

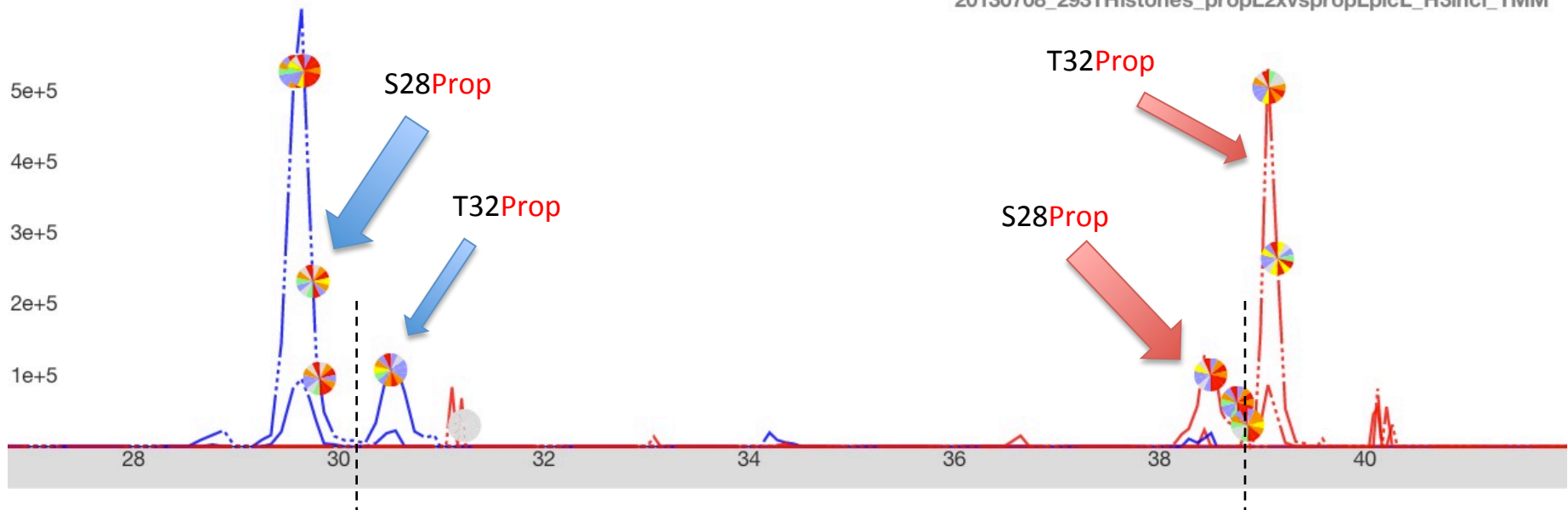
H3.1_K27-R40:

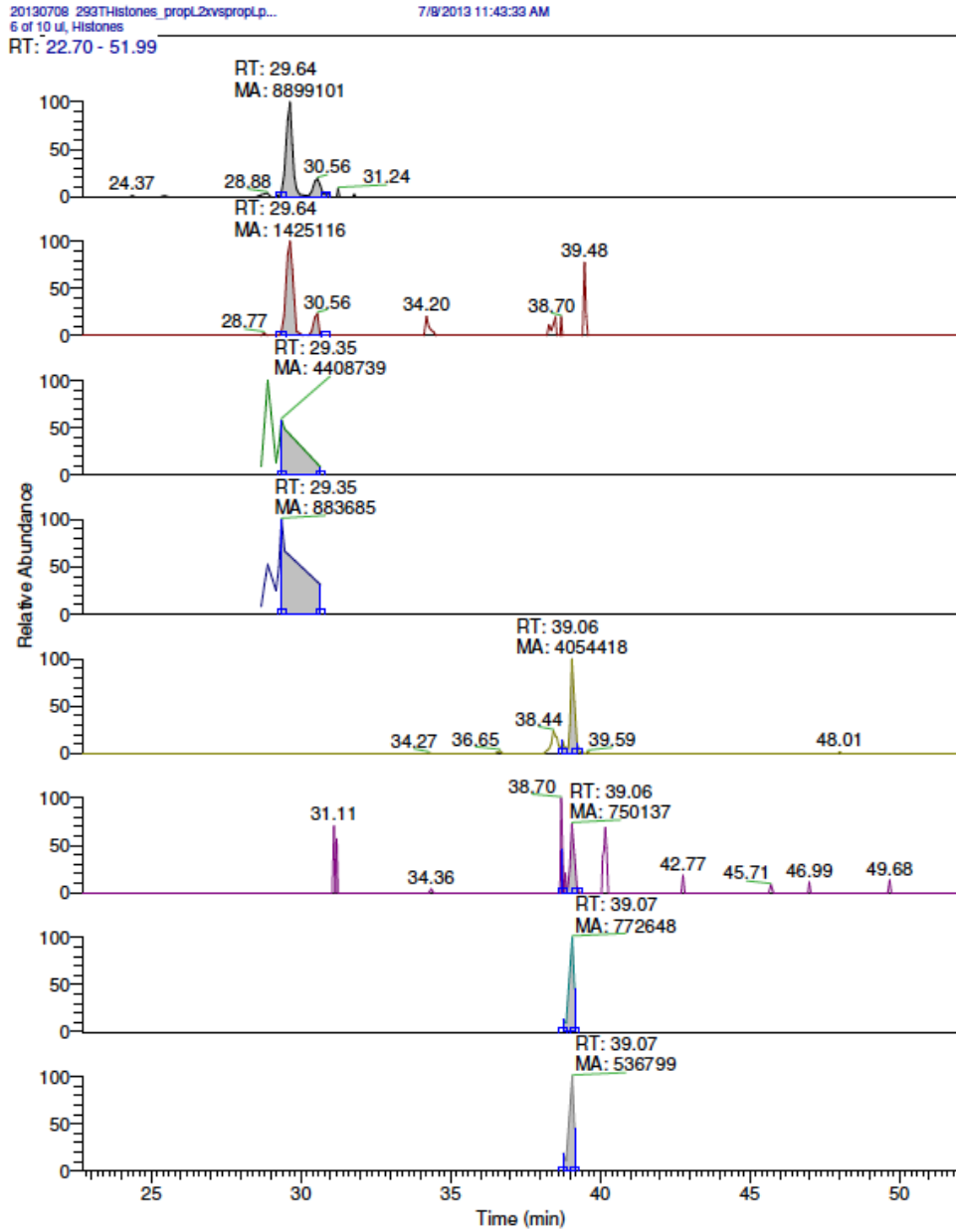
KMe3SPropAPATGGVKMe2KPHR

Overlaps with K27Me2,K36Me3, S28Prop (see page 324).

id list per inj.	peptide	2+	3+	4+
20130708_293THistone	H3.1K27Me3S28PropK36Me2 [prop_d0]	836.499	558.002	418.753
20130708_293THistone	H3.1K27Me3S28PropK36Me2 [pic,prop_d0]	868.004	579.005	434.506

20130708_293THistones_propL2xvspropLpicL_H3incl_TMM





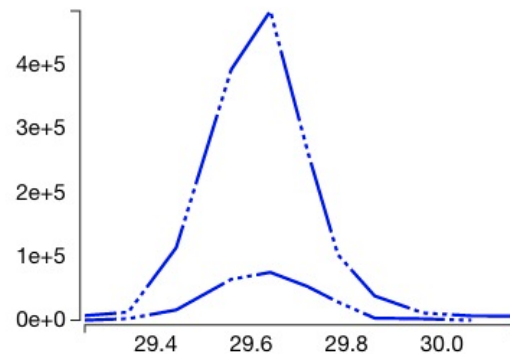
AUC calculation on MS2 level:

XIC-Prop 418.75 (4+)
 227.18, 370.23, 441.27, 481.80,
 532.32, 567.84, 616.37

XIC-PIC 434.51 (4+)
 290.19, 433.24, 481.80, 504.28,
 532.32, 567.84, 616.37

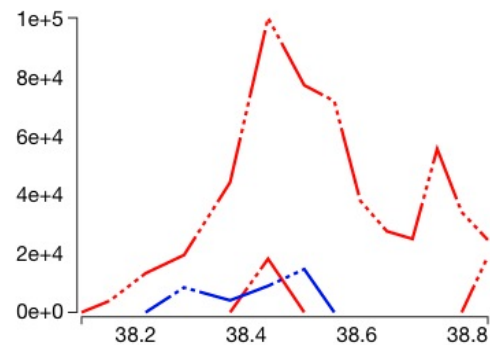
Quanti event: 29.2-30.2min >

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me2 [prop_d0]	2	836.4989	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me2 [pic,prop_d0]	2	868.0043	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me2 [prop_d0]	3	558.0017	1.2e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me2 [pic,prop_d0]	3	579.0053	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me2 [prop_d0]	4	418.7531	7.3e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me2 [pic,prop_d0]	4	434.5058	0.0e+0



Quanti event: 37.9-38.9min ✕

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me2 [prop_d0]	2	836.4989	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me2 [pic,prop_d0]	2	868.0043	7.4e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me2 [prop_d0]	3	558.0017	1.5e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me2 [pic,prop_d0]	3	579.0053	2.7e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me2 [prop_d0]	4	418.7531	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3S28PropK36Me2 [pic,prop_d0]	4	434.5058	1.8e+6



H3.1_K27-R40: Prop-KMe3SPropAPATGGVKMe2KPHR MS/MS

Experimental spectrum

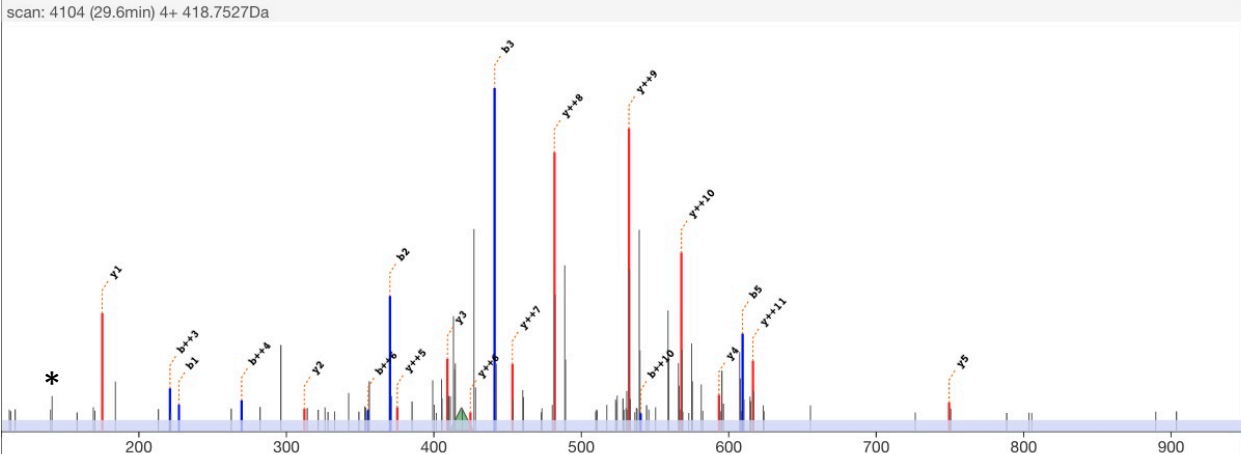
scan 4104
 retention time 29.6min
 precursor m/z 418.7527
 precursor charge 4+

Theoretical

M H⁴⁺ 418.7531
 MH Δ_{mass} Da -0.0015
 MH Δ_{mass} ppm -0.9

edit peptide

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



	b++	b		y	y++	
			Propionyl	1615.96	808.49	14
1	114.09	227.18	K			
			Trimethyl	1445.82	723.41	13
2	185.62	370.23	S			
			Propionyl	1302.76	651.89	12
3	221.14	441.27	A		616.37	11
4	269.67	538.32	P		567.84	10
5	305.18	609.36	A		532.32	9
6	355.71	710.41	T		481.80	8
7	384.22	767.43	G		453.29	7
8	412.73	824.45	G			
9	462.26	923.52	V			
10	540.33	1079.65	K	749.48	375.24	5
11	632.39	1263.77	Dimethyl	593.35	297.18	4
12	680.91	1360.82	K			
13	749.44	1497.88	Propionyl	409.23	205.12	3
14	827.49	1653.98	P			
			H	312.18	156.59	2
			R	175.12	88.06	1

* = 140Da diagnostic ion

H3.1_K27-R40: PIC-KMe3SPropAPATGGVKMe2KPHR MS/MS

Experimental spectrum

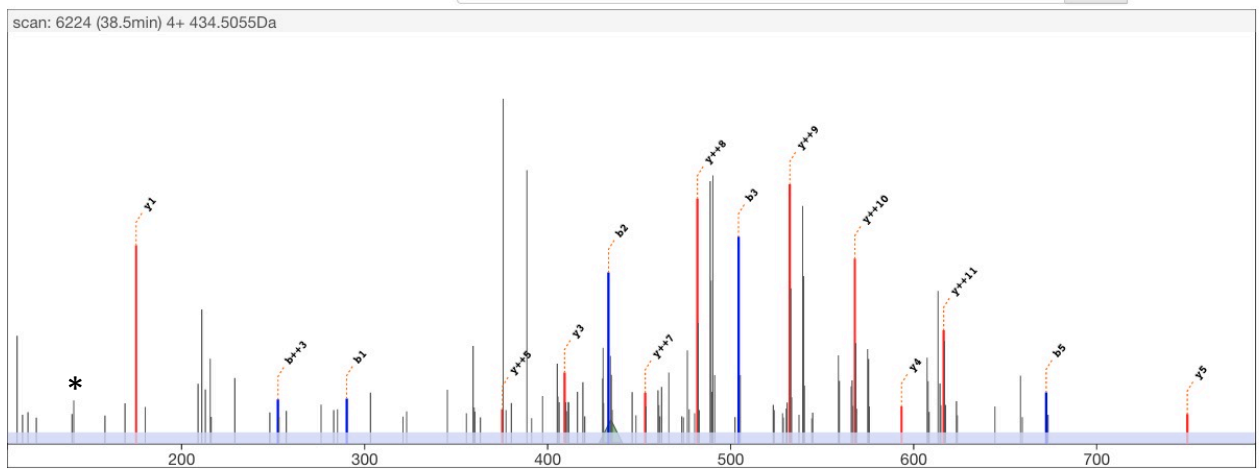
scan 6224
 retention time 38.5min
 precursor m/z 434.5055
 precursor charge 4+

Theoretical

M H⁴⁺ 434.5058
 MH Δ_{mass} Da -0.0012
 MH Δ_{mass} ppm -0.7

edit peptide

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



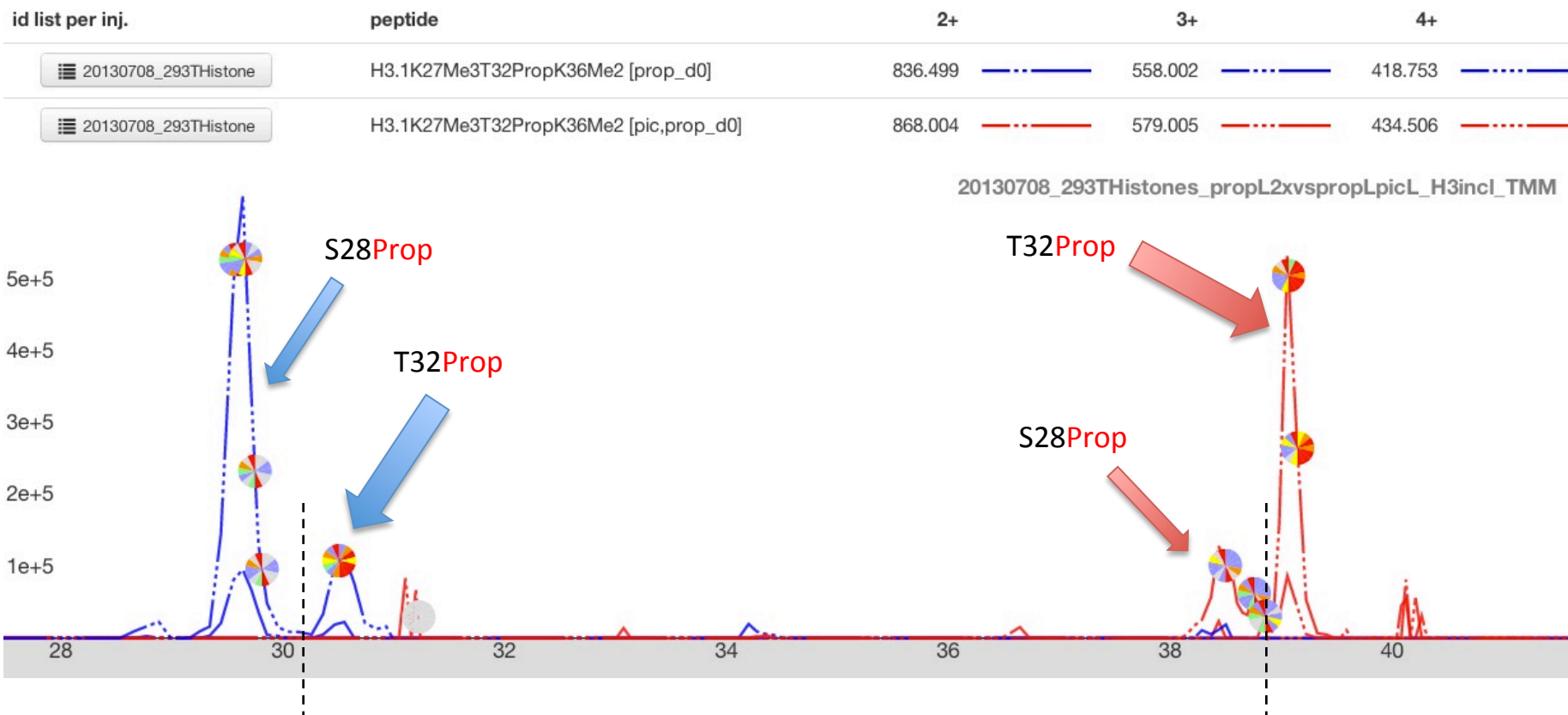
	b++	b		y	y++	
	60.53	120.04	PIC	1615.96	808.49	14
1	145.60	290.19	K	1445.82	723.41	13
2	217.13	433.24	S	1302.76	651.89	12
3	252.64	504.28	Propionyl	1231.73	616.37	11
4	301.17	601.33	A	1134.67	567.84	10
5	336.69	672.37	P	1063.64	532.32	9
6	387.21	773.42	A	962.59	481.80	8
7	415.72	830.44	T	905.57	453.29	7
8	444.23	887.46	G	848.55	424.78	6
9	493.77	986.53	V	749.48	375.24	5
10	571.83	1142.66	K	593.35	297.18	4
11	663.89	1326.78	Dimethyl	409.23	205.12	3
12	712.42	1423.83	K	312.18	156.59	2
13	780.95	1560.89	Propionyl	175.12	88.06	1
14	859.00	1716.99	P			
			H			
			R			

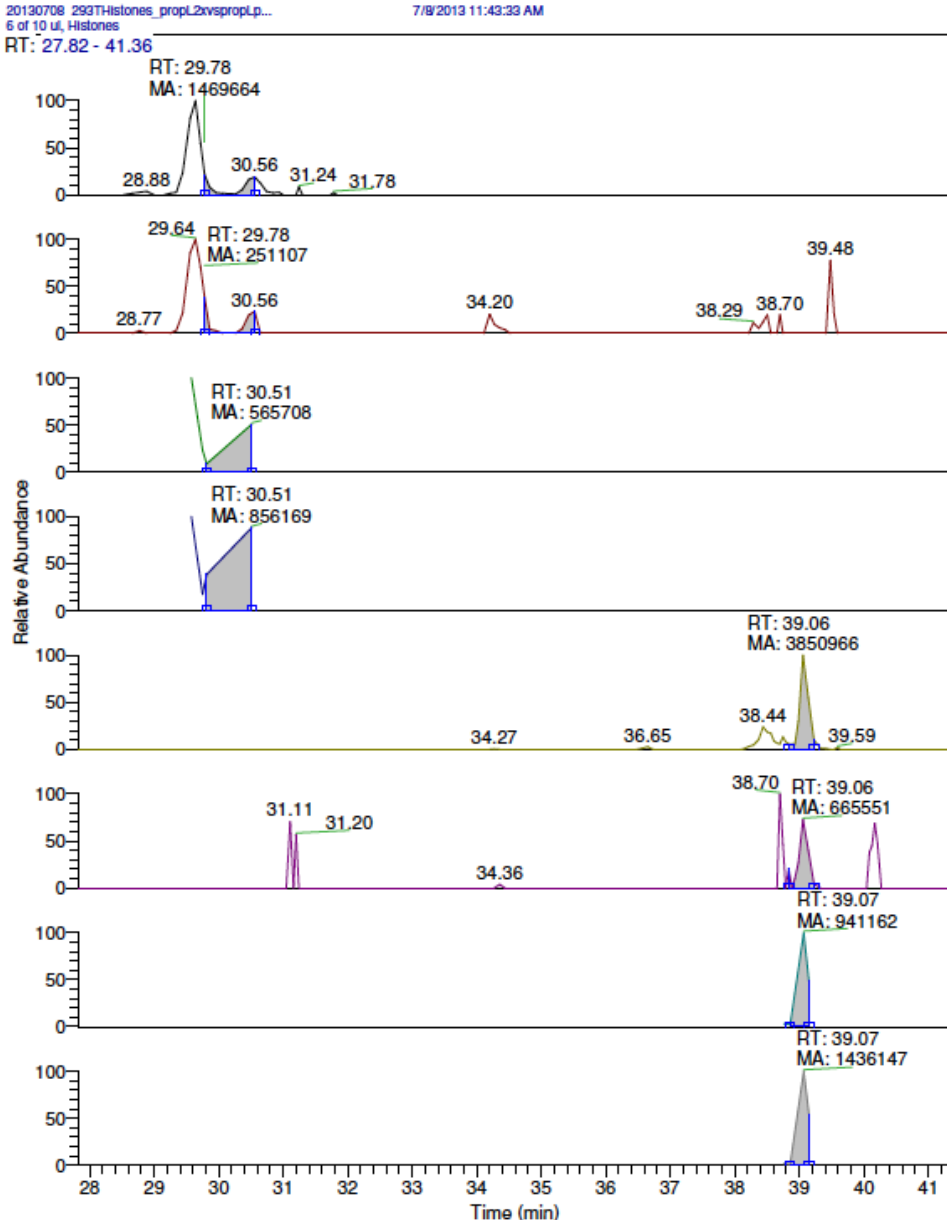
* = 140Da diagnostic ion

H3.1_K27-R40:

KMe3SAPATPropGGVKMe2KPHR

Overlaps with K27Me2,K36me3,T32Prop (see page 329).





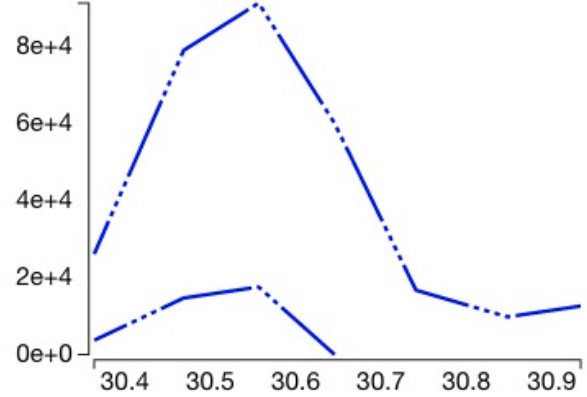
AUC calculation on MS2 level:

XIC-Prop 418.75 (4+)
 227.18, 314.21, 385.24, 481.80,
 560.34, 595.85, 644.38

XIC-PIC 434.51 (4+)
 290.19, 377.22, 448.26, 481.80,
 560.34, 595.85, 644.38

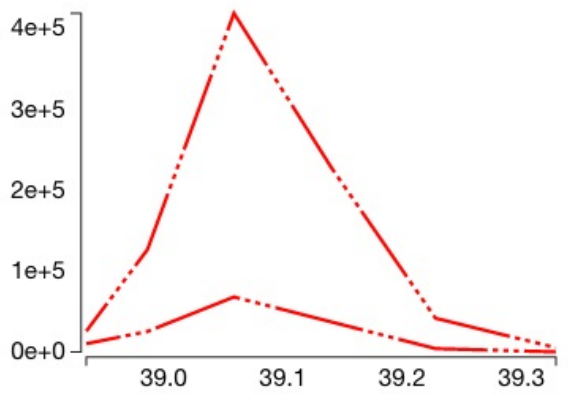
Quanti event: 30.3-31.0min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3T32PropK36Me2 [prop_d0]	2	836.4989	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3T32PropK36Me2 [pic,prop_d0]	2	868.0043	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3T32PropK36Me2 [prop_d0]	3	558.0017	1.9e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3T32PropK36Me2 [pic,prop_d0]	3	579.0053	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3T32PropK36Me2 [prop_d0]	4	418.7531	1.5e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3T32PropK36Me2 [pic,prop_d0]	4	434.5058	0.0e+0



Quanti event: 38.9-39.4min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3T32PropK36Me2 [prop_d0]	2	836.4989	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3T32PropK36Me2 [pic,prop_d0]	2	868.0043	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3T32PropK36Me2 [prop_d0]	3	558.0017	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3T32PropK36Me2 [pic,prop_d0]	3	579.0053	6.4e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3T32PropK36Me2 [prop_d0]	4	418.7531	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me3T32PropK36Me2 [pic,prop_d0]	4	434.5058	3.9e+6



H3.1_K27-R40: Prop-KMe3SAPATPropGGVKMe2KPHR MS/MS

Experimental spectrum

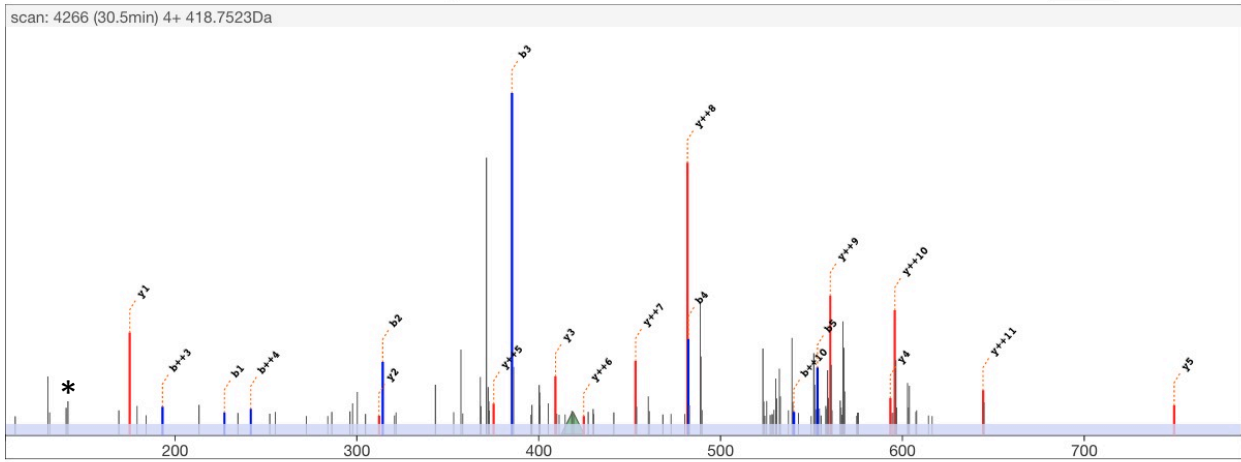
scan 4266
 retention time 30.5min
 precursor m/z 418.7523
 precursor charge 4+

Theoretical

M H⁴⁺ 418.7531
 MH Δ_{mass} Da -0.0029
 MH Δ_{mass} ppm -1.7

edit peptide

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



	b++	b		y	y++	
			Propionyl	1615.96	808.49	14
1	114.09	227.18	K			
			Trimethyl	1445.82	723.41	13
2	157.61	314.21	S	1358.79	679.90	12
3	193.13	385.24	A	1287.75	644.38	11
4	241.65	482.30	P	1190.70	595.85	10
5	277.17	553.33	A	1119.66	560.34	9
6	355.71	710.41	T	962.59	481.80	8
			Propionyl			
7	384.22	767.43	G	905.57	453.29	7
8	412.73	824.45	V	848.55	424.78	6
9	462.26	923.52	K	749.48	375.24	5
10	540.33	1079.65	Dimethyl	593.35	297.18	4
11	632.39	1263.77	Propionyl	409.23	205.12	3
12	680.91	1360.82	K			
13	749.44	1497.88	P	312.18	156.59	2
			H			
14	827.49	1653.98	R	175.12	88.06	1

* = 140Da diagnostic ion

Experimental spectrum

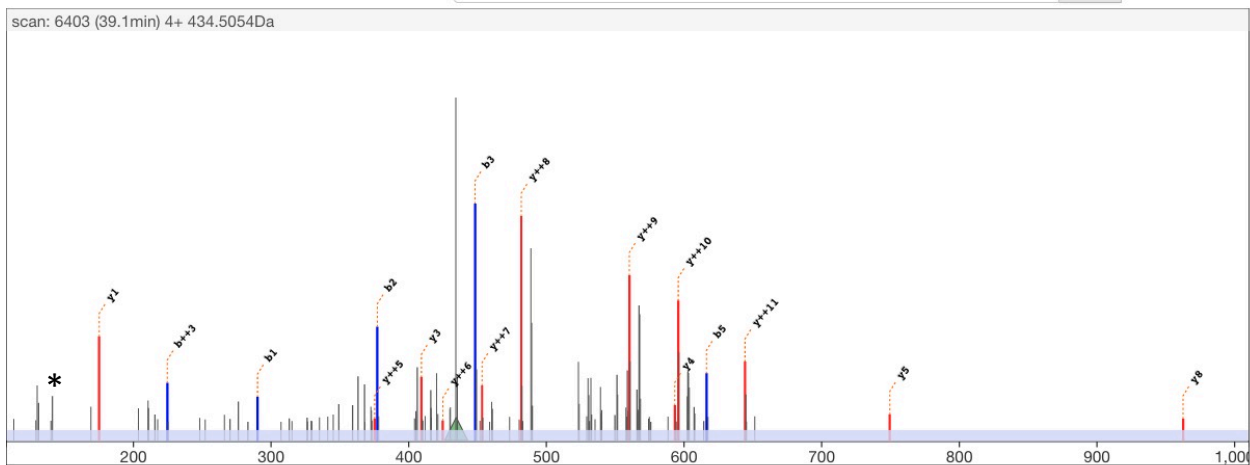
scan 6403
 retention time 39.1min
 precursor m/z 434.5054
 precursor charge 4+

Theoretical

M H⁺ 434.5058
 MH Δ_{mass} Da -0.0017
 MH Δ_{mass} ppm -1.0

edit peptide

{PIC}K{Trimethyl}SAPATPropGGVK{Dimethyl}K{Propionyl}PHR



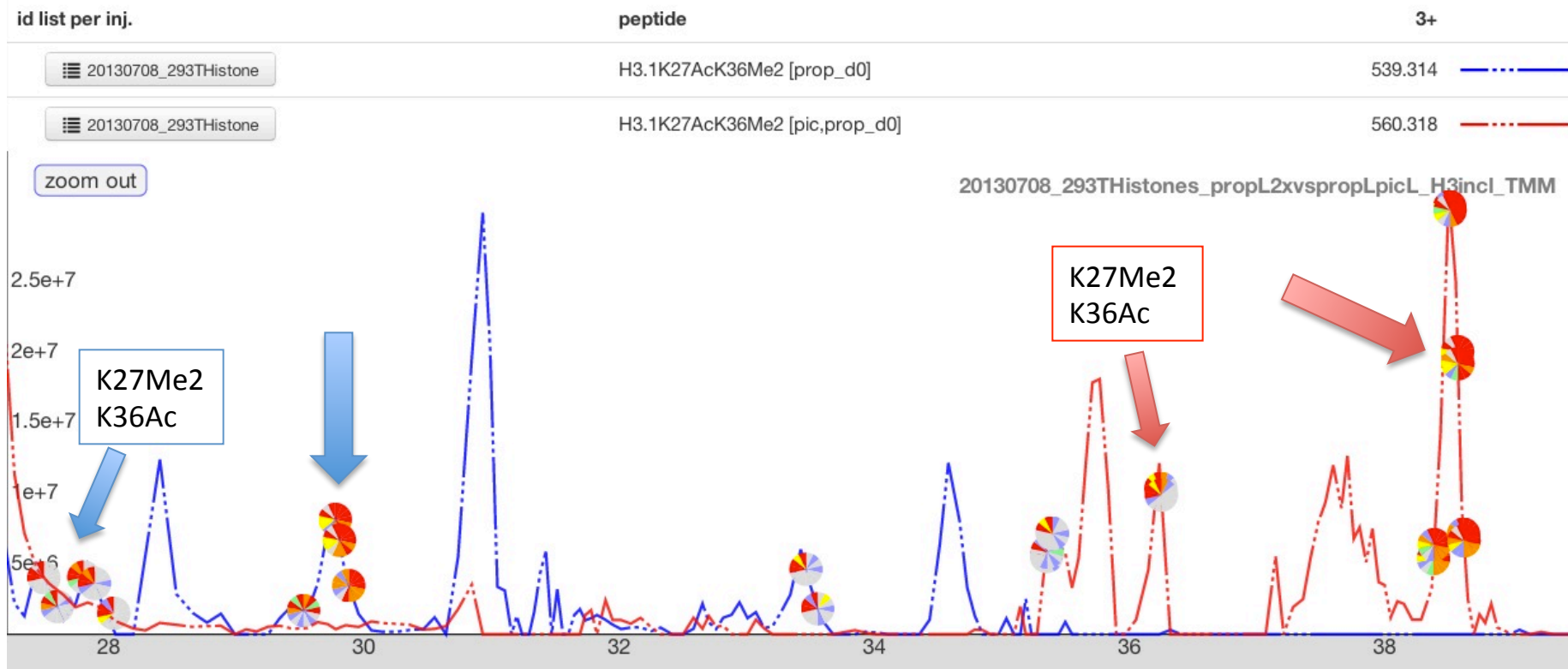
	b++	b		y	y++	
	60.53	120.04	PIC	1615.96	808.49	14
1	145.60	290.19	K Trimethyl	1445.82	723.41	13
2	189.11	377.22	S	1358.79	679.90	12
3	224.63	448.26	A	1287.75	644.38	11
4	273.16	545.31	P	1190.70	595.85	10
5	308.68	616.35	A	1119.66	560.34	9
6	387.21	773.42	T Propionyl	962.59	481.80	8
7	415.72	830.44	G	905.57	453.29	7
8	444.23	887.46	V	848.55	424.78	6
9	493.77	986.53	G	749.48	375.24	5
10	571.83	1142.66	V Dimethyl	593.35	297.18	4
11	663.89	1326.78	K Propionyl	409.23	205.12	3
12	712.42	1423.83	P	312.18	156.59	2
13	780.95	1560.89	H	175.12	88.06	1
14	859.00	1716.99	R			

* = 140Da diagnostic ion

H3.1_K27-R40:

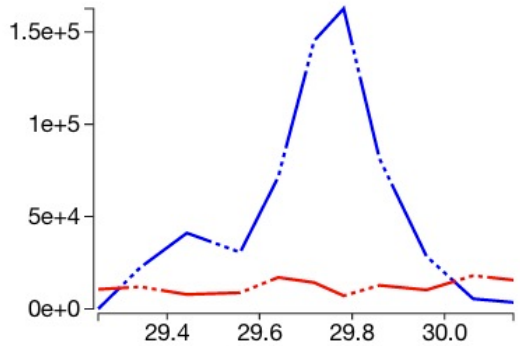
KAcSAPATGGVK**Me**2KPHR

+4 charged peptides omitted: no MS2 and peaks not overlapping/similar shape



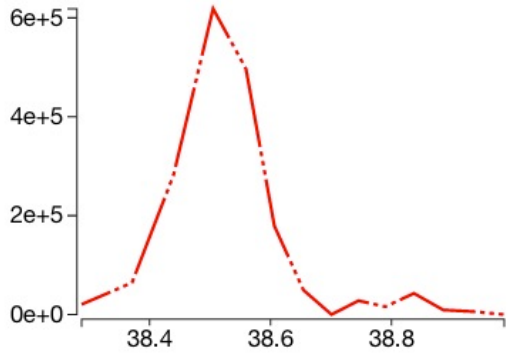
Quanti event: 29.2-30.3min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27AcK36Me2 [prop_d0]	3	539.3141	2.9e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27AcK36Me2 [pic,prop_d0]	3	560.3178	6.5e+5



Quanti event: 38.3-39.0min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27AcK36Me2 [prop_d0]	3	539.3141	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27AcK36Me2 [pic,prop_d0]	3	560.3178	6.2e+6



H3.1_K27-R40: Prop-KAcSAPATGGVKMe2KPHR MS/MS

Experimental spectrum

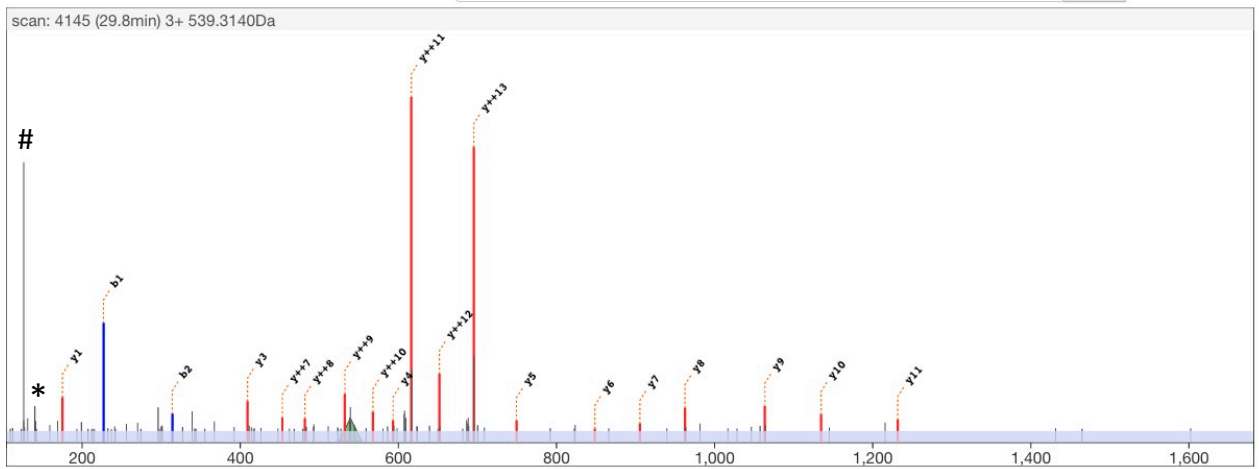
scan 4145
 retention time 29.8min
 precursor m/z 539.3140
 precursor charge 3+

Theoretical

M H³⁺ 539.3141
 MH Δ_{mass} Da -0.0005
 MH Δ_{mass} ppm -0.3

edit peptide

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



	b++	b		y	y++	
			Propionyl	1559.90	780.45	14
1	114.07	227.14	K			
			Acetyl	1389.80	695.40	13
2	157.59	314.17	S			
			A	1302.76	651.89	12
3	193.11	385.21	P	1231.73	616.37	11
			A	1134.67	567.84	10
4	241.63	482.26	T	1063.64	532.32	9
			G	962.59	481.80	8
5	277.15	553.30	V	905.57	453.29	7
			G	848.55	424.78	6
6	327.68	654.35	V	749.48	375.24	5
			Dimethyl	593.35	297.18	4
7	356.19	711.37	K	409.23	205.12	3
			Propionyl			
8	384.70	768.39	P			
			H	312.18	156.59	2
9	434.23	867.46	R	175.12	88.06	1
10	512.30	1023.58				
11	604.36	1207.70				
12	652.88	1304.76				
13	721.41	1441.82				
14	799.46	1597.92				

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

H3.1_K27-R40: PIC-KAcSAPATGGVKMe2KPHR MS/MS

Experimental spectrum

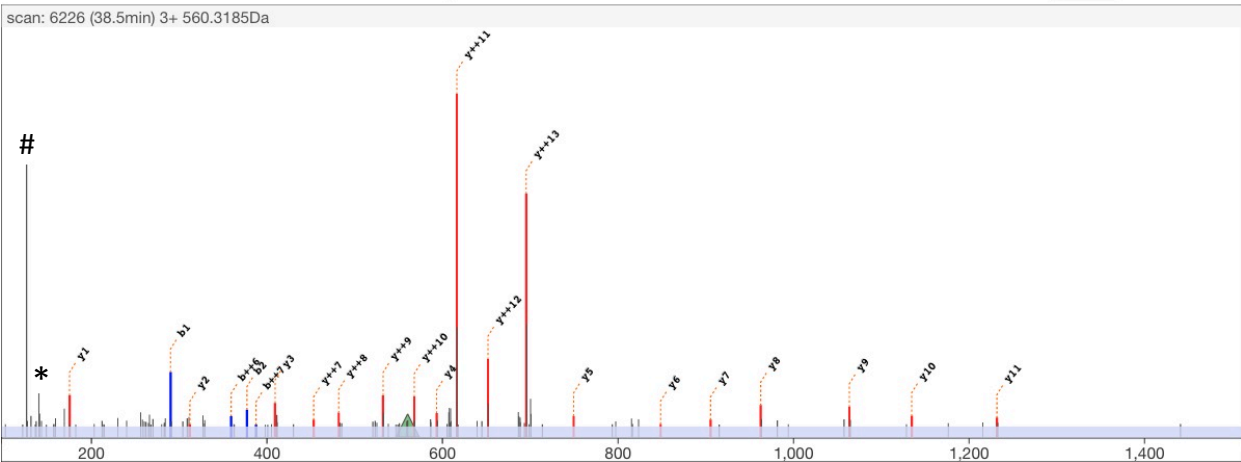
scan 6226
 retention time 38.5min
 precursor m/z 560.3185
 precursor charge 3+

Theoretical

M H³⁺ 560.3178
 MH Δ_{mass} Da 0.0023
 MH Δ_{mass} ppm 1.4

edit peptide

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



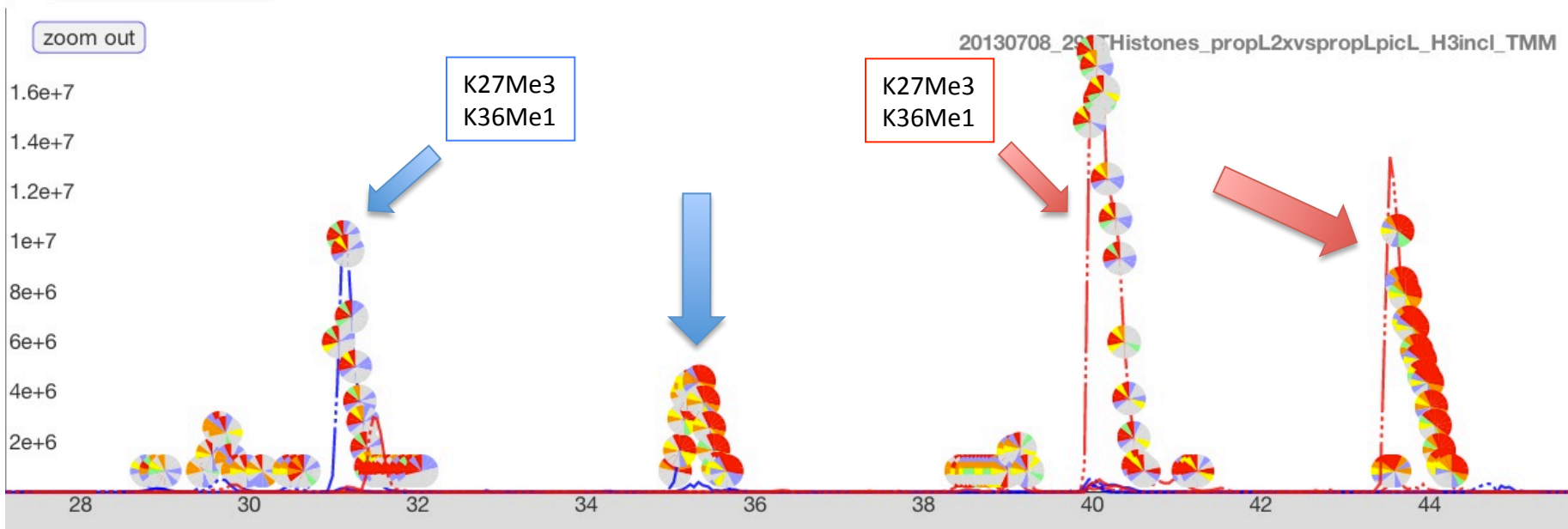
	b++	b		y	y++	
	60.53	120.04	PIC	1559.90	780.45	14
1	145.58	290.15	K	1389.80	695.40	13
2	189.09	377.18	Acetyl	1302.76	651.89	12
3	224.61	448.22	S	1231.73	616.37	11
4	273.14	545.27	A	1134.67	567.84	10
5	308.66	616.31	P	1063.64	532.32	9
6	359.18	717.36	A	962.59	481.80	8
7	387.69	774.38	T	905.57	453.29	7
8	416.20	831.40	G	848.55	424.78	6
9	465.74	930.47	V	749.48	375.24	5
10	543.80	1086.59	K	593.35	297.18	4
11	635.86	1270.72	Dimethyl	409.23	205.12	3
12	684.39	1367.77	K	312.18	156.59	2
13	752.92	1504.83	Propionyl	175.12	88.06	1
14	830.97	1660.93	P			
			H			
			R			

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

H3.1_K27-R40:

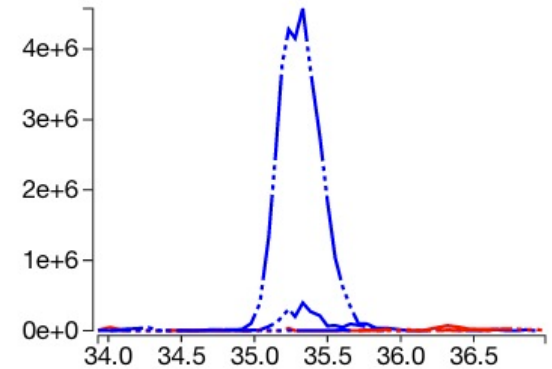
KMe1SAPATGGVKMe3KPHR

id list per inj.	peptide	2+	3+	4+	5+
20130708_293THistone	H3.1K27MeK36Me3 [prop_d0]	829.491	553.330	415.249	332.401
20130708_293THistone	H3.1K27MeK36Me3 [pic,prop_d0]	860.996	574.333	431.002	345.003



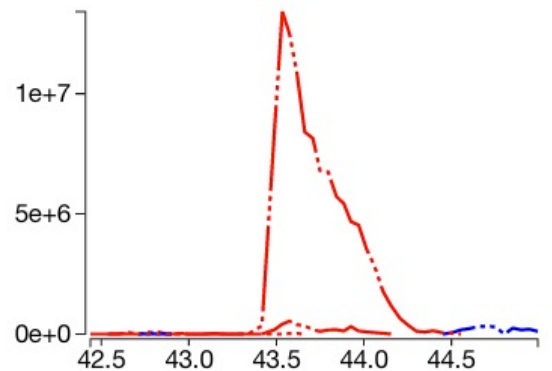
Quanti event: 33.9-37.1min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me3 [prop_d0]	2	829.4910	6.8e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me3 [pic,prop_d0]	2	860.9965	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me3 [prop_d0]	3	553.3298	9.8e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me3 [pic,prop_d0]	3	574.3334	1.4e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me3 [prop_d0]	4	415.2492	1.0e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me3 [pic,prop_d0]	4	431.0019	8.3e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me3 [prop_d0]	5	332.4008	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me3 [pic,prop_d0]	5	345.0030	0.0e+0



Quanti event: 42.4-45.0min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me3 [prop_d0]	2	829.4910	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me3 [pic,prop_d0]	2	860.9965	8.7e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me3 [prop_d0]	3	553.3298	6.1e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me3 [pic,prop_d0]	3	574.3334	2.9e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me3 [prop_d0]	4	415.2492	5.6e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me3 [pic,prop_d0]	4	431.0019	1.5e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me3 [prop_d0]	5	332.4008	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27MeK36Me3 [pic,prop_d0]	5	345.0030	0.0e+0



H3.1_K27-R40: Prop-KMe1SAPATGGVKMe3KPHR MS/MS

Experimental spectrum

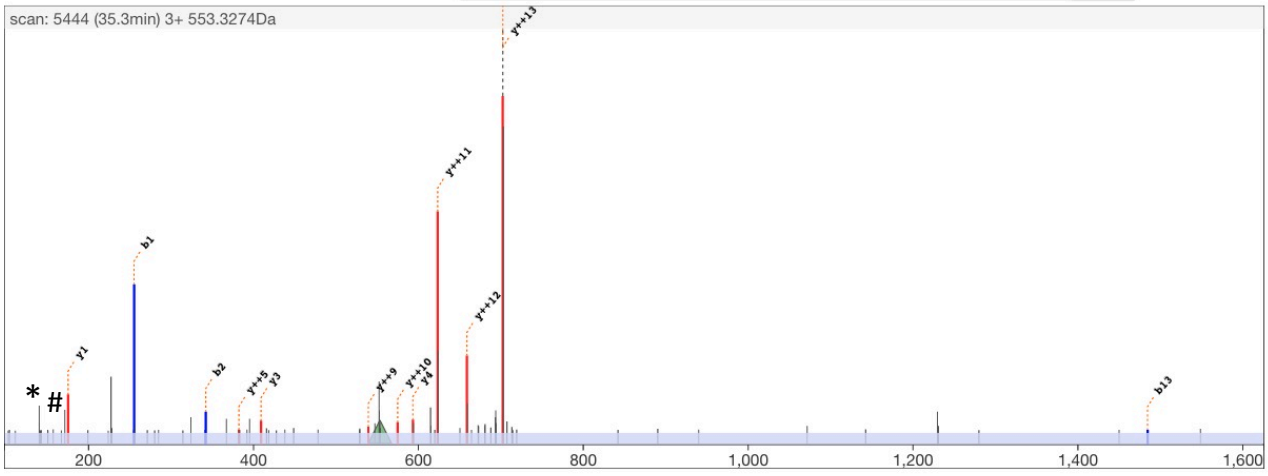
scan 5444
 retention time 35.3min
 precursor m/z 553.3274
 precursor charge 3+

Theoretical

M H³⁺ 553.3298
 MH Δ_{mass} Da -0.0072
 MH Δ_{mass} ppm -4.3

edit peptide

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



	b++	b		y	y++	
			Propionyl	1601.95	801.48	14
1	128.09	255.17	K	1403.81	702.41	13
2	171.60	342.20	Methyl,Propionyl	1316.78	658.89	12
3	207.12	413.24	S	1245.74	623.37	11
4	255.65	510.29	A	1148.69	574.85	10
5	291.17	581.33	P	1077.65	539.33	9
6	341.69	682.38	A	976.61	488.81	8
7	370.20	739.40	T	919.58	460.30	7
8	398.71	796.42	G	862.56	431.78	6
9	448.25	895.49	V	763.49	382.25	5
10	533.32	1065.63	K	593.35	297.18	4
11	625.38	1249.75	Trimethyl	409.23	205.12	3
12	673.91	1346.80	K	312.18	156.59	2
13	742.44	1483.86	Propionyl	175.12	88.06	1
14	820.49	1639.96	P			
			H			
			R			

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

H3.1_K27-R40: PIC-KMe1SAPATGGVKMe3KPHR MS/MS

Experimental spectrum

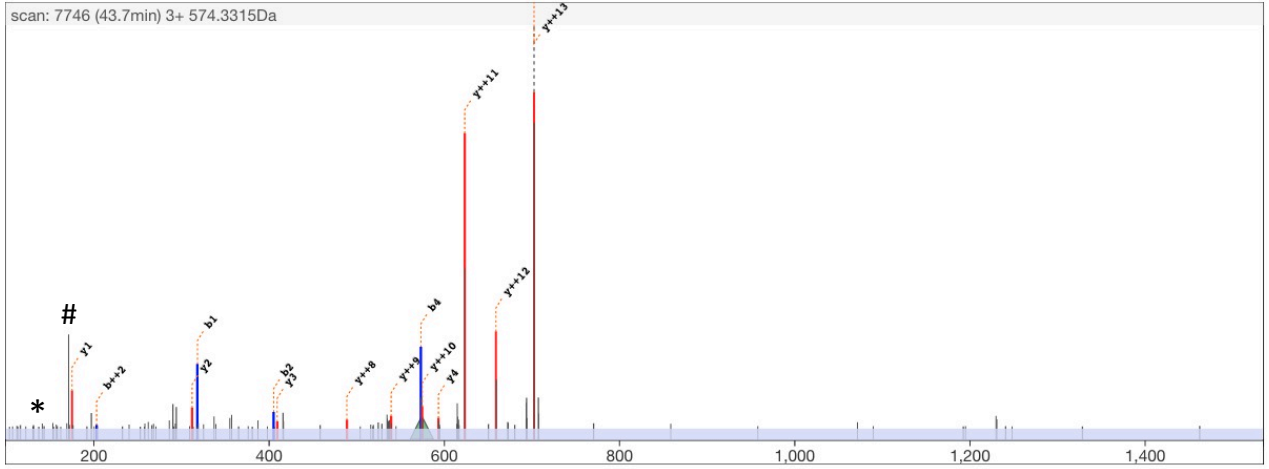
scan 7746
 retention time 43.7min
 precursor m/z 574.3315
 precursor charge 3+

Theoretical

M H³⁺ 574.3334
 MH Δ_{mass} Da -0.0058
 MH Δ_{mass} ppm -3.4

edit peptide

{PIC}K(Methyl,Propionyl)SAPATGGVK(Trimethyl)K(Propionyl)PHR



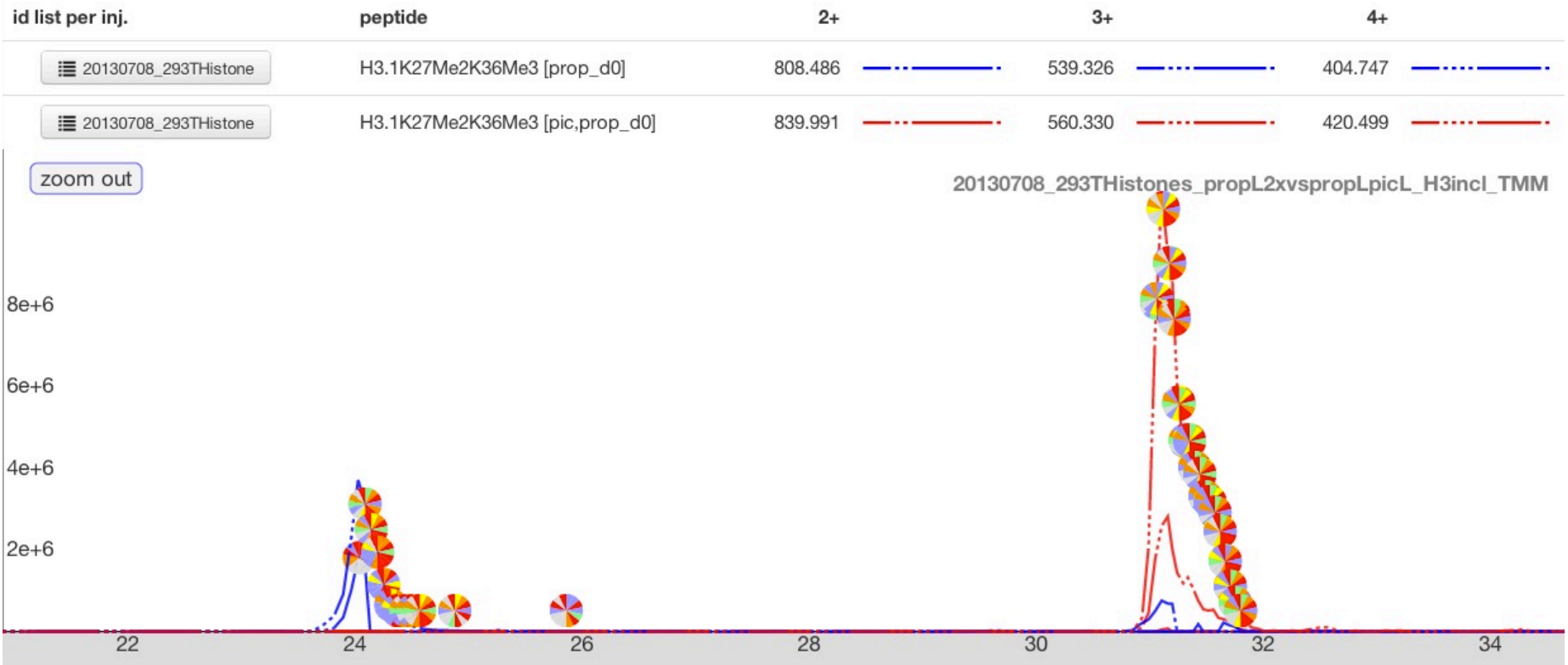
	b++	b		y	y++	
	60.53	120.04	PIC	1601.95	801.48	14
1	159.59	318.18	Methyl,Propionyl	1403.81	702.41	13
2	203.11	405.21	K	1316.78	658.89	12
3	238.63	476.25	S	1245.74	623.37	11
4	287.16	573.30	A	1148.69	574.85	10
5	322.67	644.34	P	1077.65	539.33	9
6	373.20	745.39	A	976.61	488.81	8
7	401.71	802.41	T	919.58	460.30	7
8	430.22	859.43	G	862.56	431.78	6
9	479.75	958.50	V	763.49	382.25	5
10	564.82	1128.64	K	593.35	297.18	4
11	656.88	1312.76	Trimethyl	409.23	205.12	3
12	705.41	1409.82	Propionyl	312.18	156.59	2
13	773.94	1546.87	P	175.12	88.06	1
14	851.99	1702.98	H			
			R			

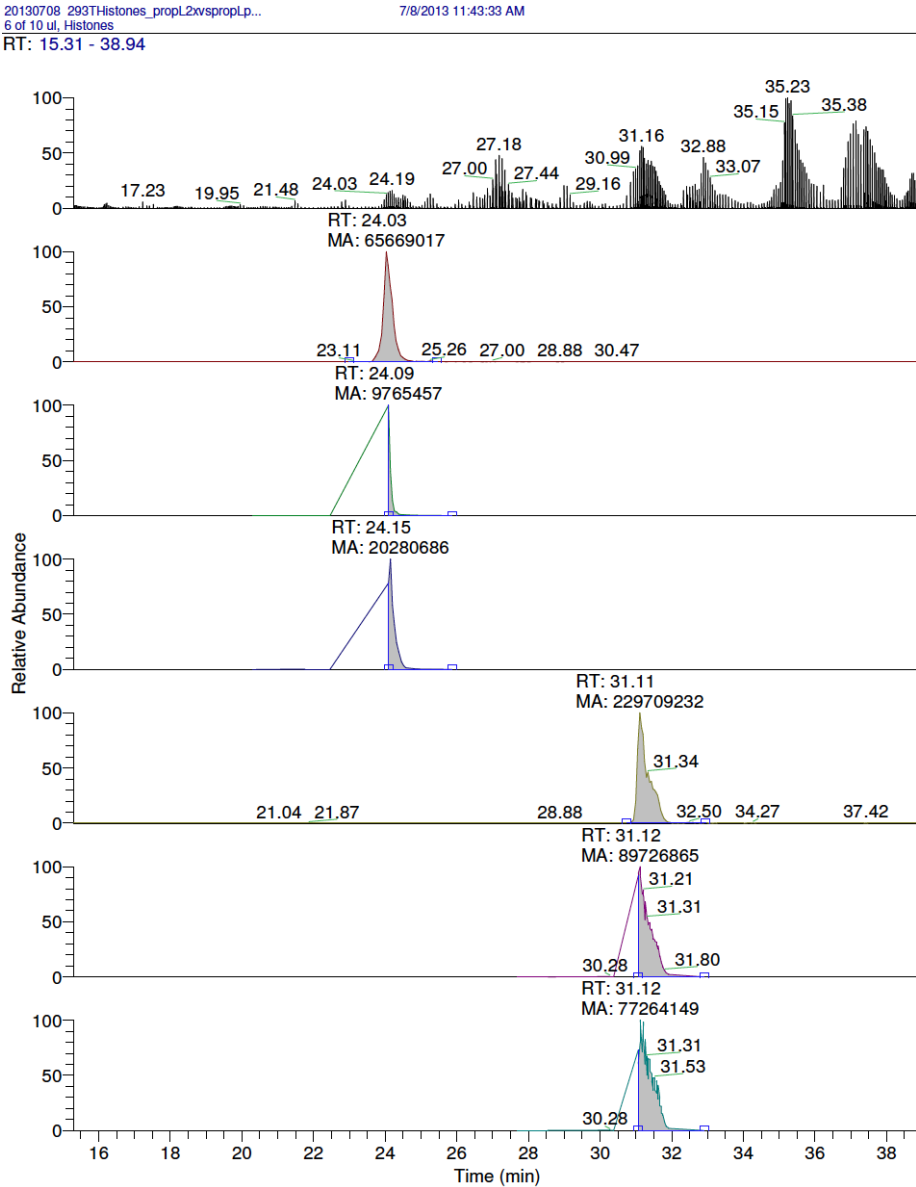
* = 140Da diagnostic ion
 # = 171Da diagnostic ion

H3.1_K27-R40:

KMe2SAPATGGVKMe3KPHR

Overlaps with K27Me3,K36me2 (see slide 296).





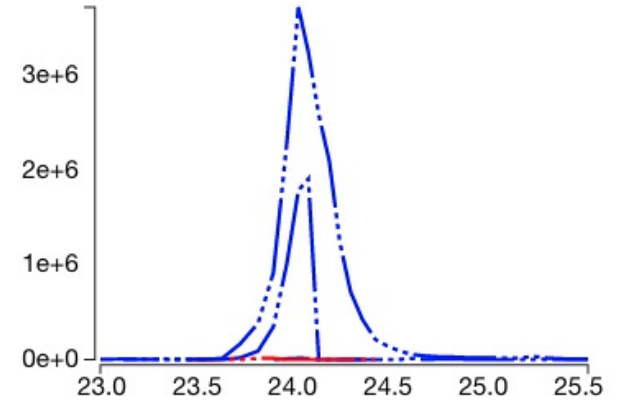
AUC calculation on MS2 level:

XIC-Prop 420.49 (4+)
 213.16, 300.19, 371.23, 488.81,
 539.33, 574.85

XIC-PIC 420.49 (4+)
 276.17, 363.20, 434.24, 488.81,
 539.33, 574.85

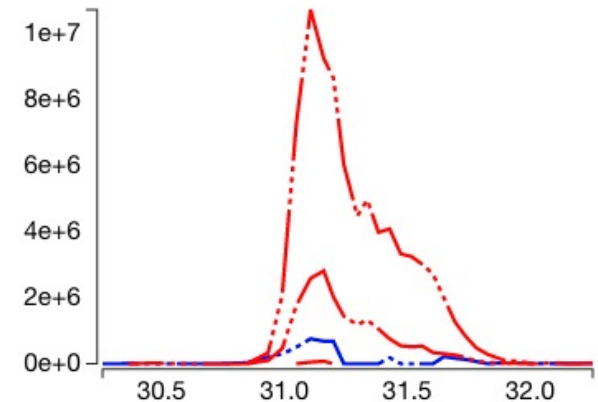
Quanti event: 23.0-25.6min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me3 [prop_d0]	2	808.4858	1.4e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me3 [pic,prop_d0]	2	839.9912	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me3 [prop_d0]	3	539.3263	1.8e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me3 [pic,prop_d0]	3	560.3299	1.8e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me3 [prop_d0]	4	404.7465	6.6e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me3 [pic,prop_d0]	4	420.4992	0.0e+0



Quanti event: 30.2-32.3min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me3 [prop_d0]	2	808.4858	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me3 [pic,prop_d0]	2	839.9912	3.7e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me3 [prop_d0]	3	539.3263	1.2e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me3 [pic,prop_d0]	3	560.3299	5.3e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me3 [prop_d0]	4	404.7465	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Me3 [pic,prop_d0]	4	420.4992	2.3e+8



H3.1_K27-R40: Prop-KMe2SAPATGGVKMe3KPHR MS/MS

Experimental spectrum

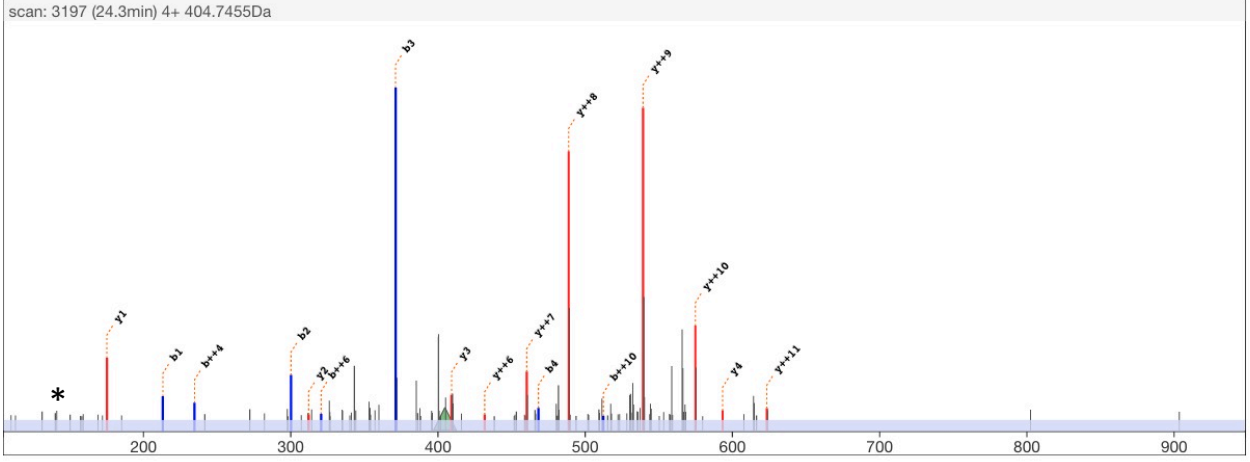
scan 3197
 retention time 24.3min
 precursor m/z 404.7455
 precursor charge 4+

Theoretical

M H⁴⁺ 404.7465
 MH Δ_{mass} Da -0.0040
 MH Δ_{mass} ppm -2.5

edit peptide

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



	b++	b		y	y++	
			Propionyl	1559.94	780.47	14
1	107.08	213.16	K	1403.81	702.41	13
2	150.60	300.19	S	1316.78	658.89	12
3	186.12	371.23	A	1245.74	623.37	11
4	234.64	468.28	P	1148.69	574.85	10
5	270.16	539.32	A	1077.65	539.33	9
6	320.69	640.37	T	976.61	488.81	8
7	349.20	697.39	G	919.58	460.30	7
8	377.71	754.41	V	862.56	431.78	6
9	427.24	853.48	G	763.49	382.25	5
10	512.31	1023.62	K	593.35	297.18	4
11	604.37	1207.74	Trimethyl	409.23	205.12	3
12	652.90	1304.79	K	312.18	156.59	2
13	721.43	1441.85	Propionyl	175.12	88.06	1
14	799.48	1597.95	P			
			H			
			R			

* = 140Da diagnostic ion

H3.1_K27-R40: PIC-KMe2SAPATGGVKMe3KPHR MS/MS

Experimental spectrum

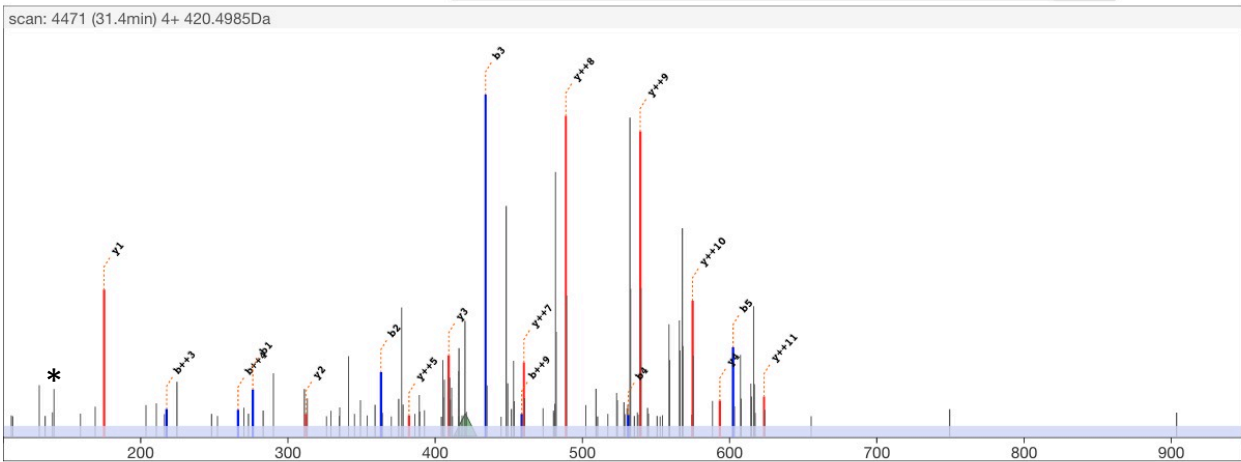
scan 4471
 retention time 31.4min
 precursor m/z 420.4985
 precursor charge 4+

Theoretical

M H⁴⁺ 420.4992
 MH Δ_{mass} Da -0.0031
 MH Δ_{mass} ppm -1.8

edit peptide

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



	b++	b		y	y++	
	60.53	120.04	PIC	1559.94	780.47	14
1	138.59	276.17	K	1403.81	702.41	13
2	182.10	363.20	S	1316.78	658.89	12
3	217.62	434.24	A	1245.74	623.37	11
4	266.15	531.29	P	1148.69	574.85	10
5	301.67	602.33	A	1077.65	539.33	9
6	352.19	703.38	T	976.61	488.81	8
7	380.70	760.40	G	919.58	460.30	7
8	409.21	817.42	G	862.56	431.78	6
9	458.75	916.49	V	763.49	382.25	5
10	543.82	1086.63	K	593.35	297.18	4
11	635.88	1270.75	K	409.23	205.12	3
12	684.41	1367.80	P	312.18	156.59	2
13	752.94	1504.86	H	175.12	88.06	1
14	830.99	1660.96	R			

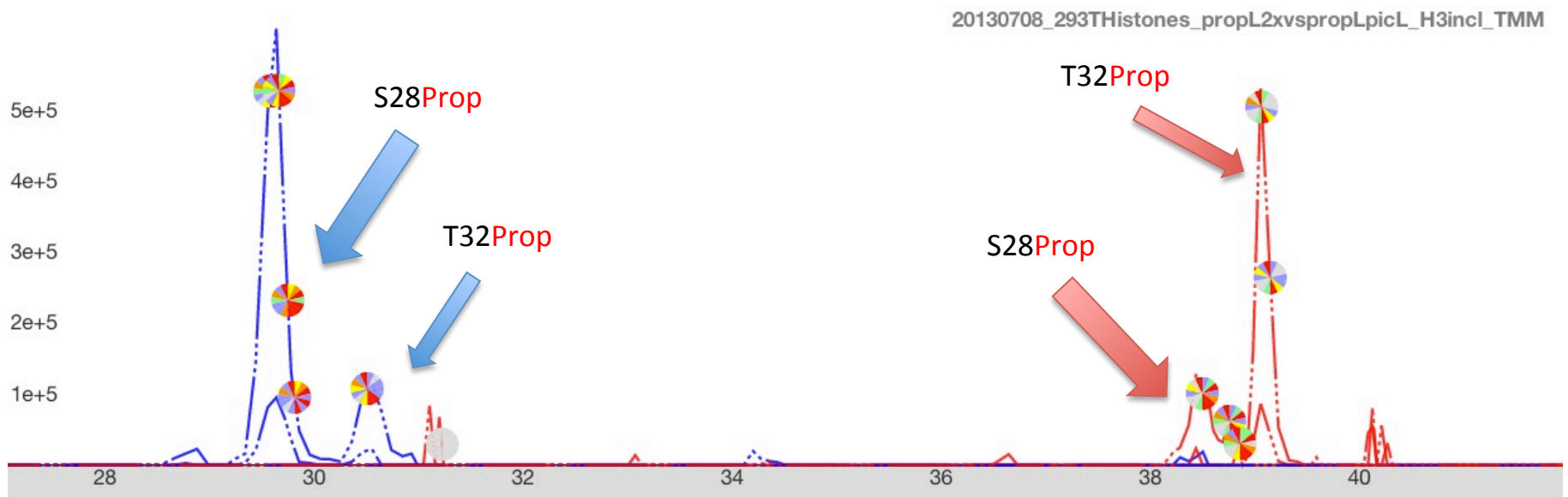
* = 140Da diagnostic ion

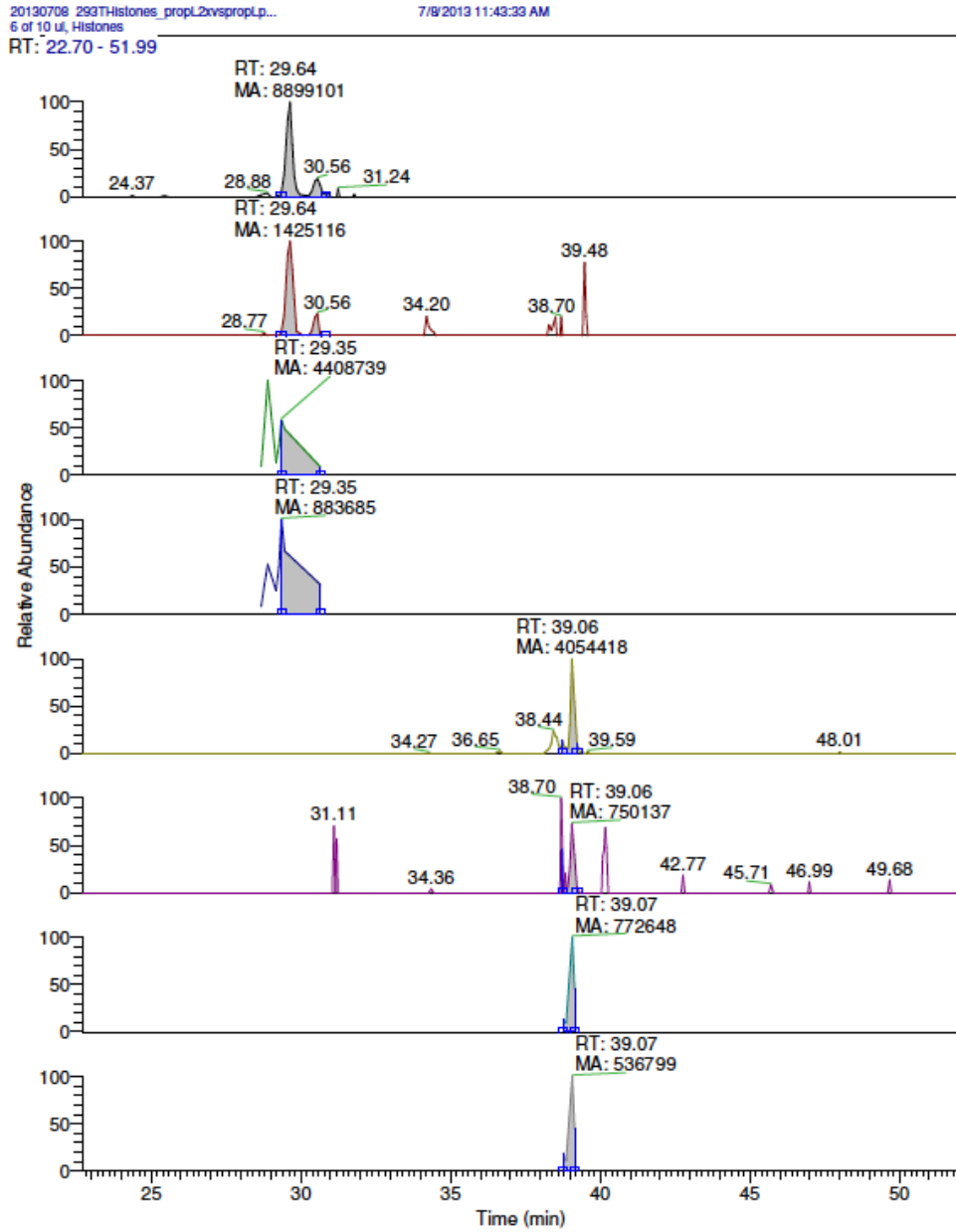
H3.1_K27-R40:

KMe2SPropAPATGGVKMe3KPHR

Overlaps with K27Me3, K36Me2, S28Prop (see page 301).

id list per inj.	peptide	2+	3+	4+
20130708_293THistone	H3.1K27Me2S28PropK36Me3 [prop_d0]	836.499	558.002	418.753
20130708_293THistone	H3.1K27Me2S28PropK36Me3 [pic,prop_d0]	868.004	579.005	434.506





AUC calculation on MS2 level:

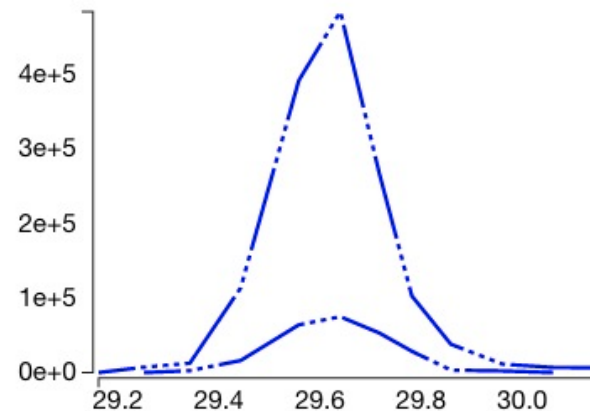
XIC-Prop 418.75 (4+)
213.16, 356.22, 427.26, 488.81,
539.33, 574.85

XIC-PIC 420.49 (4+)
276.17, 419.23, 488.81, 490.27,
539.33, 574.85

Quanti event: 29.1-30.2min

x

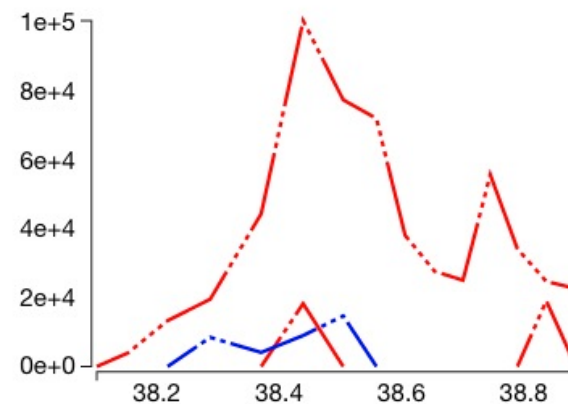
injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me3 [prop_d0]	2	836.4989	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me3 [pic,prop_d0]	2	868.0043	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me3 [prop_d0]	3	558.0017	1.2e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me3 [pic,prop_d0]	3	579.0053	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me3 [prop_d0]	4	418.7531	7.4e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me3 [pic,prop_d0]	4	434.5058	0.0e+0



Quanti event: 37.8-38.9min

x

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me3 [prop_d0]	2	836.4989	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me3 [pic,prop_d0]	2	868.0043	7.4e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me3 [prop_d0]	3	558.0017	1.5e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me3 [pic,prop_d0]	3	579.0053	5.5e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me3 [prop_d0]	4	418.7531	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2S28PropK36Me3 [pic,prop_d0]	4	434.5058	1.9e+6



H3.1_K27-R40: Prop-KMe2SPropAPATGGVKMe3KPHR MS/MS

Experimental spectrum

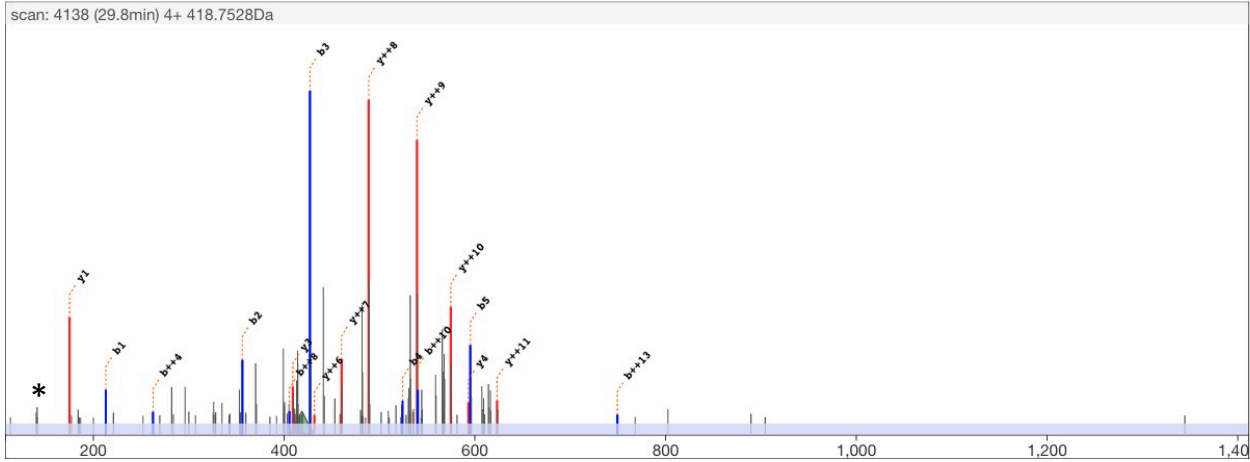
scan 4138
 retention time 29.8min
 precursor m/z 418.7528
 precursor charge 4+

Theoretical

M H⁴⁺ 418.7531
 MH Δ_{mass} Da -0.0009
 MH Δ_{mass} ppm -0.6

edit peptide

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



	b++	b		y	y++	
			Propionyl	1615.96	808.49	14
1	107.08	213.16	K			
			Dimethyl	1459.84	730.42	13
2	178.61	356.22	S			
			Propionyl	1316.78	658.89	12
3	214.13	427.26	A		623.37	11
4	262.66	524.31	P		574.85	10
5	298.18	595.34	A		539.33	9
6	348.70	696.39	T		488.81	8
7	377.21	753.41	G		460.30	7
8	405.72	810.44	V		431.78	6
9	455.26	909.50	K		382.25	5
10	540.33	1079.65	Trimethyl	593.35	297.18	4
			K			
11	632.39	1263.77	Propionyl	409.23	205.12	3
12	680.91	1360.82	P			
13	749.44	1497.88	H		175.12	2
14	827.49	1653.98	R			1

* = 140Da diagnostic ion

H3.1_K27-R40: PIC-KMe2SPropAPATGGVKMe3KPHR MS/MS

Experimental spectrum

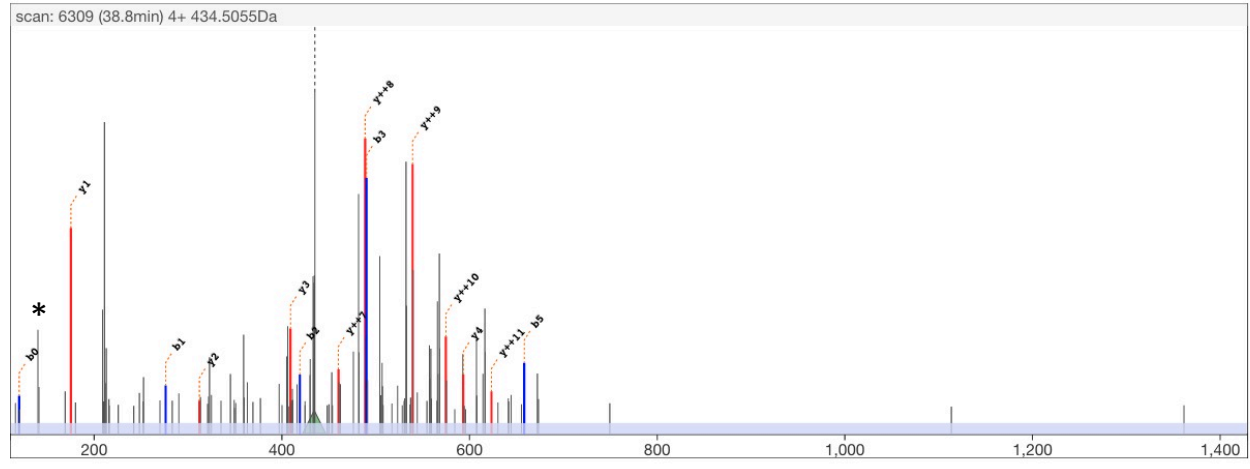
scan 6309
 retention time 38.8min
 precursor m/z 434.5055
 precursor charge 4+

Theoretical

M H⁴⁺ 434.5058
 MH Δ_{mass} Da -0.0013
 MH Δ_{mass} ppm -0.8

edit peptide

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



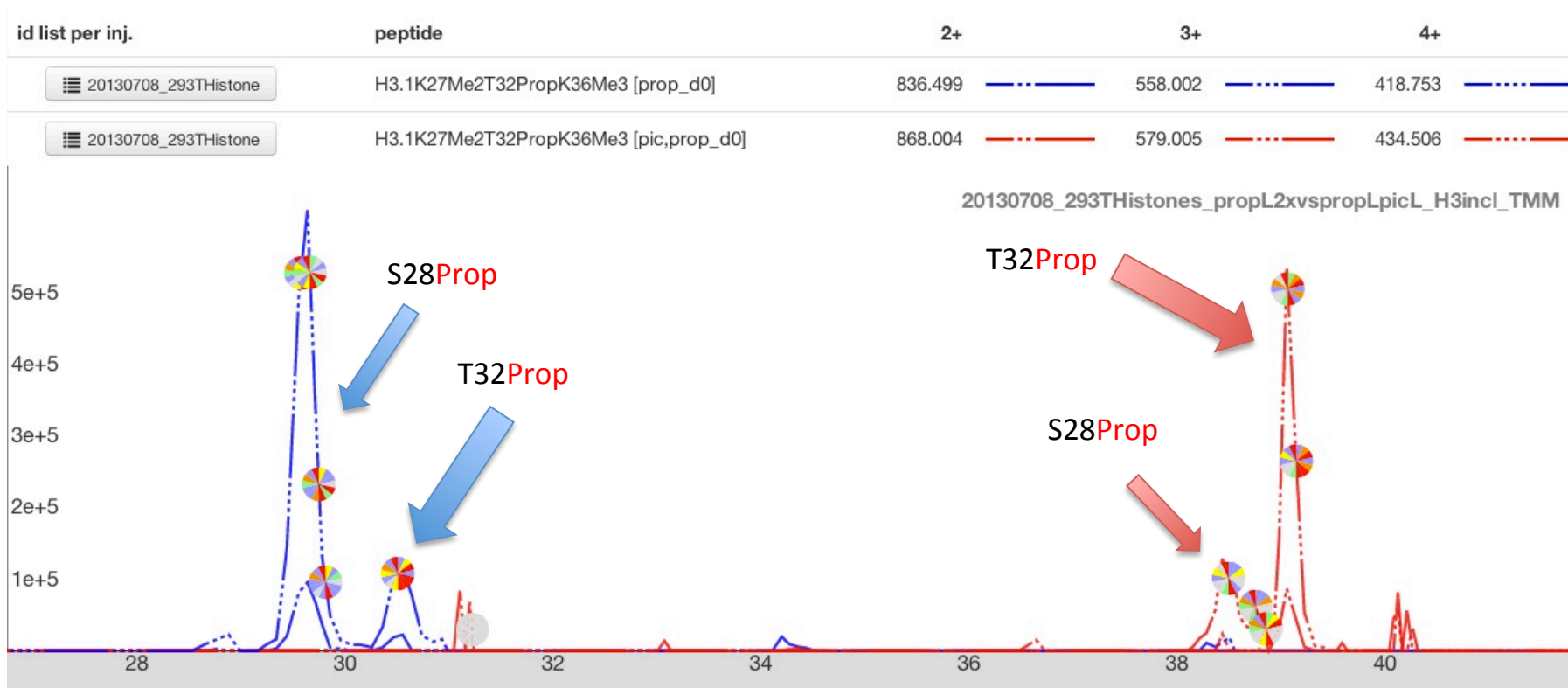
	b++	b		y	y++	
	60.53	120.04	PIC	1615.96	808.49	14
1	138.59	276.17	K	1459.84	730.42	13
2	210.12	419.23	S	1316.78	658.89	12
3	245.64	490.27	Propionyl	1245.74	623.37	11
4	294.16	587.32	A	1148.69	574.85	10
5	329.68	658.36	P	1077.65	539.33	9
6	380.21	759.40	A	976.61	488.81	8
7	408.72	816.43	T	919.58	460.30	7
8	437.23	873.45	G	862.56	431.78	6
9	486.76	972.51	V	763.49	382.25	5
10	571.83	1142.66	K	593.35	297.18	4
11	663.89	1326.78	Trimethyl	409.23	205.12	3
12	712.42	1423.83	K	312.18	156.59	2
13	780.95	1560.89	Propionyl	175.12	88.06	1
14	859.00	1716.99	P			
			H			
			R			

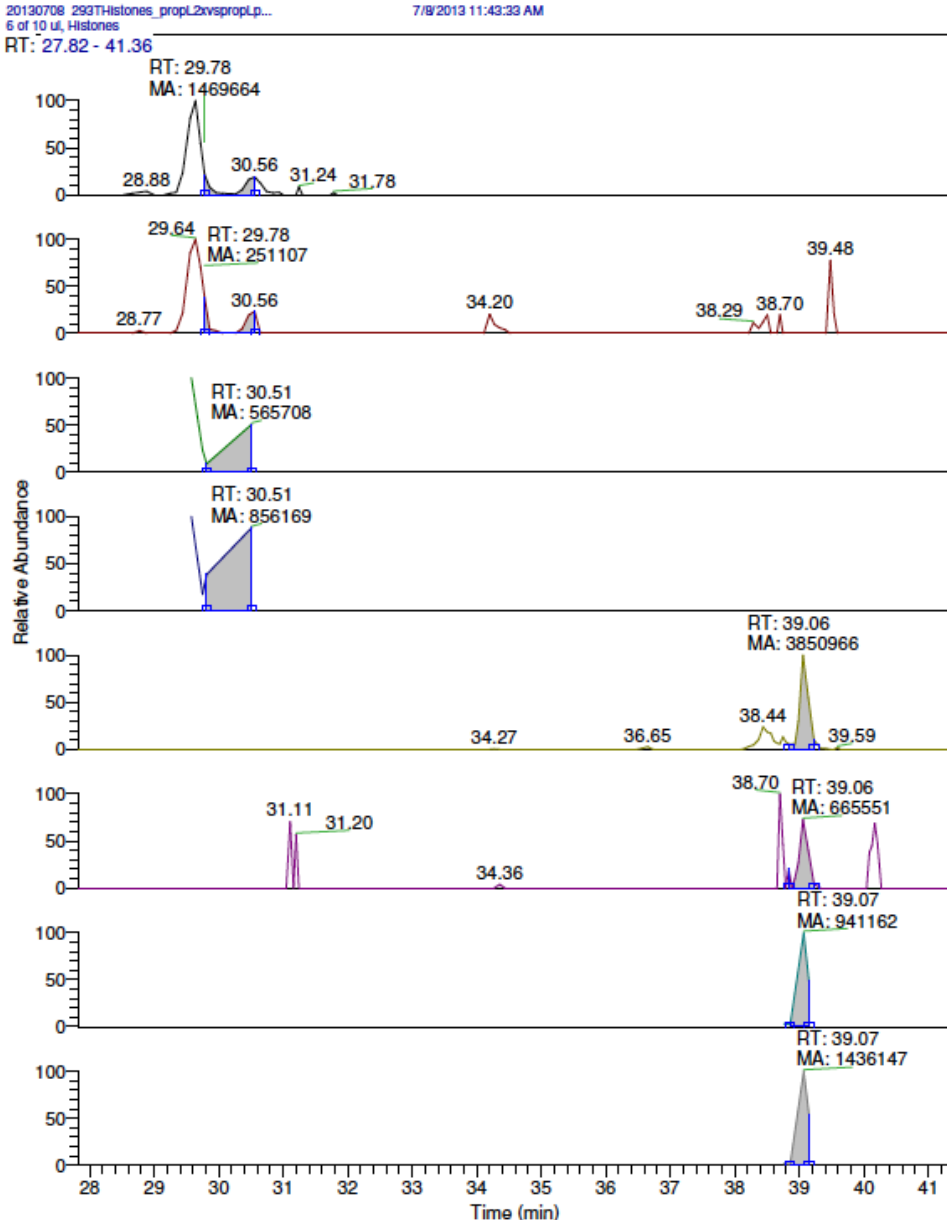
* = 140Da diagnostic ion

H3.1_K27-R40:

KMe2SAPAT**Prop**GGVK**Me3**KPHR

Overlaps with K27Me3,K36Me2,T32Prop (see page 306).





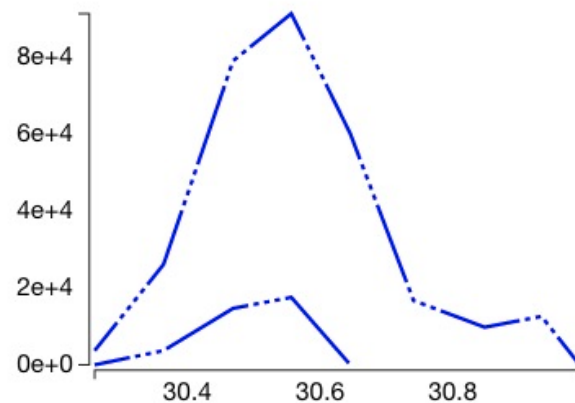
AUC calculation on MS2 level:

XIC-Prop 418.75 (4+)
 213.16, 300.19, 371.23, 488.81,
 567.34, 602.86

XIC-PIC 434.51 (4+)
 276.17, 363.20, 434.24, 488.81,
 567.34, 602.86, 651.39

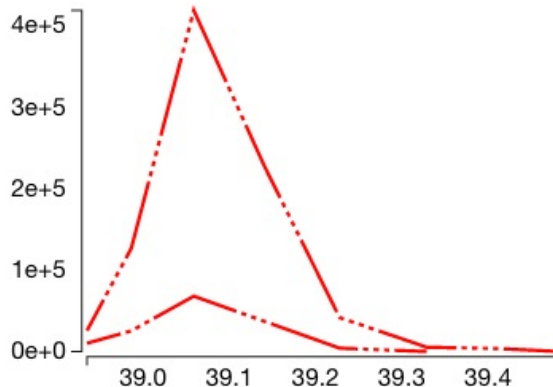
Quanti event: 30.2-31.0min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me3 [prop_d0]	2	836.4989	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me3 [pic,prop_d0]	2	868.0043	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me3 [prop_d0]	3	558.0017	2.0e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me3 [pic,prop_d0]	3	579.0053	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me3 [prop_d0]	4	418.7531	1.7e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me3 [pic,prop_d0]	4	434.5058	0.0e+0



Quanti event: 38.9-39.5min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me3 [prop_d0]	2	836.4989	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me3 [pic,prop_d0]	2	868.0043	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me3 [prop_d0]	3	558.0017	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me3 [pic,prop_d0]	3	579.0053	6.4e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me3 [prop_d0]	4	418.7531	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2T32PropK36Me3 [pic,prop_d0]	4	434.5058	3.9e+6



Experimental spectrum

scan 4266
 retention time 30.5min
 precursor m/z 418.7523
 precursor charge 4+

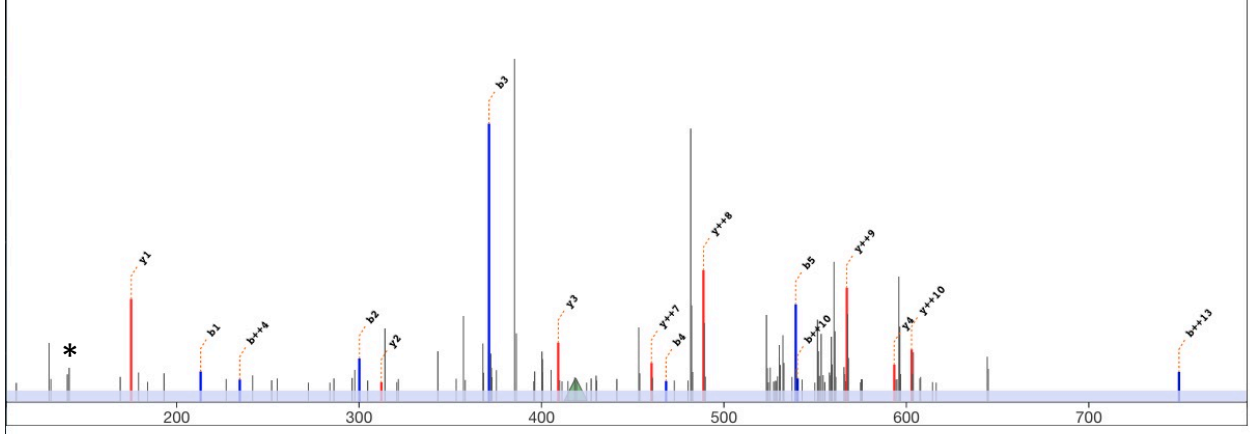
Theoretical

M H⁴⁺ 418.7531
 MH Δ_{mass} Da -0.0029
 MH Δ_{mass} ppm -1.7

edit peptide

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

scan: 4266 (30.5min) 4+ 418.7523Da



	b++	b		y	y++	
			Propionyl	1615.96	808.49	14
1	107.08	213.16	K			
			Dimethyl	1459.84	730.42	13
2	150.60	300.19	S	1372.81	686.91	12
3	186.12	371.23	A	1301.77	651.39	11
4	234.64	468.28	P	1204.72	602.86	10
5	270.16	539.32	A	1133.68	567.34	9
6	348.70	696.39	T	976.61	488.81	8
7	377.21	753.41	Propionyl	919.58	460.30	7
8	405.72	810.44	G	862.56	431.78	6
9	455.26	909.50	V	763.49	382.25	5
10	540.33	1079.65	K	593.35	297.18	4
11	632.39	1263.77	Trimethyl	409.23	205.12	3
12	680.91	1360.82	K	312.18	156.59	2
13	749.44	1497.88	Propionyl	175.12	88.06	1
14	827.49	1653.98	P			
			H			
			R			

* = 140Da diagnostic ion

H3.1_K27-R40: PIC-KMe2SAPATPropGGVKMe3KPHR MS/MS

Experimental spectrum

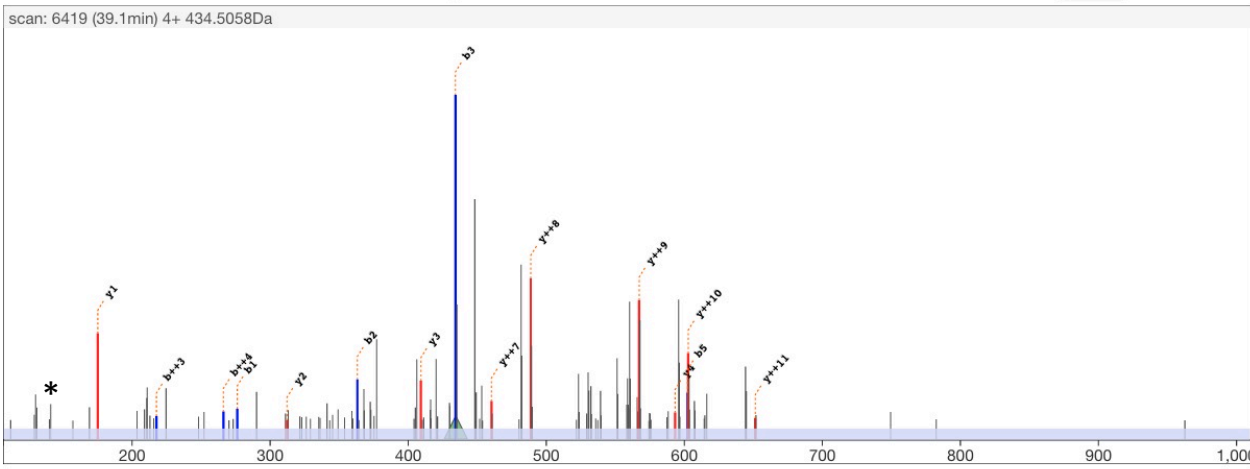
scan 6419
 retention time 39.2min
 precursor m/z 434.5058
 precursor charge 4+

Theoretical

M H⁴⁺ 434.5058
 MH Δ_{mass} Da 0.0001
 MH Δ_{mass} ppm 0.1

edit peptide

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

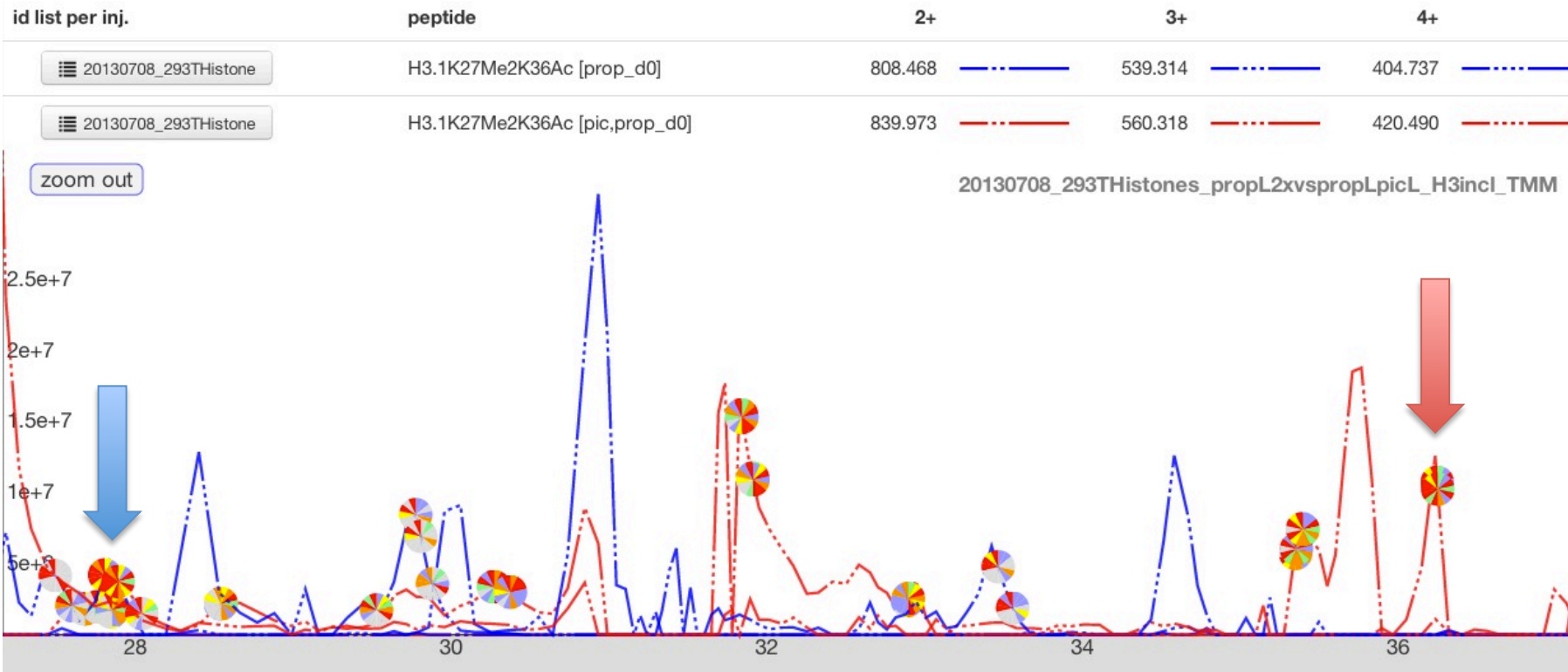


	b++	b		y	y++	
	60.53	120.04	PIC	1615.96	808.49	14
1	138.59	276.17	K	1459.84	730.42	13
2	182.10	363.20	S	1372.81	686.91	12
3	217.62	434.24	A	1301.77	651.39	11
4	266.15	531.29	P	1204.72	602.86	10
5	301.67	602.33	A	1133.68	567.34	9
6	380.21	759.40	T	976.61	488.81	8
7	408.72	816.43	G	919.58	460.30	7
8	437.23	873.45	V	862.56	431.78	6
9	486.76	972.51	K	763.49	382.25	5
10	571.83	1142.66	K	593.35	297.18	4
11	663.89	1326.78	K	409.23	205.12	3
12	712.42	1423.83	P	312.18	156.59	2
13	780.95	1560.89	H	175.12	88.06	1
14	859.00	1716.99	R			

* = 140Da diagnostic ion

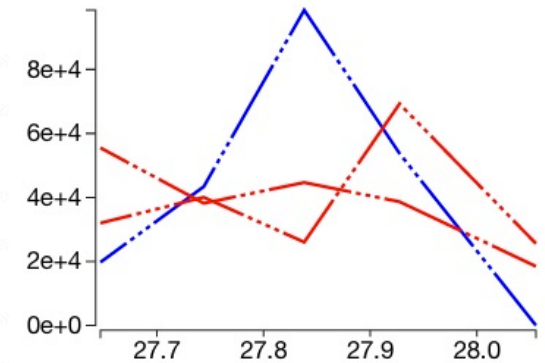
H3.1_K27-R40:

KMe2SAPATGGVKAcKPHR



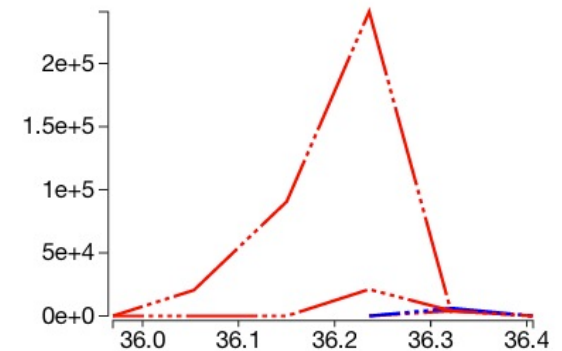
Quanti event: 27.6-28.1min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Ac [prop_d0]	2	808.4676	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Ac [pic,prop_d0]	2	839.9730	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Ac [prop_d0]	3	539.3141	1.2e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Ac [pic,prop_d0]	3	560.3178	9.5e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Ac [prop_d0]	4	404.7374	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Ac [pic,prop_d0]	4	420.4901	1.0e+6



Quanti event: 35.9-36.4min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Ac [prop_d0]	2	808.4676	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Ac [pic,prop_d0]	2	839.9730	2.1e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Ac [prop_d0]	3	539.3141	3.1e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Ac [pic,prop_d0]	3	560.3178	1.9e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Ac [prop_d0]	4	404.7374	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3.1K27Me2K36Ac [pic,prop_d0]	4	420.4901	1.3e+5



H3.1_K27-R40: Prop-KMe2SAPATGGVKAcKPHR MS/MS

Experimental spectrum

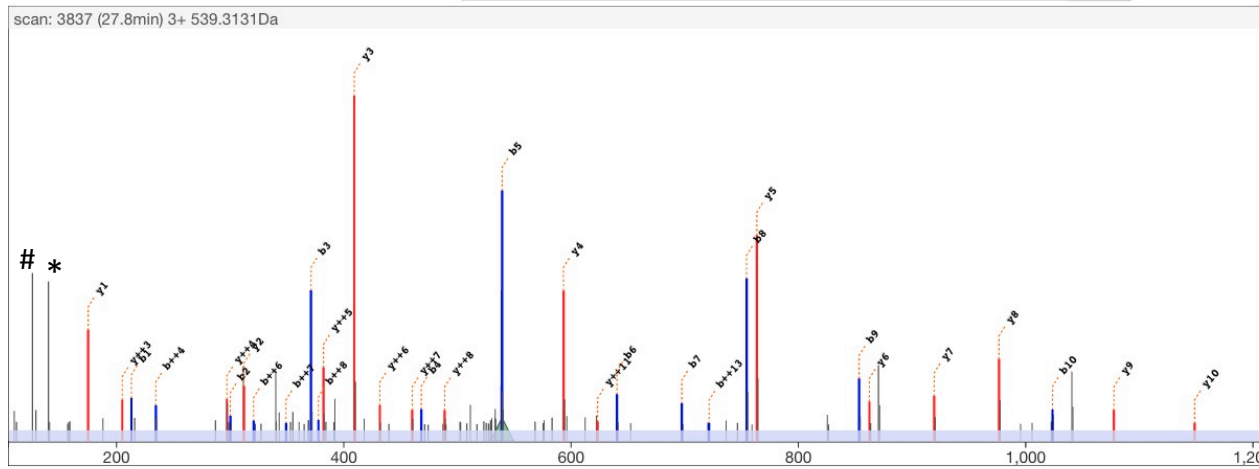
scan 3837
 retention time 27.8min
 precursor m/z 539.3131
 precursor charge 3+

Theoretical

M H³⁺ 539.3141
 MH Δ_{mass} Da -0.0031
 MH Δ_{mass} ppm -1.9

edit peptide

{Propionyl}K(Dimethyl)SAPATGGVK(Acetyl)K{Propionyl}PHR



	b++	b		y	y++	
			Propionyl	1559.90	780.45	14
1	107.08	213.16	K	1403.78	702.39	13
			Dimethyl			
2	150.60	300.19	S	1316.74	658.88	12
3	186.12	371.23	A	1245.71	623.36	11
4	234.64	468.28	P	1148.65	574.83	10
5	270.16	539.32	A	1077.62	539.31	9
6	320.69	640.37	T	976.57	488.79	8
7	349.20	697.39	G	919.55	460.28	7
8	377.71	754.41	V	862.53	431.77	6
9	427.24	853.48	K	763.46	382.23	5
10	512.30	1023.58	Acetyl	593.35	297.18	4
11	604.36	1207.70	Propionyl	409.23	205.12	3
12	652.88	1304.76	K	312.18	156.59	2
13	721.41	1441.82	P	175.12	88.06	1
14	799.46	1597.92	H			
			R			

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

Experimental spectrum

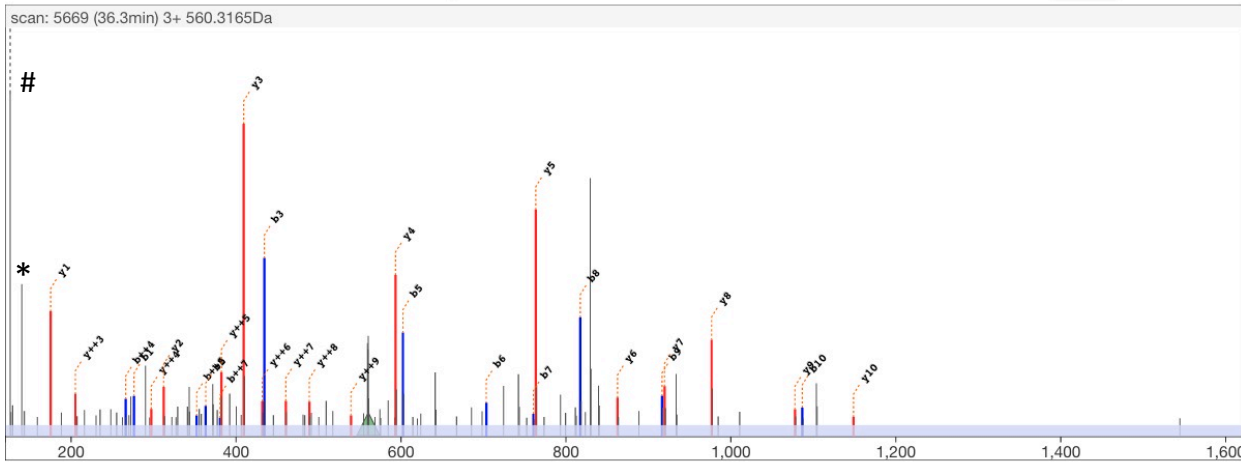
scan 5669
 retention time 36.3min
 precursor m/z 560.3165
 precursor charge 3+

Theoretical

M H³⁺ 560.3178
 MH Δ_{mass} Da -0.0037
 MH Δ_{mass} ppm -2.2

edit peptide

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



	b++	b		y	y++	
	60.53	120.04	PIC	1559.90	780.45	14
1	138.59	276.17	K	1403.78	702.39	13
2	182.10	363.20	S	1316.74	658.88	12
3	217.62	434.24	A	1245.71	623.36	11
4	266.15	531.29	P	1148.65	574.83	10
5	301.67	602.33	A	1077.62	539.31	9
6	352.19	703.38	T	976.57	488.79	8
7	380.70	760.40	G	919.55	460.28	7
8	409.21	817.42	V	862.53	431.77	6
9	458.75	916.49	K	763.46	382.23	5
10	543.80	1086.59	Acetyl	593.35	297.18	4
11	635.86	1270.72	Propionyl	409.23	205.12	3
12	684.39	1367.77	K	312.18	156.59	2
13	752.92	1504.83	P	175.12	88.06	1
14	830.97	1660.93	H			
			R			

* = 140Da diagnostic ion

= 126Da diagnostic ion