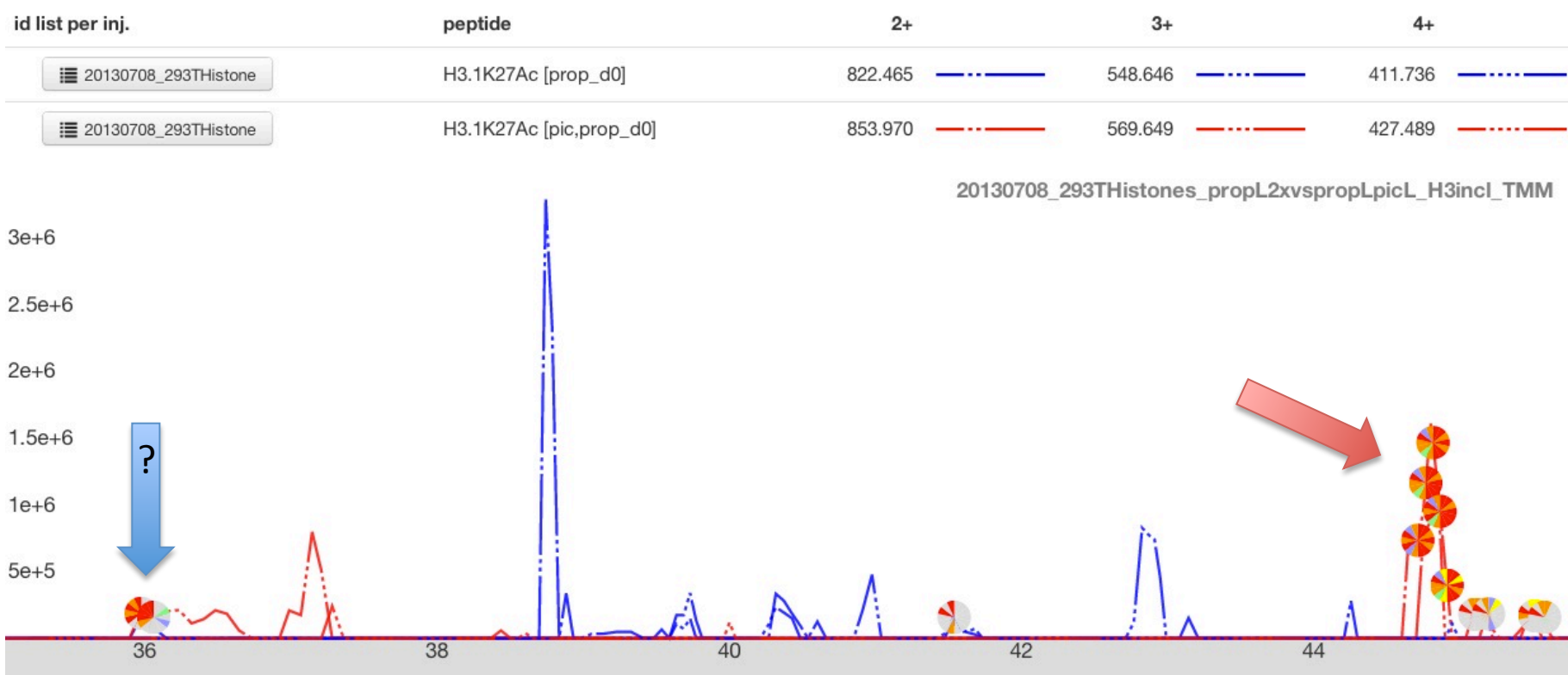
	b++	b		y	y++	
	60.53	120.04	PIC	1643.96	822.48	14
1	145.60	290.19	K	1473.82	737.41	13
2	189.11	377.22	S	1386.79	693.90	12
3	224.63	448.26	A	1315.75	658.38	11
4	273.16	545.31	P	1218.70	609.85	10
5	308.68	616.35	A	1147.66	574.33	9
6	387.21	773.42	T	990.58	495.80	8
7	415.72	830.44	G	933.56	467.29	7
8	444.23	887.46	V	876.54	438.77	6
9	493.77	986.53	K	777.47	389.24	5
10	585.83	1170.65	K	593.35	297.18	4
11	677.89	1354.77	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

H3.1_K27-R40:

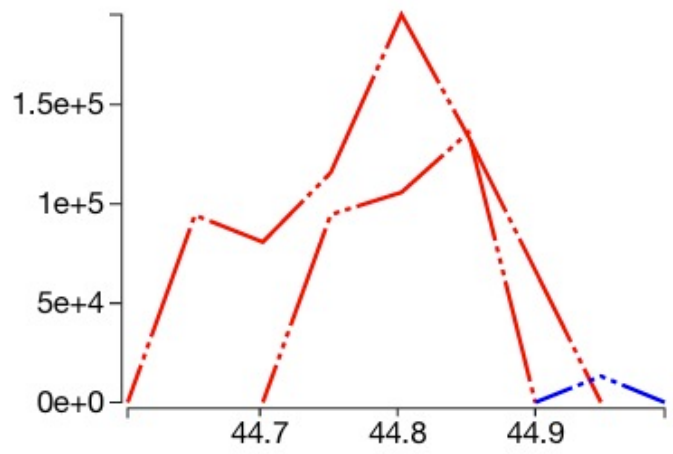
KA_cSAPATGGVKKPHR

No MS2 for Prop-only peak detected.



Quanti event: 44.5-45.0min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Ac [prop_d0]	2	822.4650	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Ac [pic,prop_d0]	2	853.9705	2.0e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Ac [prop_d0]	3	548.6458	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Ac [pic,prop_d0]	3	569.6494	1.0e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Ac [prop_d0]	4	411.7361	3.7e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Ac [pic,prop_d0]	4	427.4889	0.0e+0



No MS2 for Prop-only peak detected.

H3.1_K27-R40: PIC-KAcSAPATGGVKKPHR MS/MS

Experimental spectrum

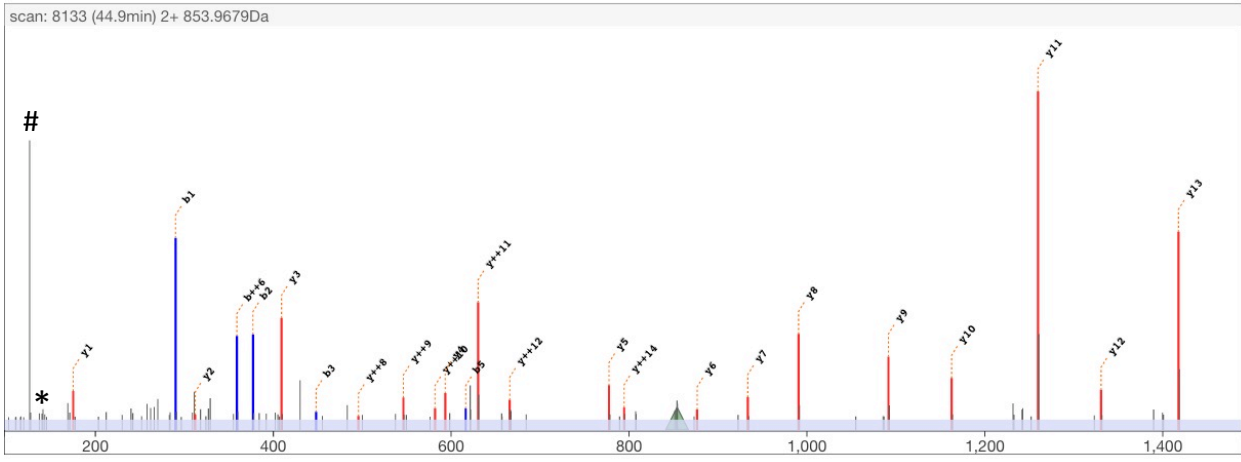
scan 8133
 retention time 44.9min
 precursor m/z 853.9679
 precursor charge 2+

Theoretical

M H²⁺ 853.9705
 MH Δ_{mass} Da -0.0052
 MH Δ_{mass} ppm -3.0

edit peptide

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



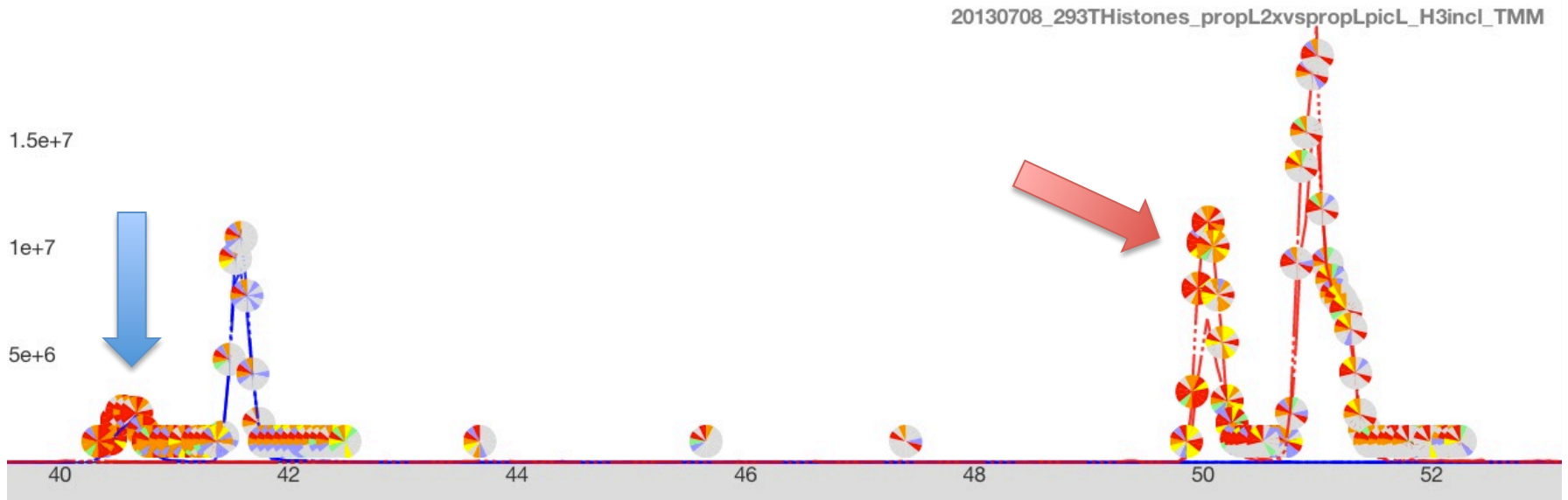
	b++	b		y	y++	
	60.53	120.04	PIC	1587.90	794.45	14
1	145.58	290.15	K	1417.79	709.40	13
2	189.09	377.18	Acetyl	1330.76	665.88	12
3	224.61	448.22	S	1259.72	630.36	11
4	273.14	545.27	A	1162.67	581.84	10
5	308.66	616.31	P	1091.63	546.32	9
6	359.18	717.36	A	990.58	495.80	8
7	387.69	774.38	T	933.56	467.29	7
8	416.20	831.40	G	876.54	438.77	6
9	465.74	930.47	V	819.52	410.25	5
10	557.80	1114.59	K	777.47	389.24	4
11	649.86	1298.71	Propionyl	593.35	297.18	3
12	698.39	1395.76	K	409.23	205.12	2
13	766.91	1532.82	Propionyl	312.18	156.59	1
14	844.97	1688.92	P	175.12	88.06	0
			H			
			R			

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

H3.1_K27-R40:

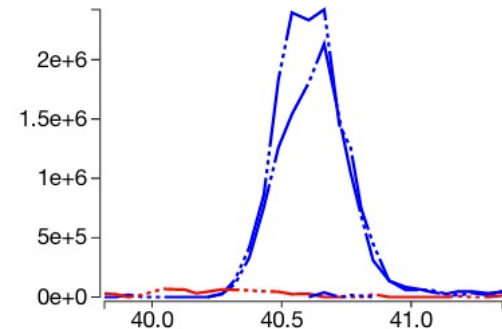
KSAPATGGVKMe1KPHR

id list per inj.	peptide	2+	3+	4+
☰ 20130708_293THistone	H3.1K36Me [prop_d0]	836.481	557.990	418.744
☰ 20130708_293THistone	H3.1K36Me [pic,prop_d0]	867.986	578.993	434.497



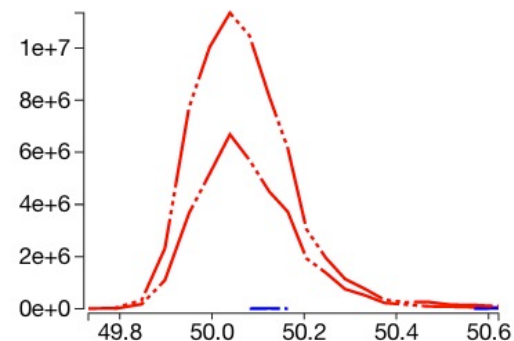
Quanti event: 39.8-41.4min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me [prop_d0]	2	836.4807	4.0e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me [pic,prop_d0]	2	867.9861	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me [prop_d0]	3	557.9895	4.9e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me [pic,prop_d0]	3	578.9932	2.2e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me [prop_d0]	4	418.7440	2.0e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me [pic,prop_d0]	4	434.4967	0.0e+0



Quanti event: 49.7-50.6min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me [prop_d0]	2	836.4807	3.3e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me [pic,prop_d0]	2	867.9861	9.4e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me [prop_d0]	3	557.9895	3.2e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me [pic,prop_d0]	3	578.9932	1.7e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me [prop_d0]	4	418.7440	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me [pic,prop_d0]	4	434.4967	0.0e+0



H3.1_K27-R40: Prop-KSAPATGGVKMe1KPHR MS/MS

Experimental spectrum

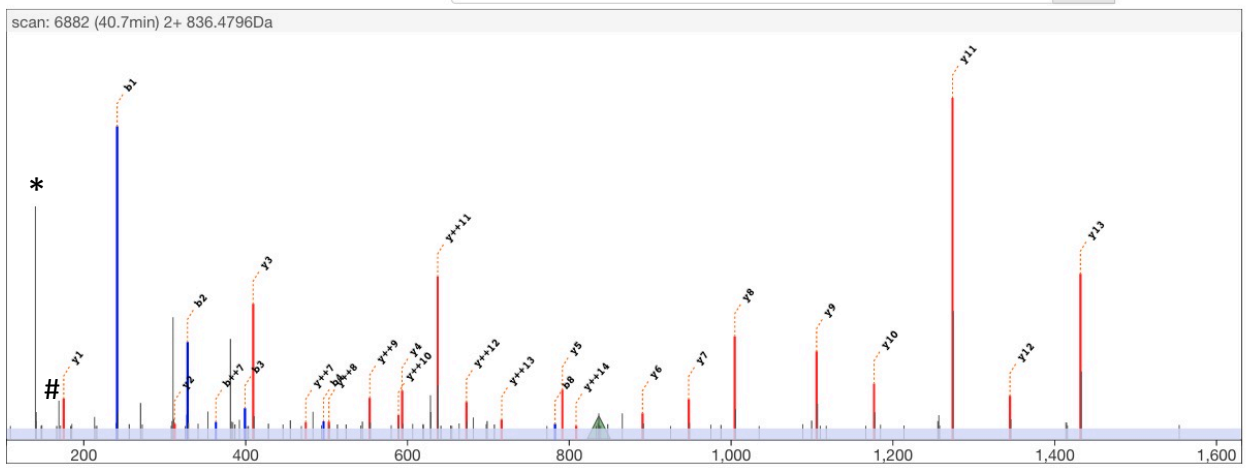
scan 6882
 retention time 40.7min
 precursor m/z 836.4796
 precursor charge 2+

Theoretical

M H²⁺ 836.4807
 MH Δ_{mass} Da -0.0022
 MH Δ_{mass} ppm -1.3

edit peptide

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



	b++	b		y	y++	
			Propionyl	1615.93	808.47	14
1	121.08	241.15	K	1431.81	716.41	13
2	164.60	328.19	S	1344.77	672.89	12
3	200.12	399.22	A	1273.74	637.37	11
4	248.64	496.28	P	1176.68	588.85	10
5	284.16	567.31	A	1105.65	553.33	9
6	334.68	668.36	T	1004.60	502.80	8
7	363.20	725.38	G	947.58	474.29	7
8	391.71	782.40	G	890.56	445.78	6
9	441.24	881.47	V	791.49	396.25	5
10	540.31	1079.61	K	593.35	297.18	4
11	632.37	1263.73	Methyl(Propionyl)K	409.23	205.12	3
12	680.90	1360.78	P	312.18	156.59	2
13	749.42	1497.84	H	175.12	88.06	1
14	827.48	1653.94	R			

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

H3.1_K27-R40: PIC-KSAPATGGVKMe1KPHR MS/MS

Experimental spectrum

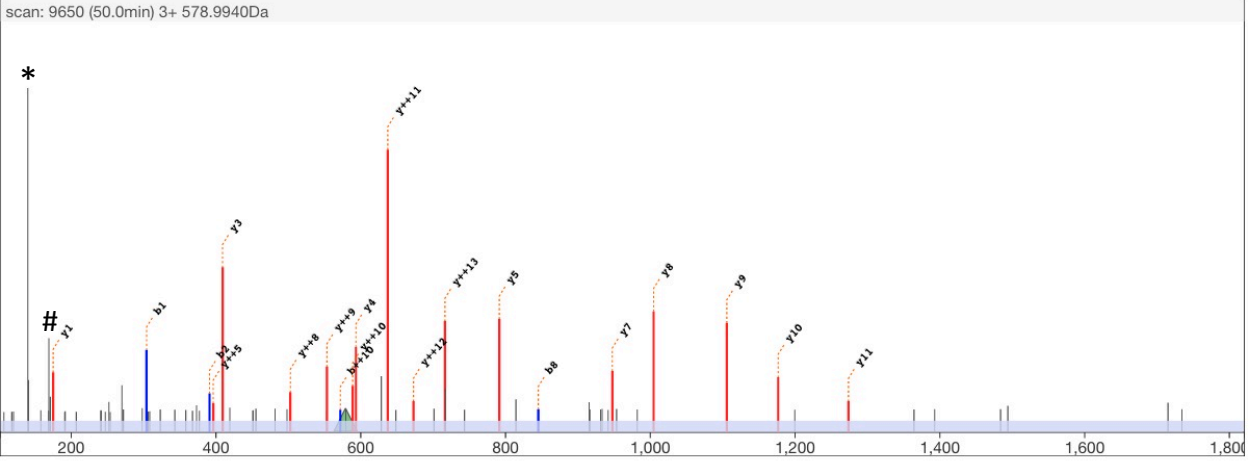
scan 9650
 retention time 50.0min
 precursor m/z 578.9940
 precursor charge 3+

Theoretical

M H³⁺ 578.9932
 MH Δ_{mass} Da 0.0025
 MH Δ_{mass} ppm 1.5

edit peptide

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



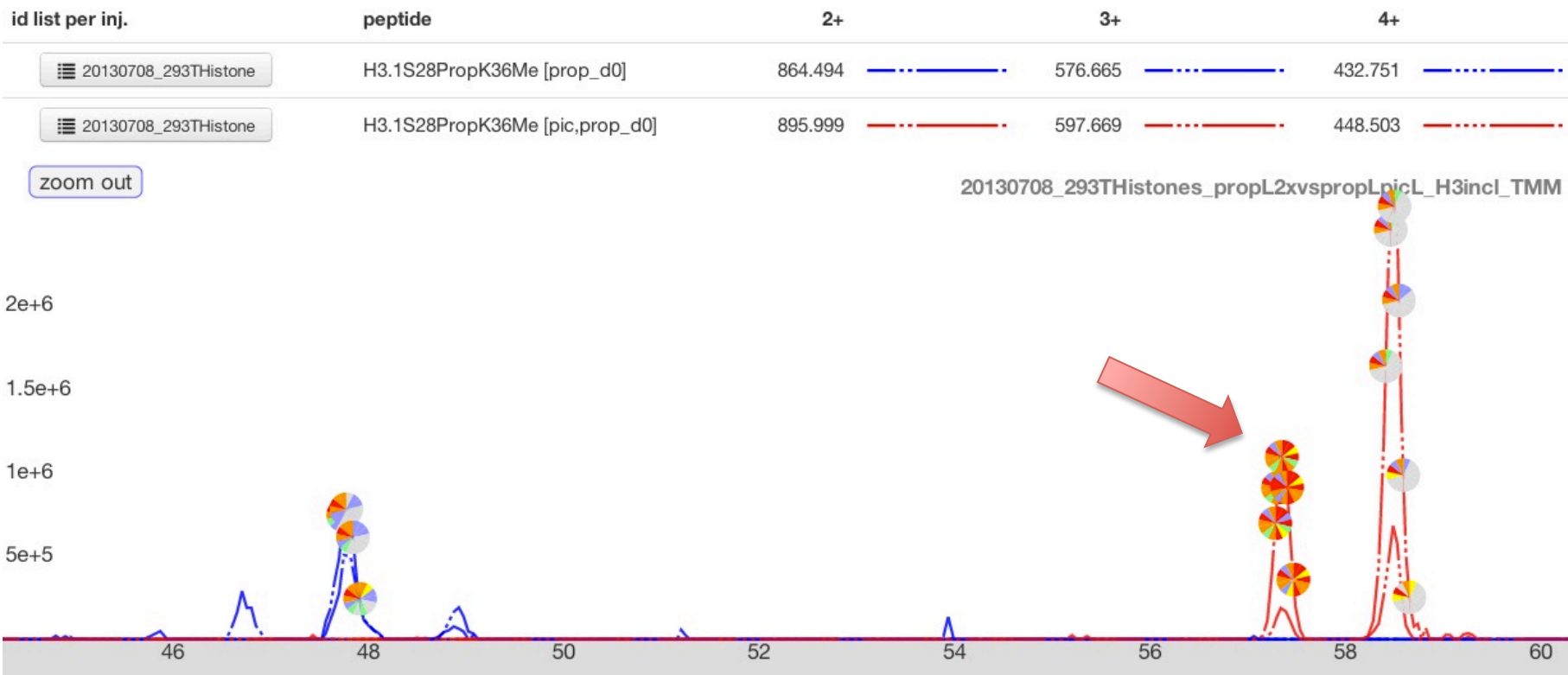
	b++	b		y	y++	
	60.53	120.04	PIC	1615.93	808.47	14
1	152.59	304.17	K	1431.81	716.41	13
2	196.10	391.20	S	1344.77	672.89	12
3	231.62	462.23	A	1273.74	637.37	11
4	280.15	559.29	P	1176.68	588.85	10
5	315.67	630.32	A	1105.65	553.33	9
6	366.19	731.37	T	1004.60	502.80	8
7	394.70	788.39	G	947.58	474.29	7
8	423.21	845.42	V	890.56	445.78	6
9	472.75	944.48	K	791.49	396.25	5
10	571.81	1142.62	Methyl,Propionyl	593.35	297.18	4
11	663.87	1326.74	K	409.23	205.12	3
12	712.40	1423.79	P	312.18	156.59	2
13	780.93	1560.85	H	175.12	88.06	1
14	858.98	1716.95	R			

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

H3.1_K27-R40:

KSProp?APATProp?GGVKMe1KPHR

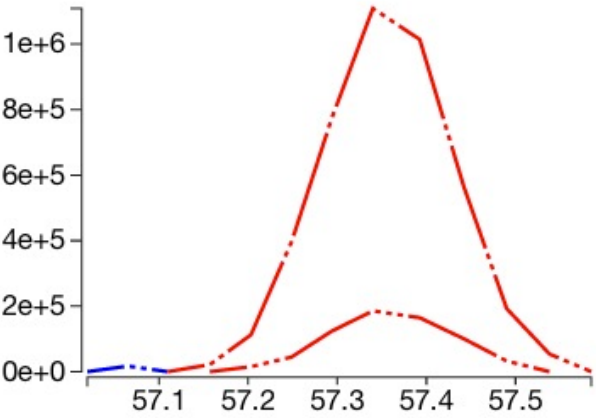
No MS2 detected for Prop-labeling. S28-prop MS2s shown.



Quanti event: 56.4-57.9min



injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1S28PropK36Me [prop_d0]	2	864.4938	4.6e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1S28PropK36Me [pic,prop_d0]	2	895.9992	1.2e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1S28PropK36Me [prop_d0]	3	576.6649	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1S28PropK36Me [pic,prop_d0]	3	597.6686	1.9e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1S28PropK36Me [prop_d0]	4	432.7505	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1S28PropK36Me [pic,prop_d0]	4	448.5033	0.0e+0



No MS2 detected for Prop-labeling.

Experimental spectrum

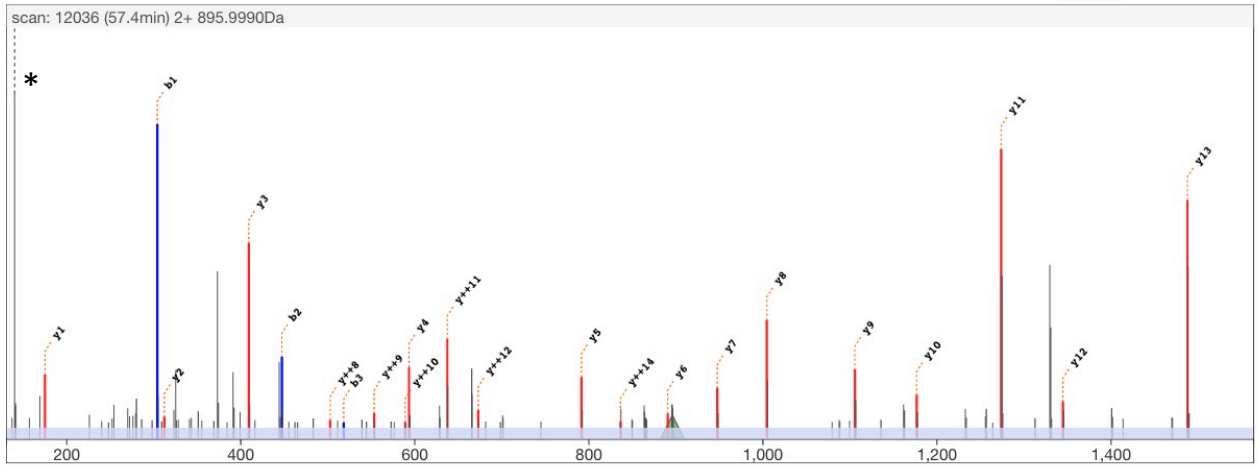
scan 12036
 retention time 57.4min
 precursor m/z 895.9990
 precursor charge 2+

Theoretical

M H²⁺ 895.9992
 MH Δ_{mass} Da -0.0005
 MH Δ_{mass} ppm -0.3

edit peptide

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



	b++	b		y	y++	
	60.53	120.04	PIC	1671.95	836.48	14
1	152.59	304.17	K	1487.83	744.42	13
2	224.12	447.22	S	1344.77	672.89	12
3	259.63	518.26	A	1273.74	637.37	11
4	308.16	615.31	P	1176.68	588.85	10
5	343.68	686.35	A	1105.65	553.33	9
6	394.20	787.40	T	1004.60	502.80	8
7	422.71	844.42	G	947.58	474.29	7
8	451.22	901.44	V	890.56	445.78	6
9	500.76	1000.51	K	791.49	396.25	5
10	599.83	1198.65	Methyl,Propionyl	593.35	297.18	4
11	691.89	1382.77	K	409.23	205.12	3
12	740.41	1479.82	P	312.18	156.59	2
13	808.94	1616.88	H	175.12	88.06	1
14	886.99	1772.98	R			

* = 140Da diagnostic ion

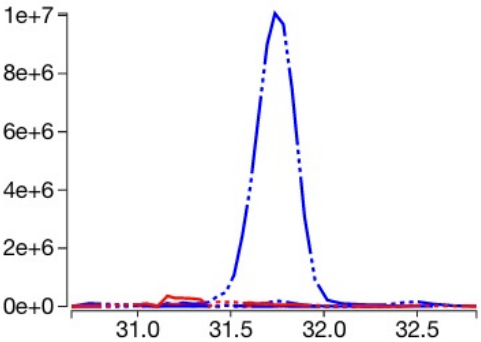
H3.1_K27-R40:

KSAPATGGVKMe2KPHR



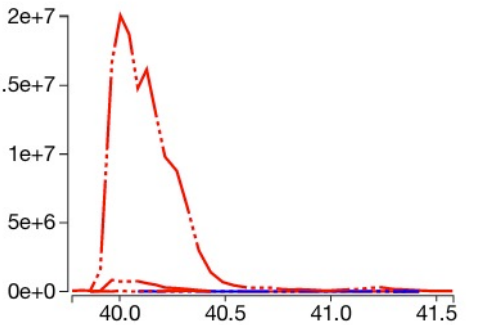
Quanti event: 30.6-32.8min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me2 [prop_d0]	2	815.4754	2.4e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me2 [pic,prop_d0]	2	846.9808	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me2 [prop_d0]	3	543.9860	1.6e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me2 [pic,prop_d0]	3	564.9897	1.1e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me2 [prop_d0]	4	408.2413	4.7e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me2 [pic,prop_d0]	4	423.9941	8.9e+6



Quanti event: 39.7-41.6min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me2 [prop_d0]	2	815.4754	1.7e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me2 [pic,prop_d0]	2	846.9808	1.4e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me2 [prop_d0]	3	543.9860	2.1e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me2 [pic,prop_d0]	3	564.9897	3.6e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me2 [prop_d0]	4	408.2413	9.0e+3
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me2 [pic,prop_d0]	4	423.9941	8.0e+5



H3.1_K27-R40: Prop-KSAPATGGVKMe2KPHR MS/MS

Experimental spectrum

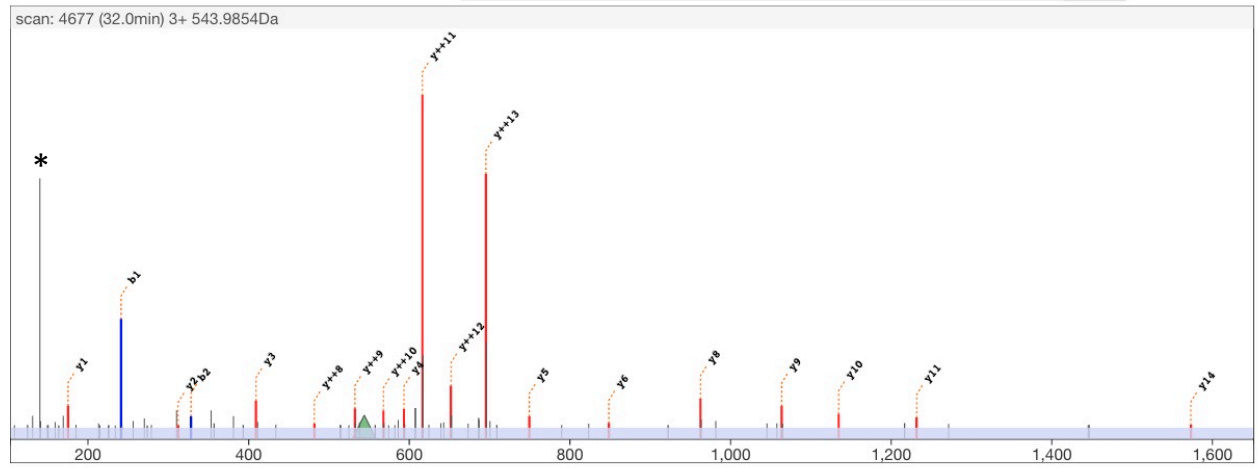
scan 4677
 retention time 32.0min
 precursor m/z 543.9854
 precursor charge 3+

Theoretical

M H³⁺ 543.9860
 MH Δ_{mass} Da -0.0018
 MH Δ_{mass} ppm -1.1

edit peptide

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



	b++	b	y	y++	
			1573.92	787.46	14
1	121.08	241.15	1389.80	695.40	13
2	164.60	328.19	1302.76	651.89	12
3	200.12	399.22	1231.73	616.37	11
4	248.64	496.28	1134.67	567.84	10
5	284.16	567.31	1063.64	532.32	9
6	334.68	668.36	962.59	481.80	8
7	363.20	725.38	905.57	453.29	7
8	391.71	782.40	848.55	424.78	6
9	441.24	881.47	749.48	375.24	5
10	519.30	1037.60	593.35	297.18	4
11	611.36	1221.72	409.23	205.12	3
12	659.89	1318.77	312.18	156.59	2
13	728.42	1455.83	175.12	88.06	1
14	806.47	1611.93			

* = 140Da diagnostic ion

H3.1_K27-R40: PIC-KSAPATGGVKMe2KPHR MS/MS

Experimental spectrum

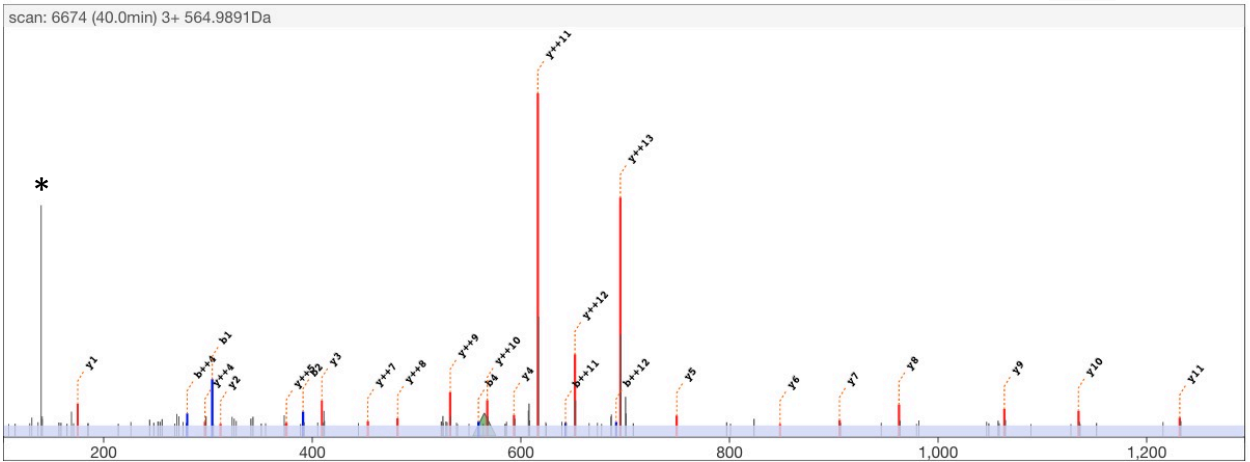
scan 6674
retention time 40.1min
precursor m/z 564.9891
precursor charge 3+

Theoretical

MH³⁺ 564.9897
MH Δ_{mass} Da -0.0015
MH Δ_{mass} ppm -0.9

edit peptide

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

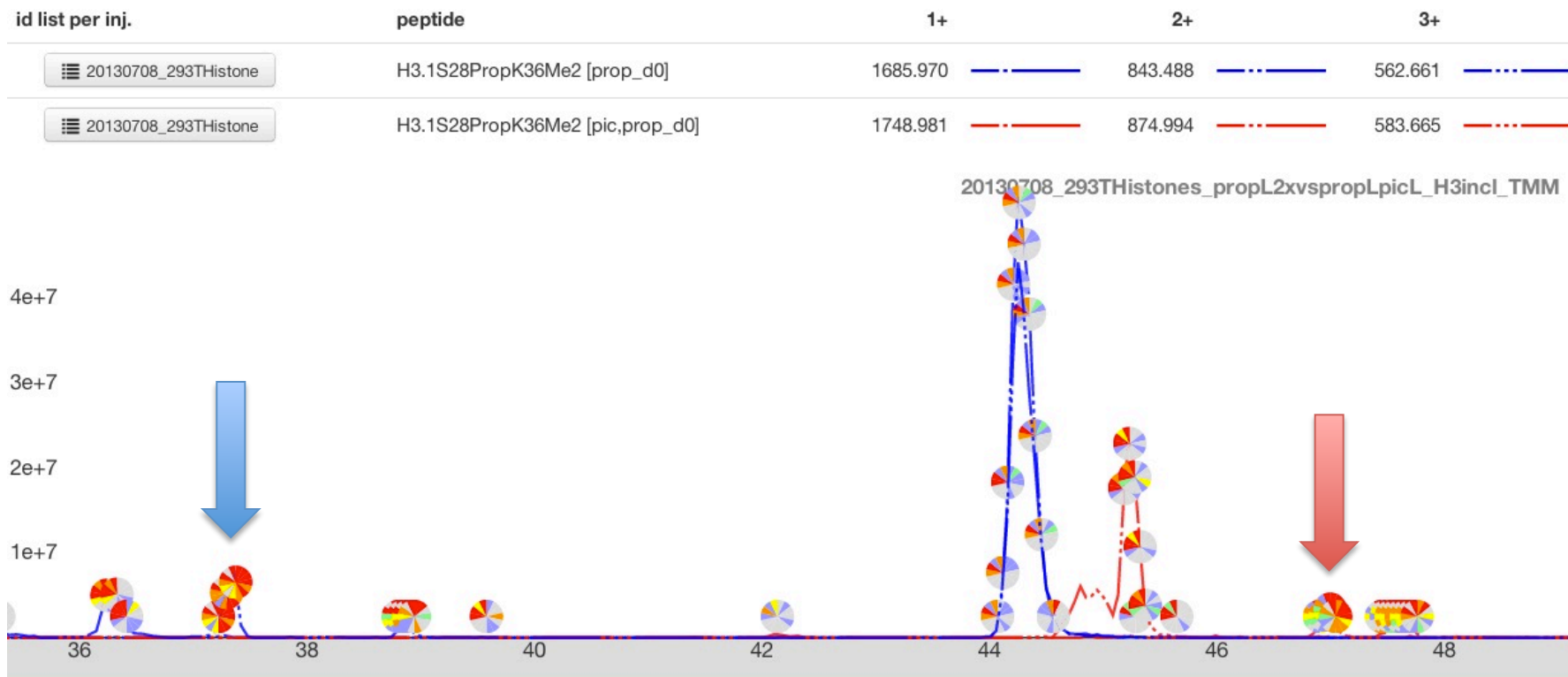


	b++	b		y	y++	
	60.53	120.04		1573.92	787.46	14
1	152.59	304.17	PIC	1389.80	695.40	13
2	196.10	391.20	Propionyl	1302.76	651.89	12
3	231.62	462.23	S	1231.73	616.37	11
4	280.15	559.29	A	1134.67	567.84	10
5	315.67	630.32	P	1063.64	532.32	9
6	366.19	731.37	A	962.59	481.80	8
7	394.70	788.39	T	905.57	453.29	7
8	423.21	845.42	G	848.55	424.78	6
9	472.75	944.48	V	749.48	375.24	5
10	550.81	1100.61	K	593.35	297.18	4
11	642.87	1284.73	Dimethyl	409.23	205.12	3
12	691.40	1381.78	Propionyl	312.18	156.59	2
13	759.93	1518.84	P	175.12	88.06	1
14	837.98	1674.94	H			
			R			

* = 140Da diagnostic ion

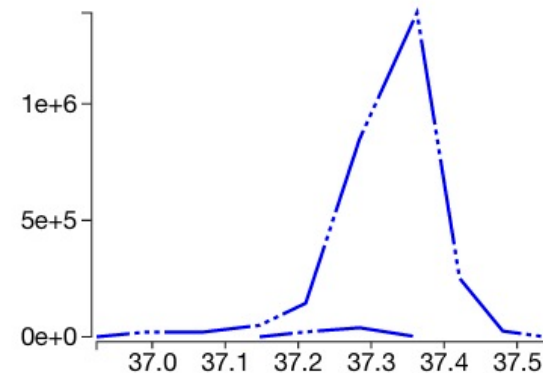
H3.1_K27-R40:

KS**Prop**APATGGVK**Me2**KPHR



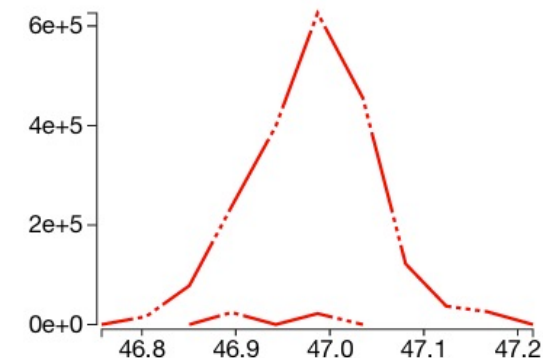
Quanti event: 36.9-37.6min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1S28PropK36Me2 [prop_d0]	1	1685.9697	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1S28PropK36Me2 [pic,prop_d0]	1	1748.9806	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1S28PropK36Me2 [prop_d0]	2	843.4885	2.7e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1S28PropK36Me2 [pic,prop_d0]	2	874.9939	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1S28PropK36Me2 [prop_d0]	3	562.6614	1.2e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1S28PropK36Me2 [pic,prop_d0]	3	583.6651	0.0e+0



Quanti event: 46.7-47.3min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1S28PropK36Me2 [prop_d0]	1	1685.9697	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1S28PropK36Me2 [pic,prop_d0]	1	1748.9806	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1S28PropK36Me2 [prop_d0]	2	843.4885	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1S28PropK36Me2 [pic,prop_d0]	2	874.9939	1.3e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1S28PropK36Me2 [prop_d0]	3	562.6614	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1S28PropK36Me2 [pic,prop_d0]	3	583.6651	5.5e+6



Experimental spectrum

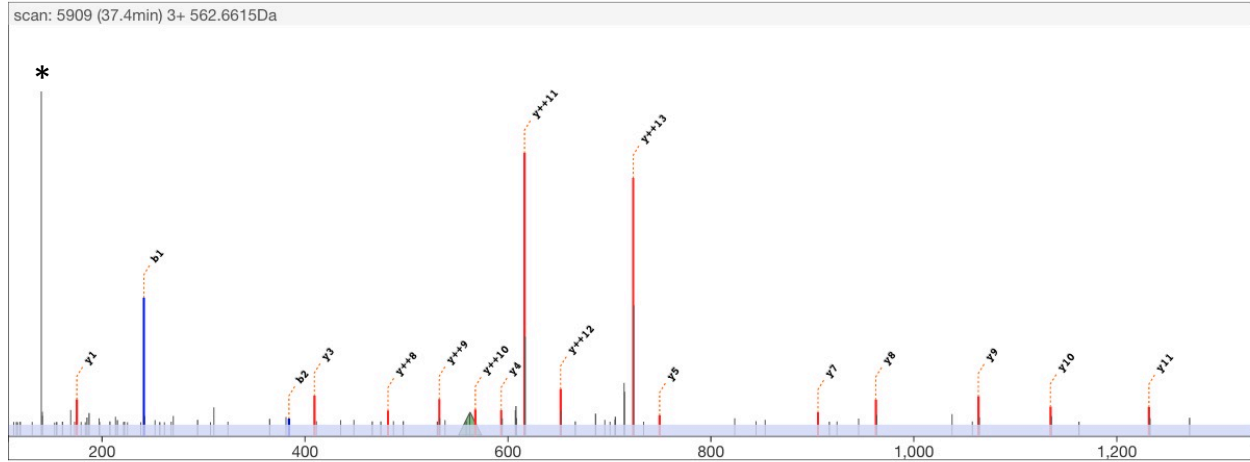
scan 5909
 retention time 37.4min
 precursor m/z 562.6615
 precursor charge 3+

Theoretical

M H³⁺ 562.6614
 MH Δ_{mass} Da 0.0002
 MH Δ_{mass} ppm 0.1

edit peptide

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



	b++	b	y	y++	
			1629.94	815.48	14
1	121.08	241.15	1445.82	723.41	13
2	192.61	384.21	1302.76	651.89	12
3	228.13	455.25	1231.73	616.37	11
4	276.66	552.30	1134.67	567.84	10
5	312.17	623.34	1063.64	532.32	9
6	362.70	724.39	962.59	481.80	8
7	391.21	781.41	905.57	453.29	7
8	419.72	838.43	848.55	424.78	6
9	469.25	937.50	749.48	375.24	5
10	547.32	1093.63	593.35	297.18	4
11	639.38	1277.75	409.23	205.12	3
12	687.90	1374.80	312.18	156.59	2
13	756.43	1511.86	175.12	88.06	1
14	834.48	1667.96			

* = 140Da diagnostic ion

H3.1_K27-R40: PIC-KSPropAPATGGVKMe2KPHR MS/MS

Experimental spectrum

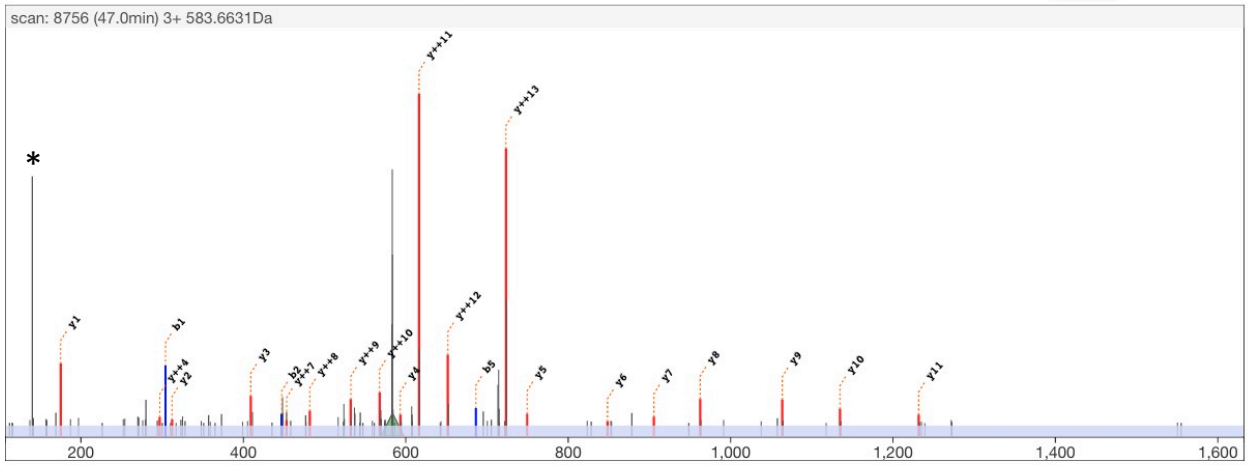
scan 8756
 retention time 47.0min
 precursor m/z 583.6631
 precursor charge 3+

Theoretical

M H³⁺ 583.6651
 MH Δ_{mass} Da -0.0057
 MH Δ_{mass} ppm -3.3

edit peptide

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

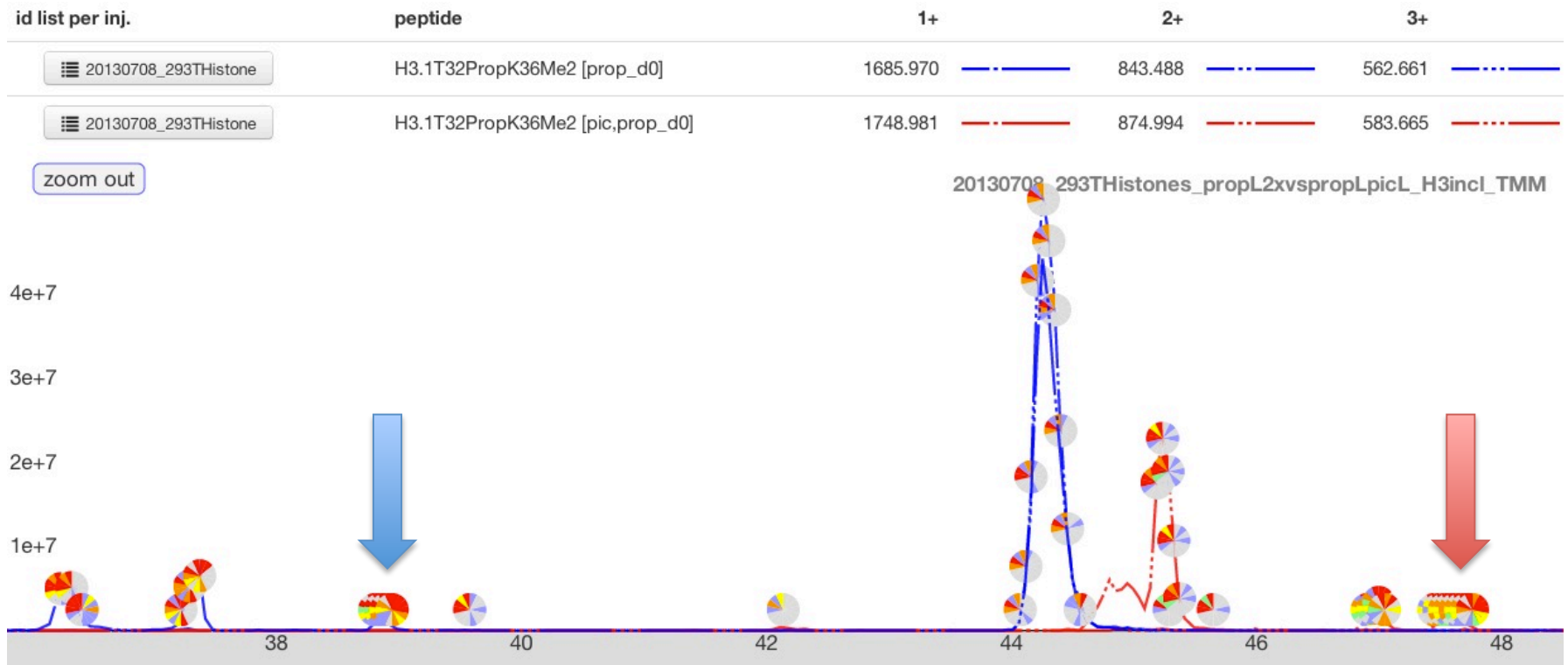


* = 140Da diagnostic ion

	b++	b		y	y++	
	60.53	120.04	PIC	1629.94	815.48	14
1	152.59	304.17	K	1445.82	723.41	13
2	224.12	447.22	S	1302.76	651.89	12
3	259.63	518.26	Propionyl	1231.73	616.37	11
4	308.16	615.31	A	1134.67	567.84	10
5	343.68	686.35	P	1063.64	532.32	9
6	394.20	787.40	A	962.59	481.80	8
7	422.71	844.42	T	905.57	453.29	7
8	451.22	901.44	G	848.55	424.78	6
9	500.76	1000.51	V	749.48	375.24	5
10	578.82	1156.64	K	593.35	297.18	4
11	670.88	1340.76	Dimethyl	409.23	205.12	3
12	719.41	1437.81	K	312.18	156.59	2
13	787.94	1574.87	Propionyl	175.12	88.06	1
14	865.99	1730.97	P			
			H			
			R			

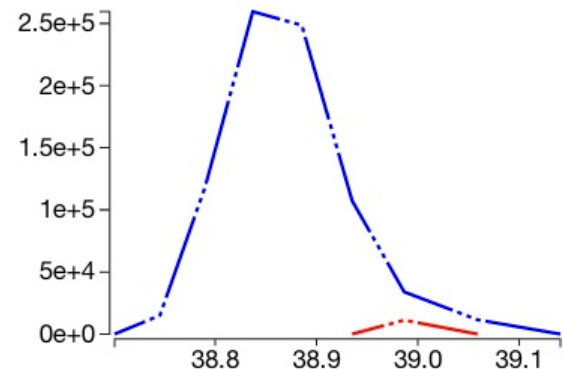
H3.1_K27-R40:

KSAPATPropGGVKMe2KPHR



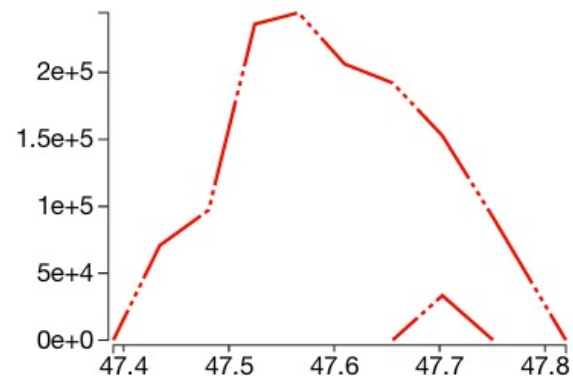
Quanti event: 38.7-39.2min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T32PropK36Me2 [prop_d0]	1	1685.9697	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T32PropK36Me2 [pic,prop_d0]	1	1748.9806	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T32PropK36Me2 [prop_d0]	2	843.4885	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T32PropK36Me2 [pic,prop_d0]	2	874.9939	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T32PropK36Me2 [prop_d0]	3	562.6614	2.3e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T32PropK36Me2 [pic,prop_d0]	3	583.6651	4.2e+4



Quanti event: 47.3-47.9min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T32PropK36Me2 [prop_d0]	1	1685.9697	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T32PropK36Me2 [pic,prop_d0]	1	1748.9806	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T32PropK36Me2 [prop_d0]	2	843.4885	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T32PropK36Me2 [pic,prop_d0]	2	874.9939	9.5e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T32PropK36Me2 [prop_d0]	3	562.6614	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1T32PropK36Me2 [pic,prop_d0]	3	583.6651	3.5e+6



H3.1_K27-R40: Prop-KSAPATPropGGVKMe2KPHR MS/MS

Experimental spectrum

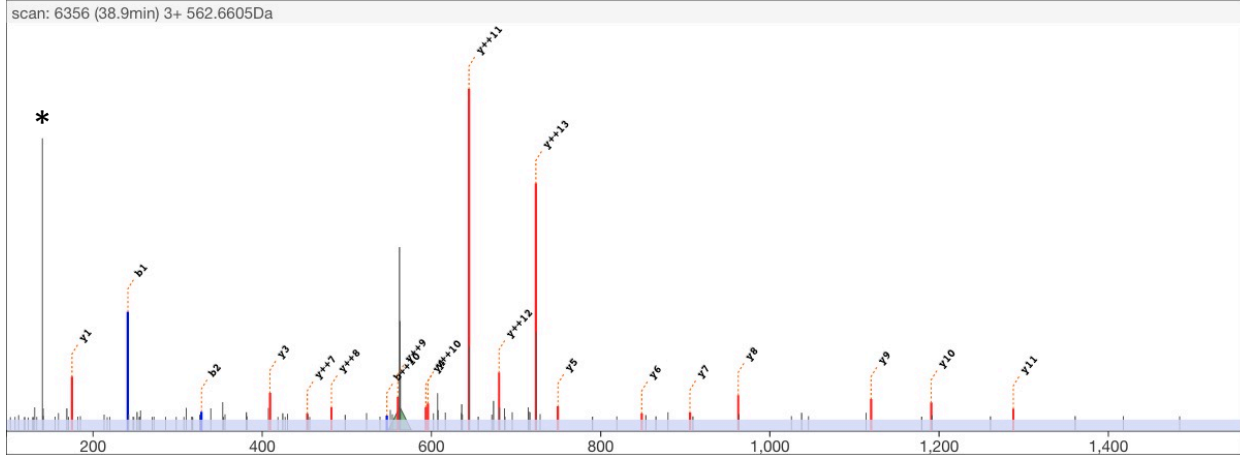
scan 6356
 retention time 38.9min
 precursor m/z 562.6605
 precursor charge 3+

Theoretical

M H³⁺ 562.6614
 MH Δ_{mass} Da -0.0027
 MH Δ_{mass} ppm -1.6

edit peptide

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



	b++	b		y	y++	
			Propionyl	1629.94	815.48	14
1	121.08	241.15	K			
			Propionyl	1445.82	723.41	13
2	164.60	328.19	S			
			A	1358.79	679.90	12
3	200.12	399.22	P	1287.75	644.38	11
			A	1190.70	595.85	10
4	248.64	496.28	T	1119.66	560.34	9
5	284.16	567.31	G			
			Propionyl	962.59	481.80	8
6	362.70	724.39	V			
7	391.21	781.41	G	905.57	453.29	7
8	419.72	838.43	V	848.55	424.78	6
9	469.25	937.50	K			
			Dimethyl	749.48	375.24	5
10	547.32	1093.63	K	593.35	297.18	4
11	639.38	1277.75	Propionyl	409.23	205.12	3
12	687.90	1374.80	P			
			H	312.18	156.59	2
13	756.43	1511.86	R	175.12	88.06	1
14	834.48	1667.96				

* = 140Da diagnostic ion

H3.1_K27-R40: PIC-KSAPATPropGGVKMe2KPHR MS/MS

Experimental spectrum

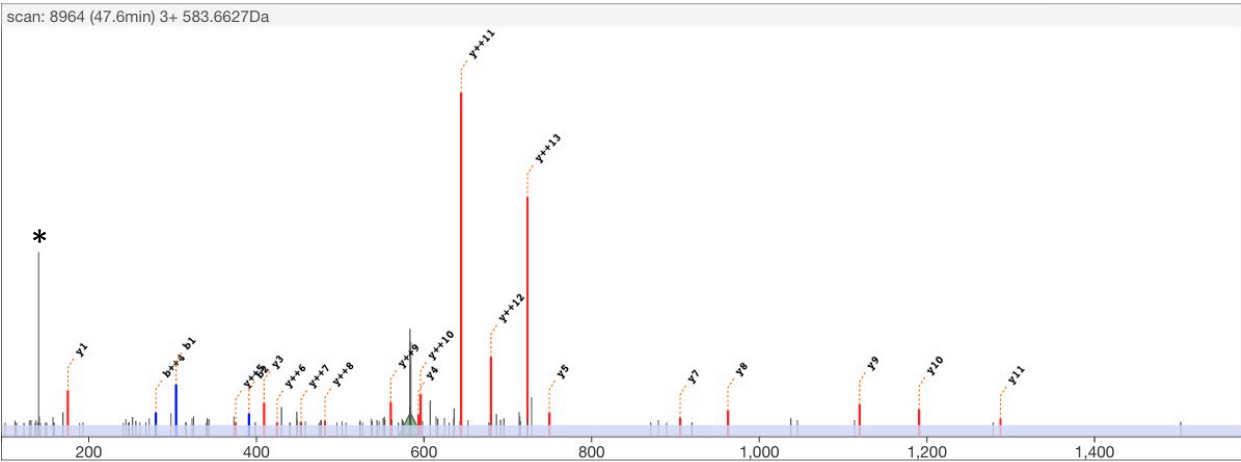
scan 8964
 retention time 47.6min
 precursor m/z 583.6627
 precursor charge 3+

Theoretical

M H³⁺ 583.6651
 MH Δ_{mass} Da -0.0070
 MH Δ_{mass} ppm -4.0

edit peptide

(PIC)K(Propionyl)SAPAT(Propionyl)GGVK(Dimethyl)K(Propionyl)PHR



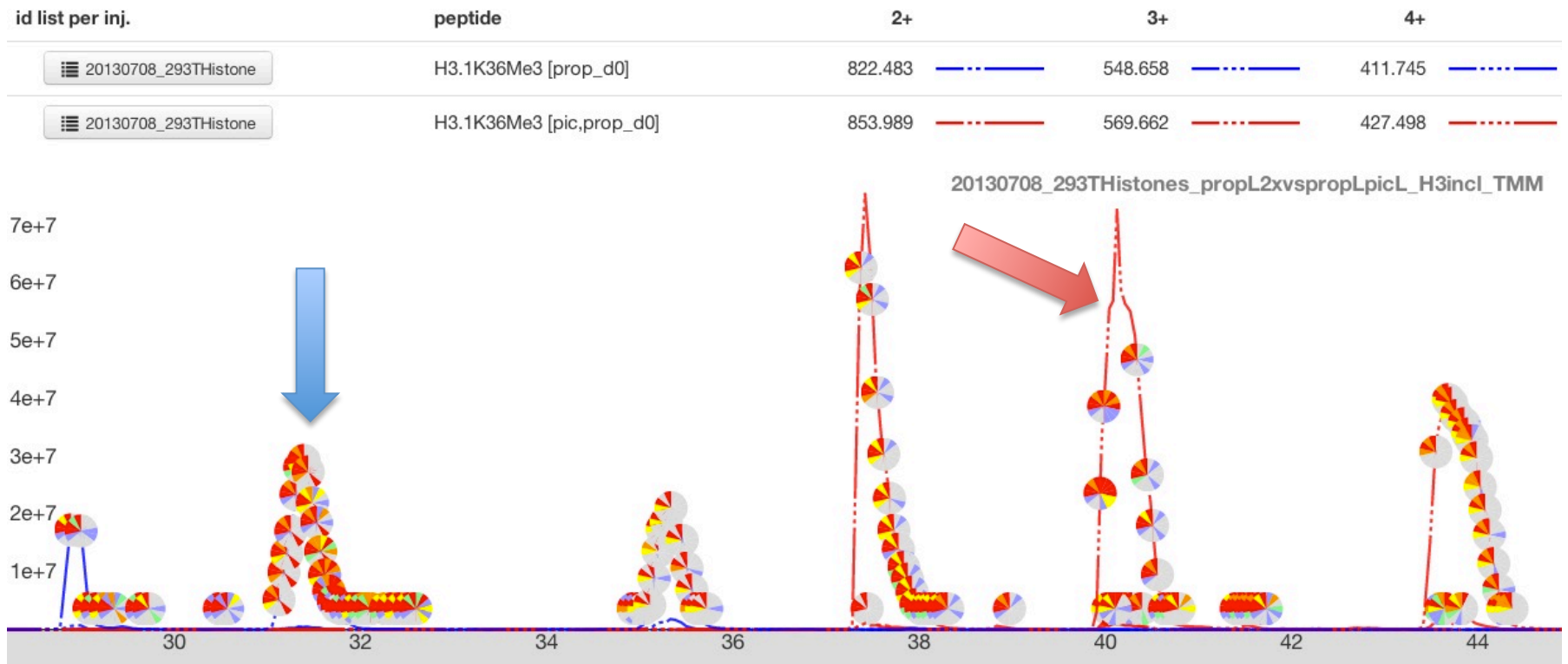
	b++	b		y	y++	
	60.53	120.04	PIC	1629.94	815.48	14
1	152.59	304.17	K	1445.82	723.41	13
2	196.10	391.20	S	1358.79	679.90	12
3	231.62	462.23	A	1287.75	644.38	11
4	280.15	559.29	P	1190.70	595.85	10
5	315.67	630.32	A	1119.66	560.34	9
6	394.20	787.40	T	962.59	481.80	8
7	422.71	844.42	G	905.57	453.29	7
8	451.22	901.44	G	848.55	424.78	6
9	500.76	1000.51	V	749.48	375.24	5
10	578.82	1156.64	K	593.35	297.18	4
11	670.88	1340.76	K	409.23	205.12	3
12	719.41	1437.81	P	312.18	156.59	2
13	787.94	1574.87	H	175.12	88.06	1
14	865.99	1730.97	R			

* = 140Da diagnostic ion

H3.1_K27-R40:

KSAPATGGVKMe3KPHR

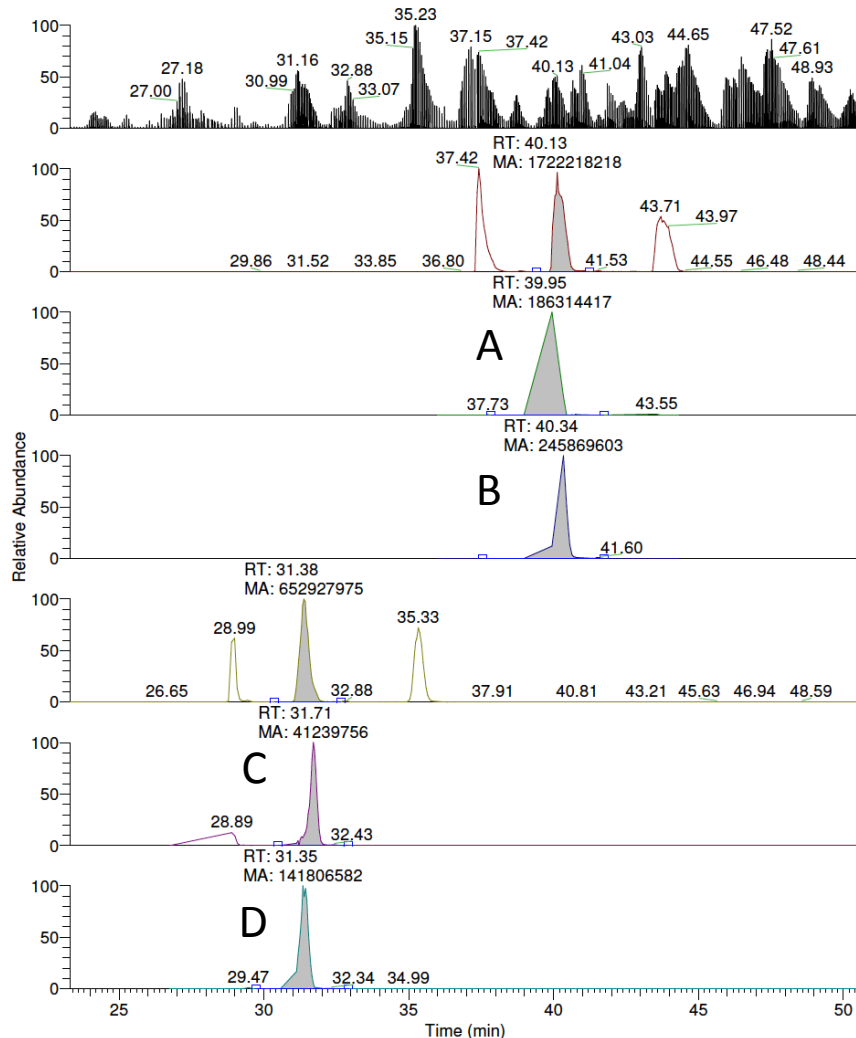
Overlaps with K27me2K36me1 (page 259). AUC determined on MS2 level (see page 244).



H3.1_K27-R40: KSAPATGGVKMe3KPHR

20130708_293THistones_propL2xvspropLp... 7/8/2013 11:43:33 AM

6 of 10 ul, Histones
RT: 23.31 - 50.59



PIC

Prop

AUC calculation on MS2 level:

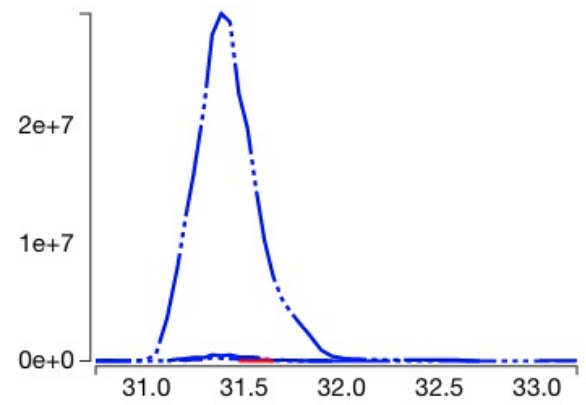
XIC-PIC 569.66 (3+)
574.85, 623.38, 658.89, 702.41

XIC-Prop 548.658 (3+)
539.33, 623.37, 658.89, 702.41,
1051.61, 1235.74

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

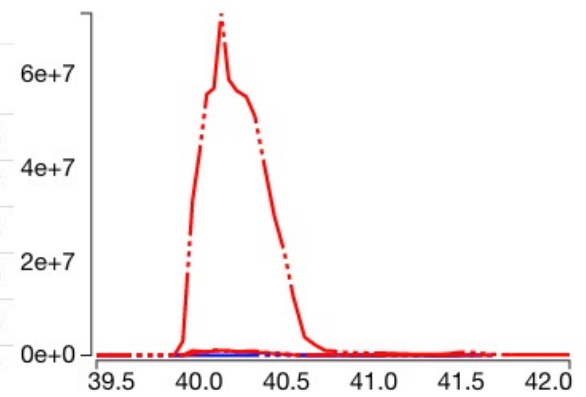
Quanti event: 30.7-33.2min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me3 [prop_d0]	2	822.4832	5.1e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me3 [pic,prop_d0]	2	853.9887	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me3 [prop_d0]	3	548.6579	6.5e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me3 [pic,prop_d0]	3	569.6615	4.2e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me3 [prop_d0]	4	411.7452	1.0e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me3 [pic,prop_d0]	4	427.4980	2.7e+4



Quanti event: 39.4-42.2min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me3 [prop_d0]	2	822.4832	9.0e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me3 [pic,prop_d0]	2	853.9887	2.5e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me3 [prop_d0]	3	548.6579	2.8e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me3 [pic,prop_d0]	3	569.6615	1.7e+9
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me3 [prop_d0]	4	411.7452	1.7e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Me3 [pic,prop_d0]	4	427.4980	2.7e+7



H3.1_K27-R40: Prop-KSAPATGGVKMe3KPHR MS/MS

Experimental spectrum

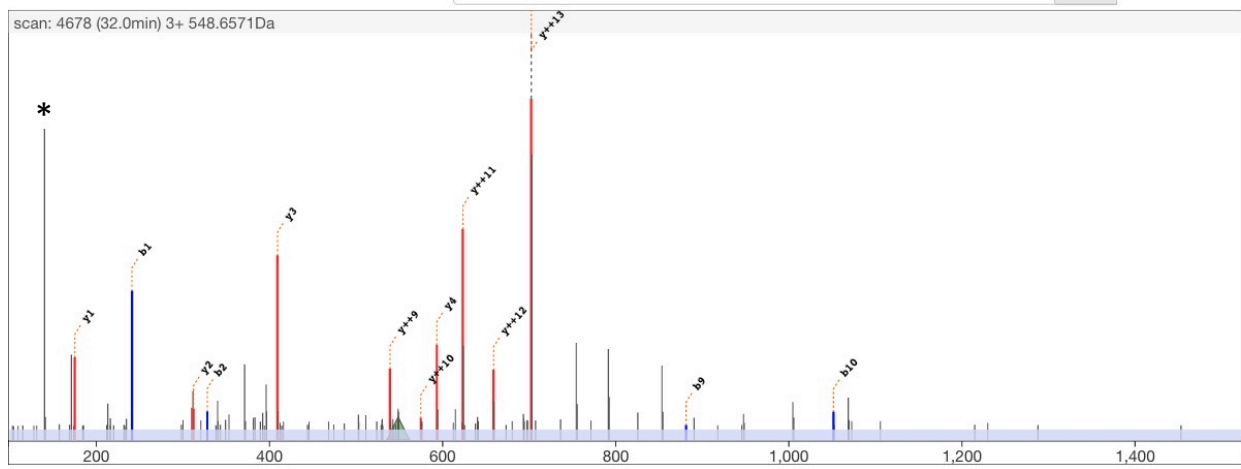
scan 4678
 retention time 32.0min
 precursor m/z 548.6571
 precursor charge 3+

Theoretical

M H³⁺ 548.6579
 MH Δ_{mass} Da -0.0024
 MH Δ_{mass} ppm -1.5

edit peptide

{Propionyl}K{Propionyl}SAPATGGVK{Trimethyl}K{Propionyl}PHR



	b++	b		y	y++	
			Propionyl	1587.93	794.47	14
1	121.08	241.15	K	1403.81	702.41	13
2	164.60	328.19	S	1316.78	658.89	12
3	200.12	399.22	A	1245.74	623.37	11
4	248.64	496.28	P	1148.69	574.85	10
5	284.16	567.31	A	1077.65	539.33	9
6	334.68	668.36	T	976.61	488.81	8
7	363.20	725.38	G	919.58	460.30	7
8	391.71	782.40	V	862.56	431.78	6
9	441.24	881.47	K	763.49	382.25	5
10	526.31	1051.61	Trimethyl K	593.35	297.18	4
11	618.37	1235.74	Propionyl K	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

H3.1_K27-R40: PIC-KSAPATGGVKMe3KPHR MS/MS

Experimental spectrum

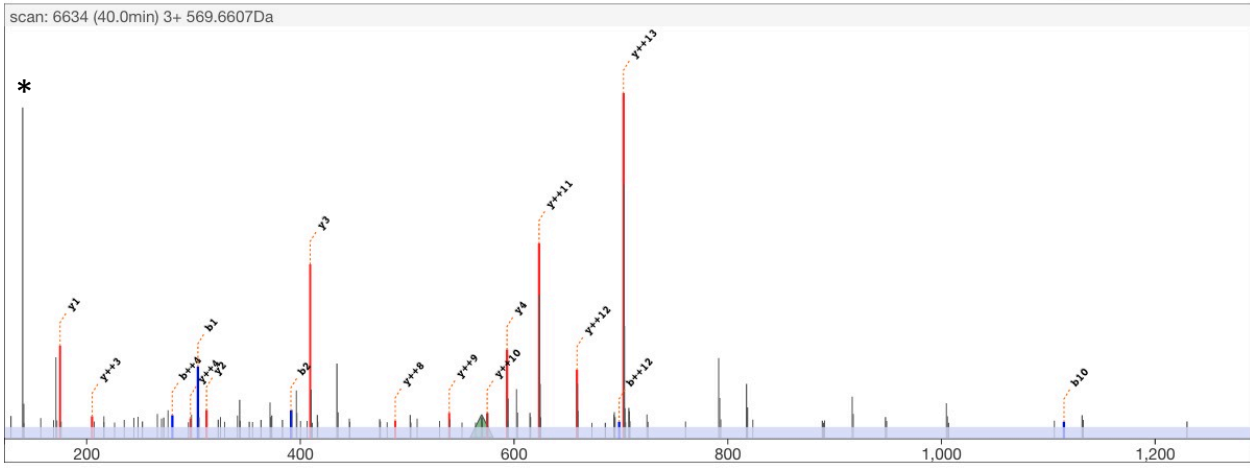
scan 6634
 retention time 39.9min
 precursor m/z 569.6607
 precursor charge 3+

Theoretical

M H³⁺ 569.6615
 MH Δ_{mass} Da -0.0025
 MH Δ_{mass} ppm -1.5

edit peptide

{PIC}K{Propionyl}SAPATGGVK{Trimethyl}K{Propionyl}PHR

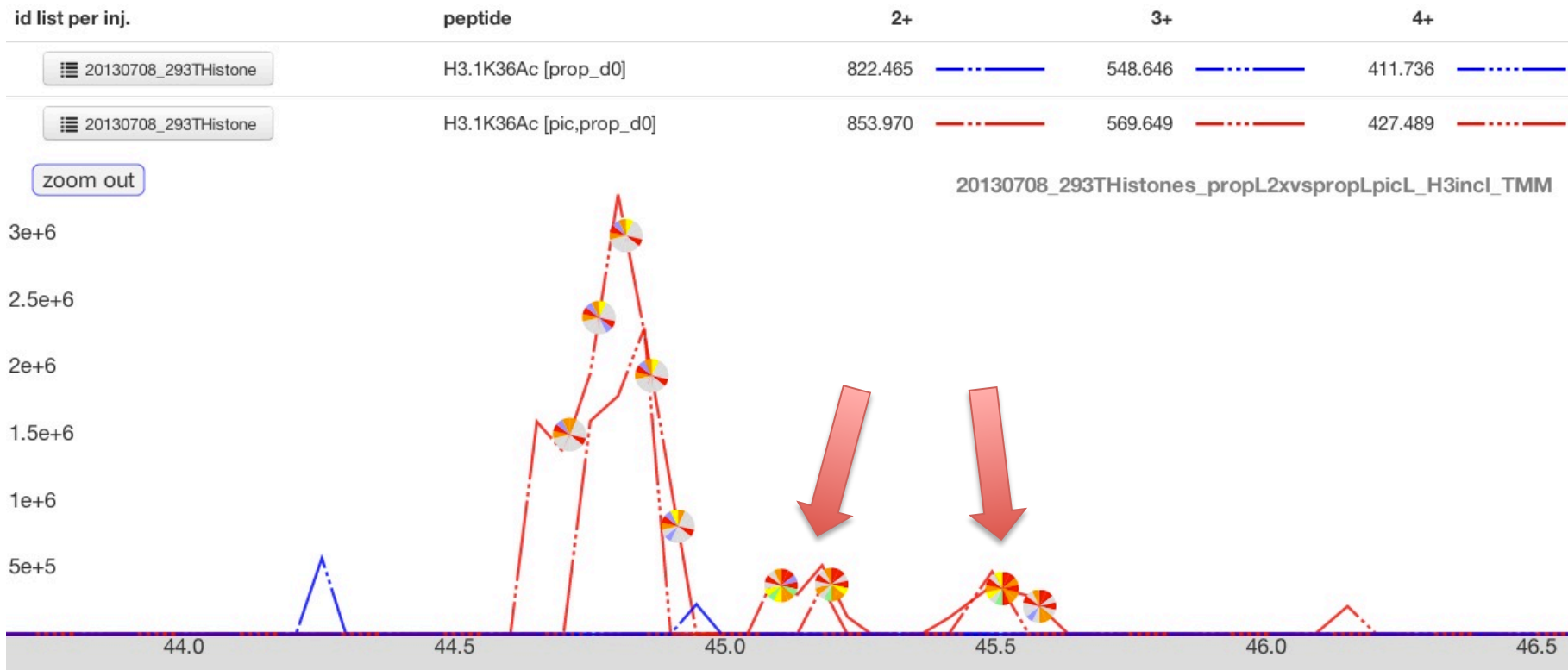


	b++	b		y	y++	
	60.53	120.04	PIC	1587.93	794.47	14
1	152.59	304.17	K	1403.81	702.41	13
2	196.10	391.20	S	1316.78	658.89	12
3	231.62	462.23	A	1245.74	623.37	11
4	280.15	559.29	P	1148.69	574.85	10
5	315.67	630.32	A	1077.65	539.33	9
6	366.19	731.37	T	976.61	488.81	8
7	394.70	788.39	G	919.58	460.30	7
8	423.21	845.42	V	862.56	431.78	6
9	472.75	944.48	K	763.49	382.25	5
10	557.82	1114.63	Trimethyl	593.35	297.18	4
11	649.88	1298.75	K	409.23	205.12	3
12	698.40	1395.80	Propionyl	312.18	156.59	2
13	766.93	1532.86	P	175.12	88.06	1
14	844.98	1688.96	H			
			R			

* = 140Da diagnostic ion

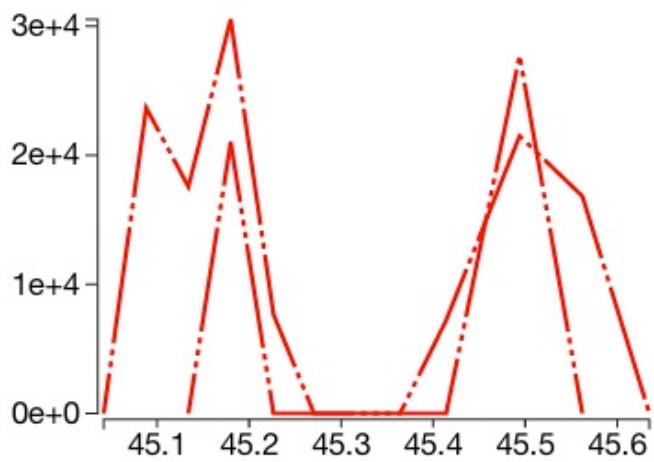
H3.1_K27-R40: KSAPATGGVK**Ac**KPHR

No MS2 for Prop-peak detected.



Quanti event: 45.0-45.7min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Ac [prop_d0]	2	822.4650	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Ac [pic,prop_d0]	2	853.9705	4.1e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Ac [prop_d0]	3	548.6458	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Ac [pic,prop_d0]	3	569.6494	1.8e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Ac [prop_d0]	4	411.7361	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K36Ac [pic,prop_d0]	4	427.4889	0.0e+0



Prop-only peak not detected.

H3.1_K27-R40: PIC-KSAPATGGVKAcKPHR MS/MS

Experimental spectrum

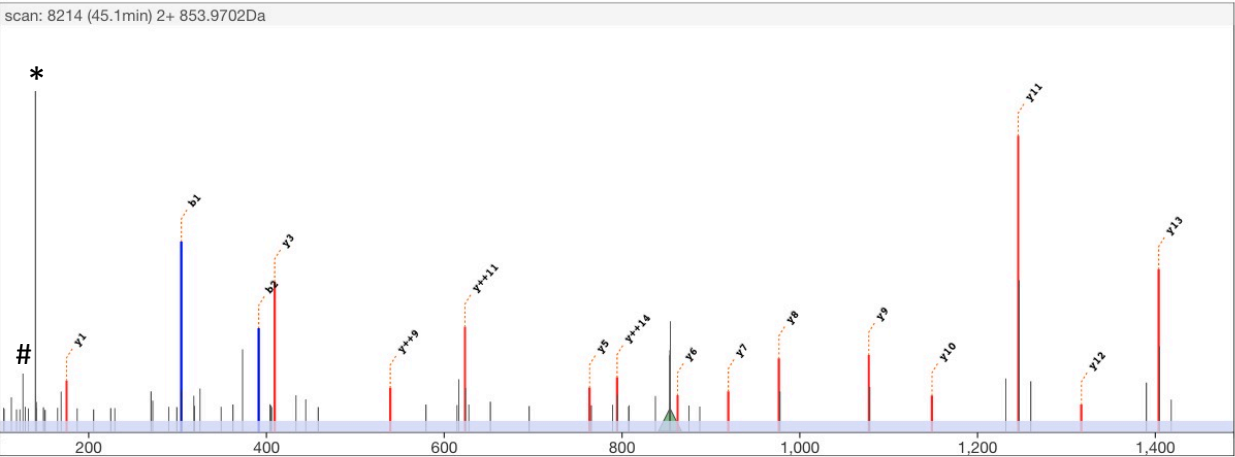
scan 8214
 retention time 45.1min
 precursor m/z 853.9702
 precursor charge 2+

Theoretical

M H²⁺ 853.9705
 MH Δ_{mass} Da -0.0006
 MH Δ_{mass} ppm -0.4

edit peptide

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



	b++	b		y	y++	
	60.53	120.04	PIC	1587.90	794.45	14
1	152.59	304.17	K	1403.78	702.39	13
2	196.10	391.20	S	1316.74	658.88	12
3	231.62	462.23	A	1245.71	623.36	11
4	280.15	559.29	P	1148.65	574.83	10
5	315.67	630.32	A	1077.62	539.31	9
6	366.19	731.37	T	976.57	488.79	8
7	394.70	788.39	G	919.55	460.28	7
8	423.21	845.42	V	862.53	431.77	6
9	472.75	944.48	K	763.46	382.23	5
10	557.80	1114.59	Acetyl	593.35	297.18	4
11	649.86	1298.71	K	409.23	205.12	3
12	698.39	1395.76	Propionyl	312.18	156.59	2
13	766.91	1532.82	P	175.12	88.06	1
14	844.97	1688.92	H			
			R			

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