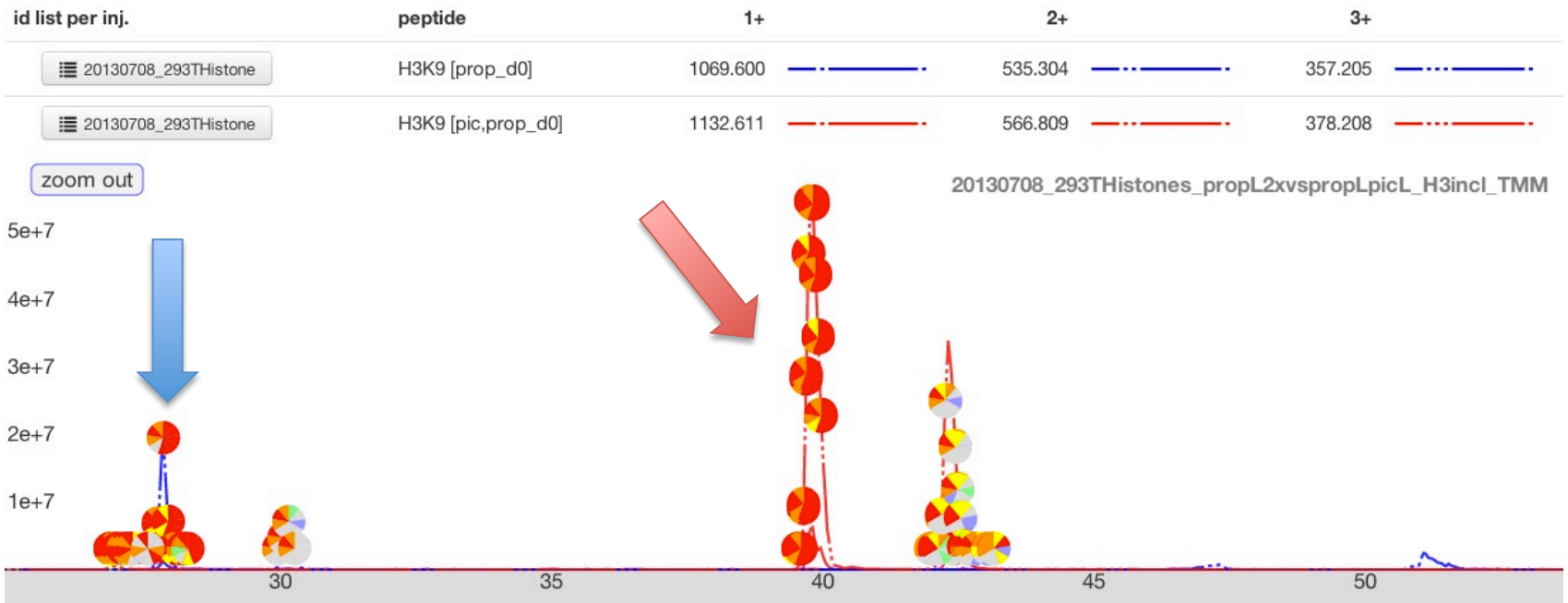


H3_K9-R17

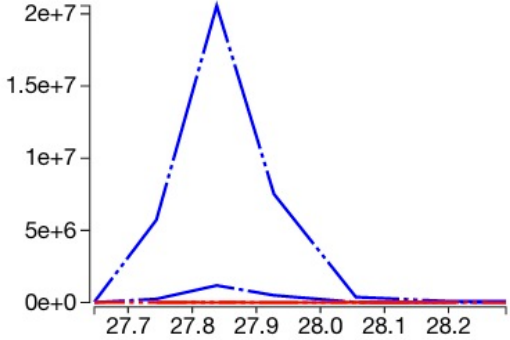
KSTGGKAPR

H3_K9-R17: KSTGGKAPR



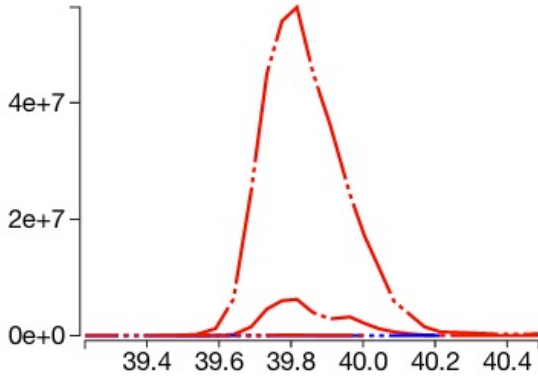
Quanti event: 27.6-28.3min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9 [prop_d0]	1	1069.6000	1.1e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9 [pic,prop_d0]	1	1132.6109	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9 [prop_d0]	2	535.3037	2.0e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9 [pic,prop_d0]	2	566.8091	1.4e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9 [prop_d0]	3	357.2049	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9 [pic,prop_d0]	3	378.2085	6.3e+4



Quanti event: 39.1-40.5min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9 [prop_d0]	1	1069.6000	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9 [pic,prop_d0]	1	1132.6109	8.8e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9 [prop_d0]	2	535.3037	6.5e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9 [pic,prop_d0]	2	566.8091	9.0e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9 [prop_d0]	3	357.2049	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9 [pic,prop_d0]	3	378.2085	9.4e+5



Experimental spectrum

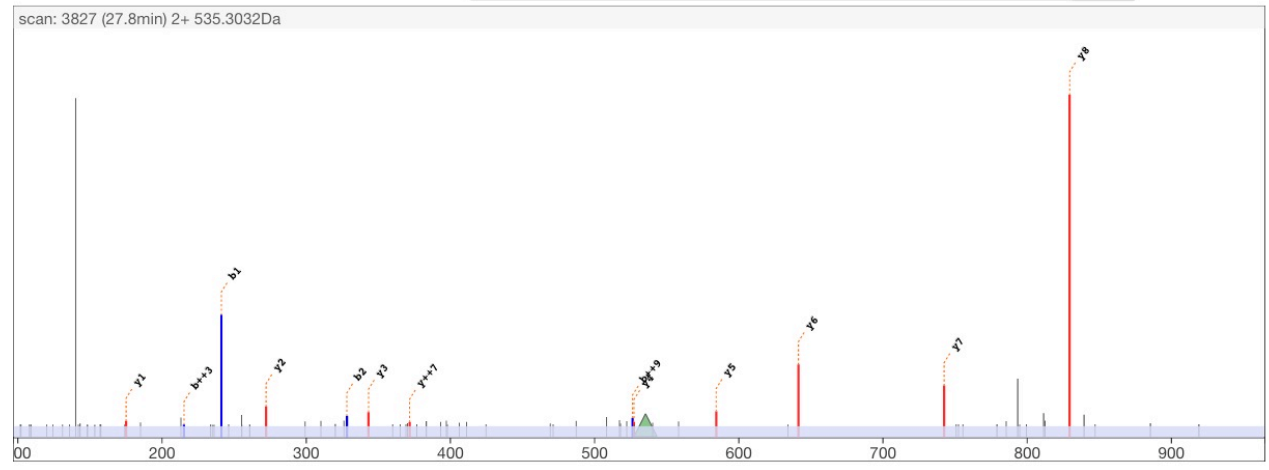
scan 3827
 retention time 27.8min
 precursor m/z 535.3032
 precursor charge 2+

Theoretical

M H²⁺ 535.3037
 MH Δ_{mass} Da -0.0010
 MH Δ_{mass} ppm -0.9

edit peptide

{Propionyl}K{Propionyl}STGGK{Propionyl}APR align



140Da diagnostic ion

	b++	b		y	y++	
			Propionyl	1013.57	507.29	9
1	121.08	241.15	K	829.45	415.23	8
2	164.60	328.19	S	742.42	371.71	7
3	215.12	429.23	T	641.37	321.19	6
4	243.63	486.26	G	584.35	292.68	5
5	272.14	543.28	G	527.33	264.17	4
6	364.20	727.40	K	343.21	172.11	3
7	399.72	798.44	Propionyl	272.17	136.59	2
8	448.25	895.49	A	175.12	88.06	1
9	526.30	1051.59	P			
			R			

H3_K9-R17: PIC-KSTGGKAPR MS/MS

Experimental spectrum

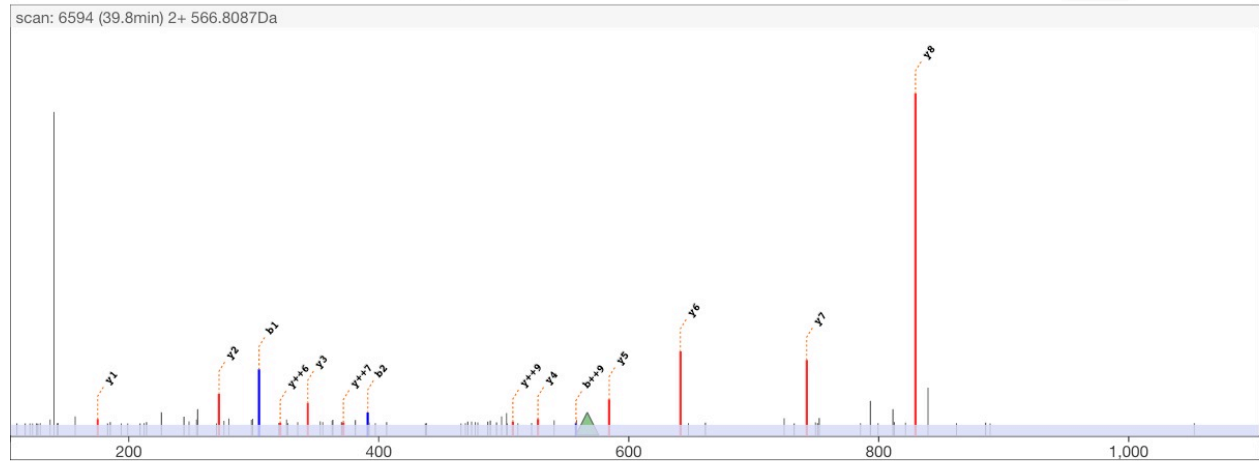
scan 6594
 retention time 39.8min
 precursor m/z 566.8087
 precursor charge 2+

Theoretical

M H²⁺ 566.8091
 MH Δ_{mass} Da -0.0008
 MH Δ_{mass} ppm -0.7

edit peptide

{PIC}K{Propionyl}STGGK{Propionyl}APR align

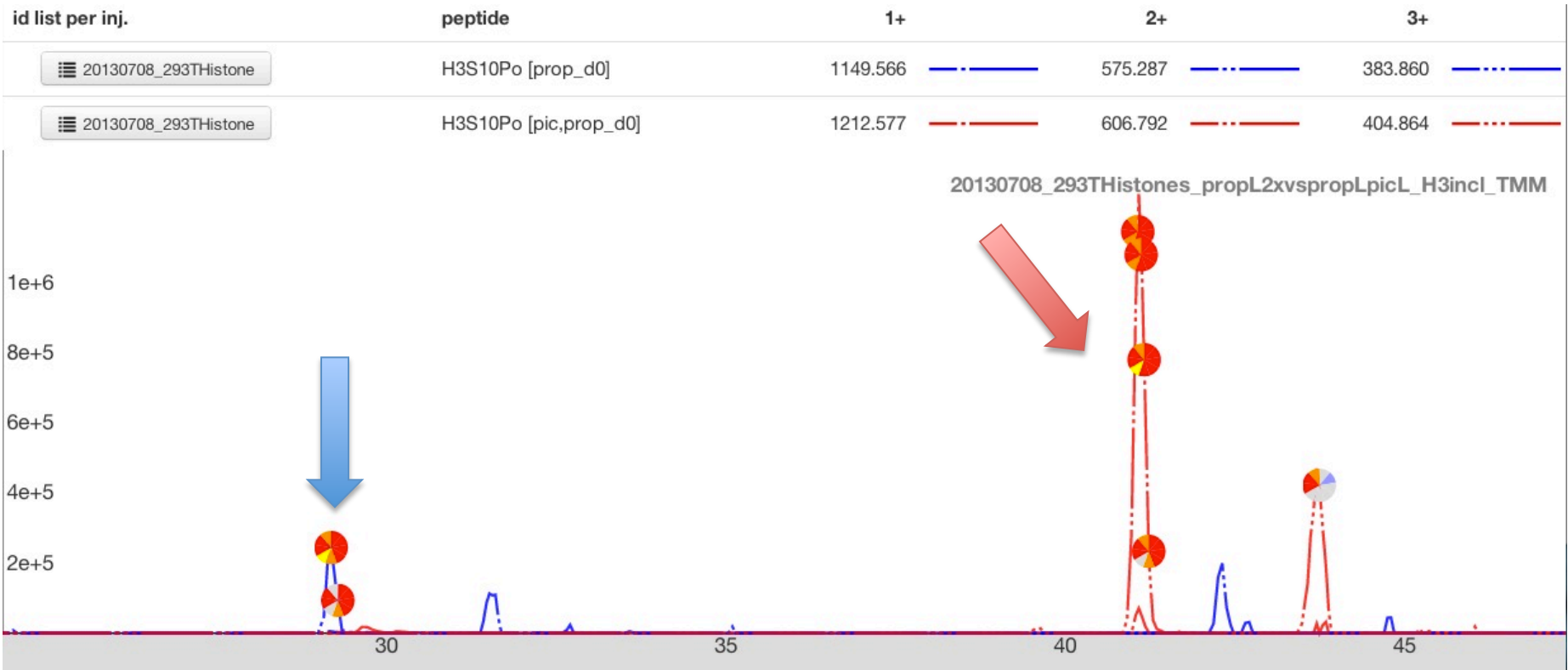


↑
 140Da diagnostic ion

	b++	b		y	y++	
	60.53	120.04	PIC	1013.57	507.29	9
1	152.59	304.17	K	829.45	415.23	8
2	196.10	391.20	Propionyl			
			S	742.42	371.71	7
3	246.63	492.25	T	641.37	321.19	6
4	275.14	549.27	G	584.35	292.68	5
5	303.65	606.29	K	527.33	264.17	4
6	395.71	790.41	Propionyl			
			K	343.21	172.11	3
7	431.23	861.45	A	272.17	136.59	2
8	479.75	958.50	P	175.12	88.06	1
9	557.80	1114.60	R			

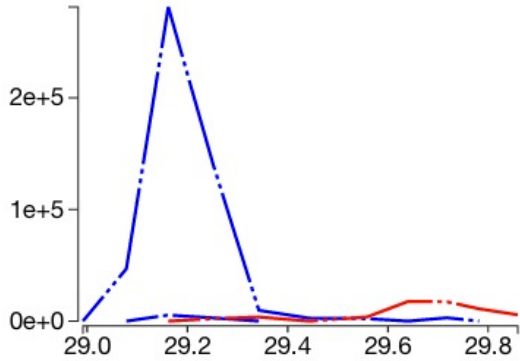
H3_K9-R17:

KS^PoTGGKAPR



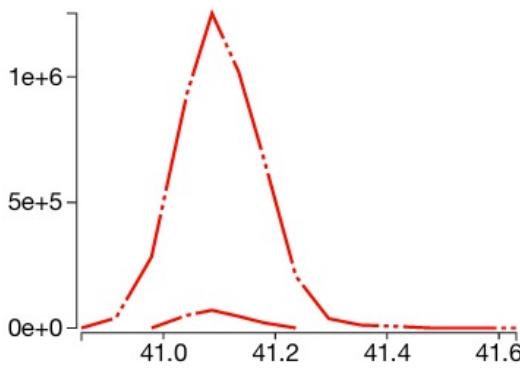
Quanti event: 28.8-29.9min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Po [prop_d0]	1	1149.5664	4.4e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Po [pic,prop_d0]	1	1212.5773	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Po [prop_d0]	2	575.2868	2.6e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Po [pic,prop_d0]	2	606.7923	2.7e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Po [prop_d0]	3	383.8603	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Po [pic,prop_d0]	3	404.8639	0.0e+0



Quanti event: 40.7-41.7min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Po [prop_d0]	1	1149.5664	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Po [pic,prop_d0]	1	1212.5773	5.6e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Po [prop_d0]	2	575.2868	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Po [pic,prop_d0]	2	606.7923	1.4e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Po [prop_d0]	3	383.8603	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Po [pic,prop_d0]	3	404.8639	0.0e+0



H3_K9-R17: Prop-KSPoTGGKAPR MS/MS

Experimental spectrum

scan 4041
 retention time 29.2min
 precursor m/z 575.2859
 precursor charge 2+

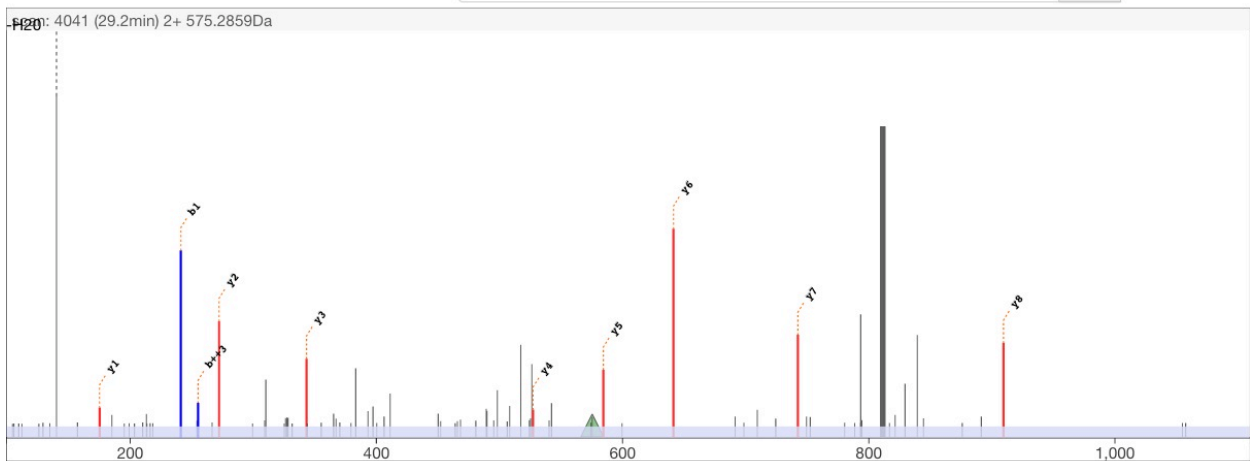
Theoretical

M H²⁺ 575.2868
 MH Δ_{mass} Da -0.0019
 MH Δ_{mass} ppm -1.6

edit peptide

{Propionyl}K{Propionyl}S{Phospho}TGGK{Propionyl}APR align

140Da diagnostic ion



Anchor		Current	
click on peak		mouse over peak	
m/z	909.4182	m/z	811.4407
intensity	5692	intensity	20427
int. rank	6	int. rank	84

Explanation?
 delta mass could be...
 $\Delta_{m/z}$ -97.97742

Tune the seq
 Align anchor peak

b2,y3,y5++

match

↑
 y8 – H3PO4

	b++	b		y	y++	
			Propionyl	1093.54	547.27	9
1	121.08	241.15	K			
			Propionyl	909.42	455.21	8
2	204.58	408.15	S			
			Phospho	742.42	371.71	7
3	255.10	509.20	T			
			G	641.37	321.19	6
4	283.61	566.22	K			
			Propionyl	584.35	292.68	5
5	312.13	623.24	K			
			Propionyl	527.33	264.17	4
6	404.19	807.36	K			
			Propionyl	343.21	172.11	3
7	439.70	878.40	A			
			P	272.17	136.59	2
8	488.23	975.45	R			
				175.12	88.06	1
9	566.28	1131.56				

140Da diagnostic ion



Experimental spectrum

scan 7004
 retention time 41.1min
 precursor m/z 606.7916
 precursor charge 2+

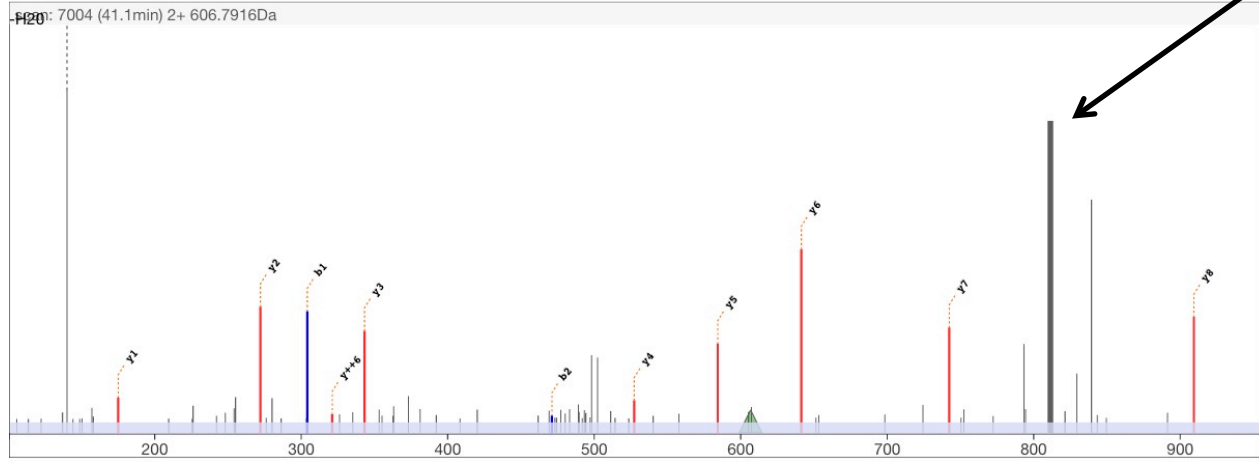
Theoretical

M H²⁺ 606.7923
 MH Δ_{mass} Da -0.0014
 MH Δ_{mass} ppm -1.2

edit peptide

{PIC}K{Propionyl}S{Phospho}TGGK{Propionyl}APR align

y8 – H3PO4



	b++	b		y	y++	
	60.53	120.04	PIC	1093.54	547.27	9
1	152.59	304.17	K	909.42	455.21	8
2	236.09	471.16	S	742.42	371.71	7
3	286.61	572.21	Phospho	641.37	321.19	6
4	315.12	629.23	T	584.35	292.68	5
5	343.63	686.25	G	527.33	264.17	4
6	435.69	870.38	K	343.21	172.11	3
7	471.21	941.41	Propionyl	272.17	136.59	2
8	519.74	1038.47	A	175.12	88.06	1
9	597.79	1194.57	P			
			R			

Anchor

click on peak
 m/z 909.4173
 intensity 26401
 int. rank 4

Current

mouse over peak
 m/z 811.4409
 intensity 75425
 int. rank 75

Explanation?

delta mass could be...
 Δ_{m/z} -97.97644

Tune the seq

Align anchor peak

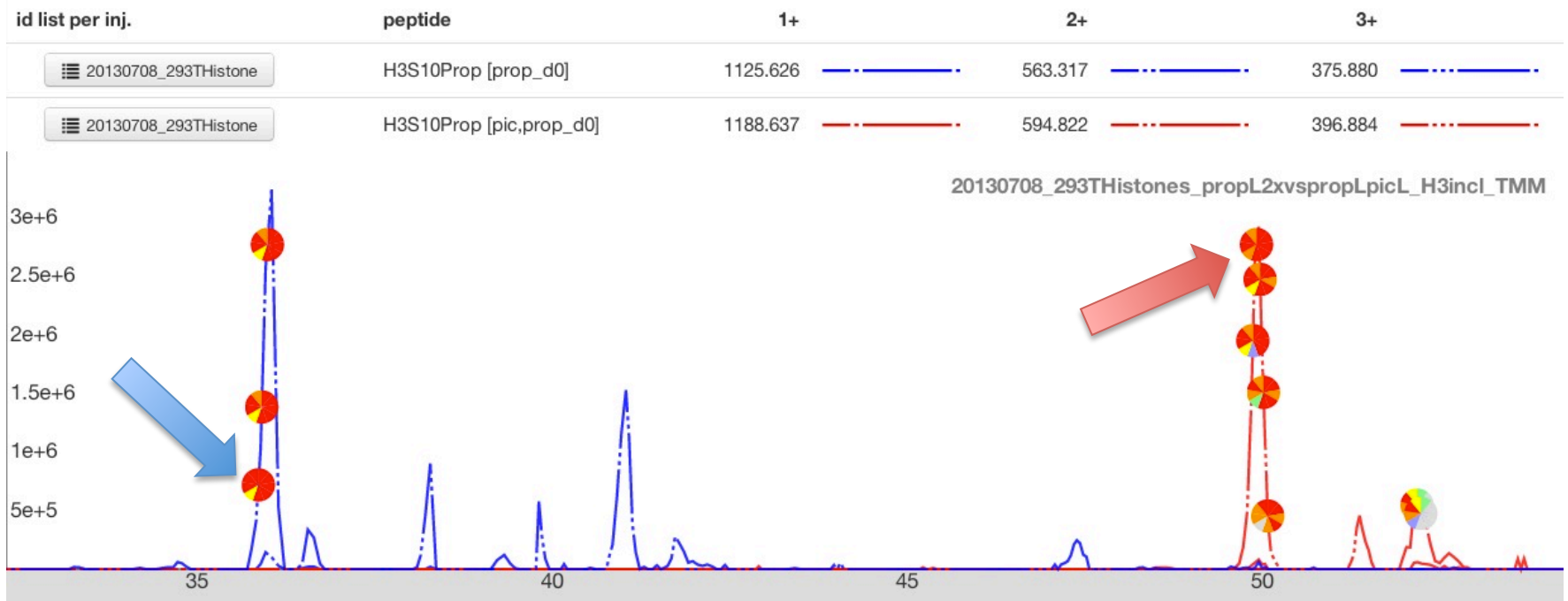
b2,y3,y5++

match

H3_K9-R17:

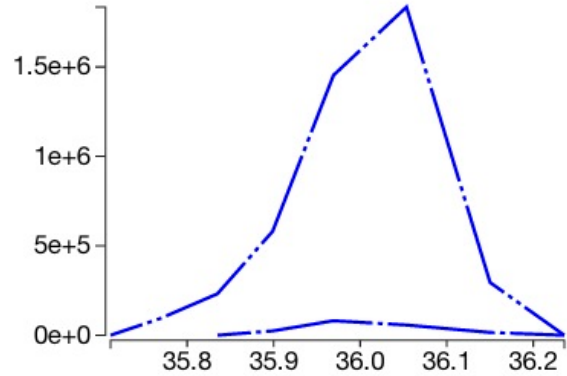
KSPropTGGKAPR

Mixed peaks for S10/T11-propionylation, only S10-prop data shown.



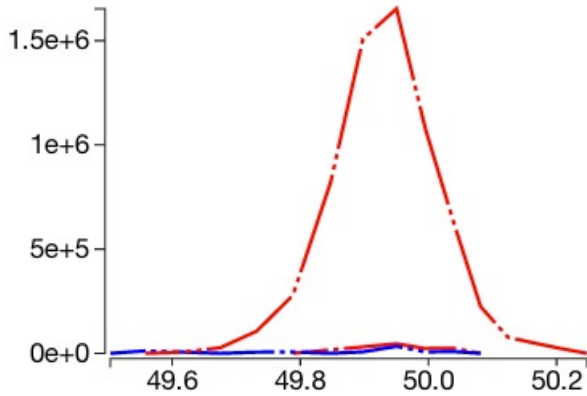
Quanti event: 35.7-36.3min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Prop [prop_d0]	1	1125.6263	8.7e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Prop [pic,prop_d0]	1	1188.6372	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Prop [prop_d0]	2	563.3168	2.2e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Prop [pic,prop_d0]	2	594.8222	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Prop [prop_d0]	3	375.8803	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Prop [pic,prop_d0]	3	396.8839	0.0e+0



Quanti event: 49.5-50.3min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Prop [prop_d0]	1	1125.6263	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Prop [pic,prop_d0]	1	1188.6372	4.1e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Prop [prop_d0]	2	563.3168	2.7e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Prop [pic,prop_d0]	2	594.8222	1.9e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Prop [prop_d0]	3	375.8803	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10Prop [pic,prop_d0]	3	396.8839	0.0e+0



Experimental spectrum

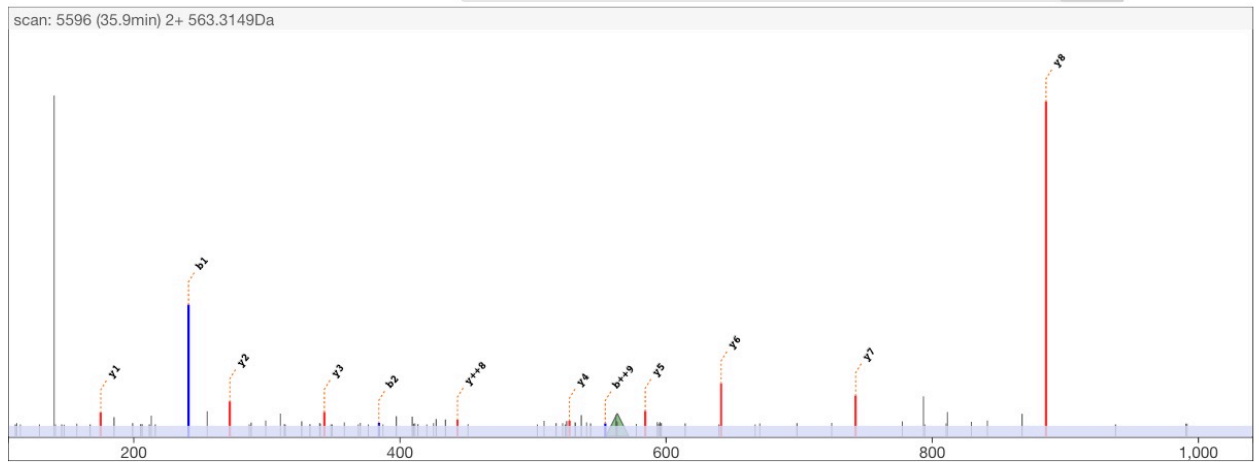
scan 5596
 retention time 35.9min
 precursor m/z 563.3149
 precursor charge 2+

Theoretical

M H²⁺ 563.3168
 MH Δ_{mass} Da -0.0036
 MH Δ_{mass} ppm -3.2

edit peptide

{Propionyl}K{Propionyl}S{Propionyl}TGGK{Propionyl}APR align



140Da diagnostic ion

	b++	b		y	y++	
			Propionyl	1069.60	535.30	9
1	121.08	241.15	K			
			Propionyl	885.48	443.24	8
2	192.61	384.21	S			
			Propionyl	742.42	371.71	7
3	243.13	485.26	T			
			G	641.37	321.19	6
4	271.64	542.28	G	584.35	292.68	5
			K	527.33	264.17	4
5	300.16	599.30	Propionyl			
6	392.22	783.42	A	343.21	172.11	3
			P	272.17	136.59	2
7	427.73	854.46	R	175.12	88.06	1
8	476.26	951.51				
9	554.31	1107.62				

Experimental spectrum

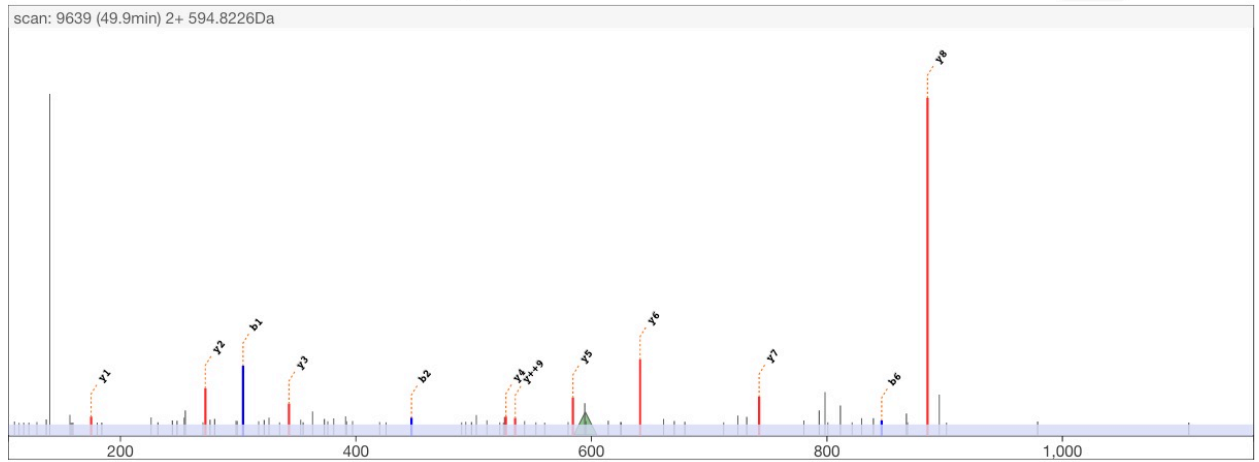
scan 9639
 retention time 49.9min
 precursor m/z 594.8226
 precursor charge 2+

Theoretical

M H²⁺ 594.8222
 MH Δ_{mass} Da 0.0008
 MH Δ_{mass} ppm 0.7

edit peptide

{PIC}K{Propionyl}S{Propionyl}TGGK{Propionyl}APR

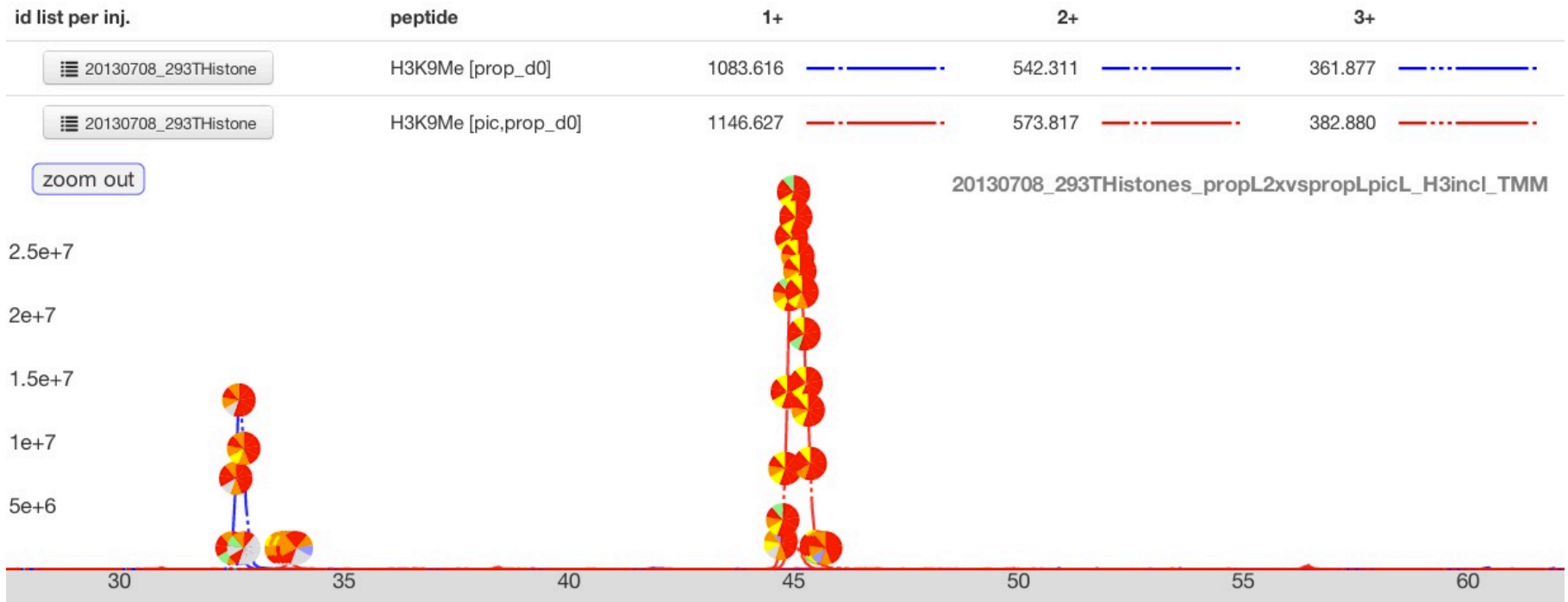


140Da diagnostic ion

	b++	b		y	y++	
	60.53	120.04	PIC	1069.60	535.30	9
1	152.59	304.17	K	885.48	443.24	8
2	224.12	447.22	Propionyl S	742.42	371.71	7
3	274.64	548.27	T	641.37	321.19	6
4	303.15	605.29	G	584.35	292.68	5
5	331.66	662.31	G	527.33	264.17	4
6	423.72	846.44	Propionyl K	343.21	172.11	3
7	459.24	917.47	A	272.17	136.59	2
8	507.77	1014.53	P	175.12	88.06	1
9	585.82	1170.63	R			

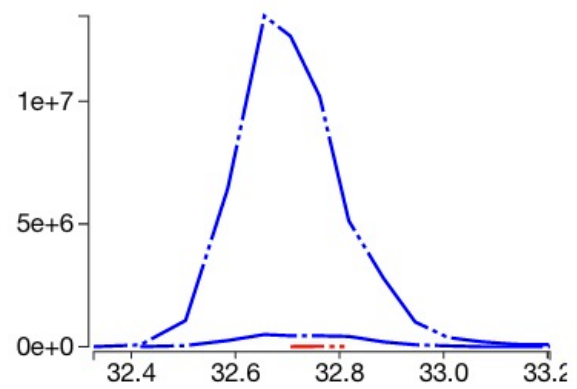
H3_K9-R17:

KMe1STGGKAPR



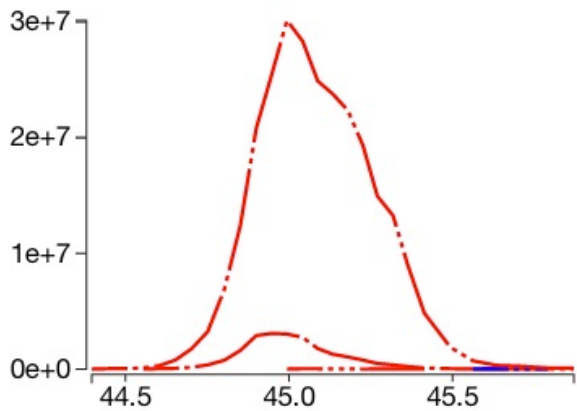
Quanti event: 32.3-33.3min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me [prop_d0]	1	1083.6157	8.8e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me [pic,prop_d0]	1	1146.6266	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me [prop_d0]	2	542.3115	1.9e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me [pic,prop_d0]	2	573.8169	5.8e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me [prop_d0]	3	361.8767	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me [pic,prop_d0]	3	382.8804	0.0e+0



Quanti event: 44.3-45.9min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me [prop_d0]	1	1083.6157	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me [pic,prop_d0]	1	1146.6266	6.0e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me [prop_d0]	2	542.3115	9.1e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me [pic,prop_d0]	2	573.8169	7.6e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me [prop_d0]	3	361.8767	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me [pic,prop_d0]	3	382.8804	3.7e+5



H3_K9-R17: Prop-KMe1STGGKAPR MS/MS

Experimental spectrum

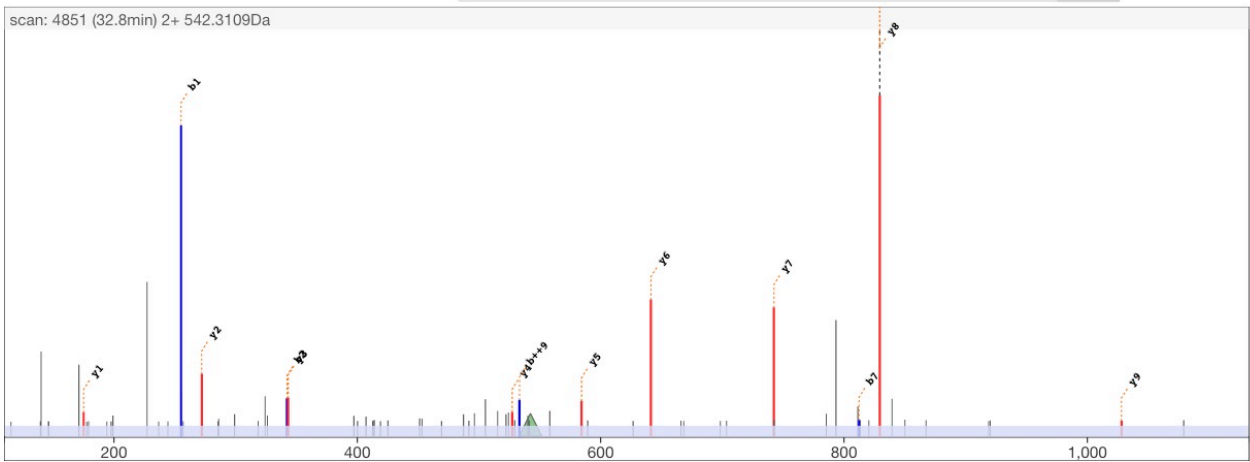
scan 4851
 retention time 32.8min
 precursor m/z 542.3109
 precursor charge 2+

Theoretical

M H²⁺ 542.3115
 MH Δ_{mass} Da -0.0011
 MH Δ_{mass} ppm -1.0

edit peptide

{Propionyl}K[Methyl,Propionyl]STGGK{Propionyl}APR align



↑
 140Da diagnostic ion

↙
 171Da diagnostic ion

	b++	b		y	y++	
			Propionyl	1027.59	514.30	9
1	128.09	255.17	K	829.45	415.23	8
2	171.60	342.20	Methyl,Propionyl	742.42	371.71	7
3	222.13	443.25	S	641.37	321.19	6
4	250.64	500.27	T	584.35	292.68	5
5	279.15	557.29	G	527.33	264.17	4
6	371.21	741.41	G	343.21	172.11	3
7	406.73	812.45	K	272.17	136.59	2
8	455.26	909.50	Propionyl	175.12	88.06	1
9	533.31	1065.61	A			
			P			
			R			

H3_K9-R17: Prop-KMe1STGGKAPR MS/MS

Experimental spectrum

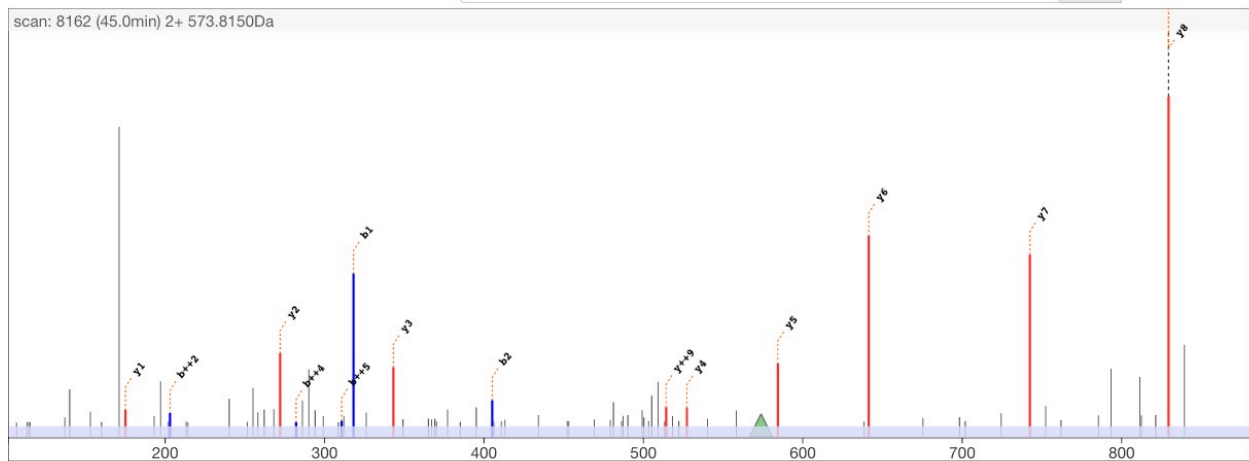
scan 8162
 retention time 45.0min
 precursor m/z 573.8150
 precursor charge 2+

Theoretical

M H²⁺ 573.8169
 MH Δ_{mass} Da -0.0039
 MH Δ_{mass} ppm -3.4

edit peptide

{PIC}K{Methyl,Propionyl}STGGK{Propionyl}APR align



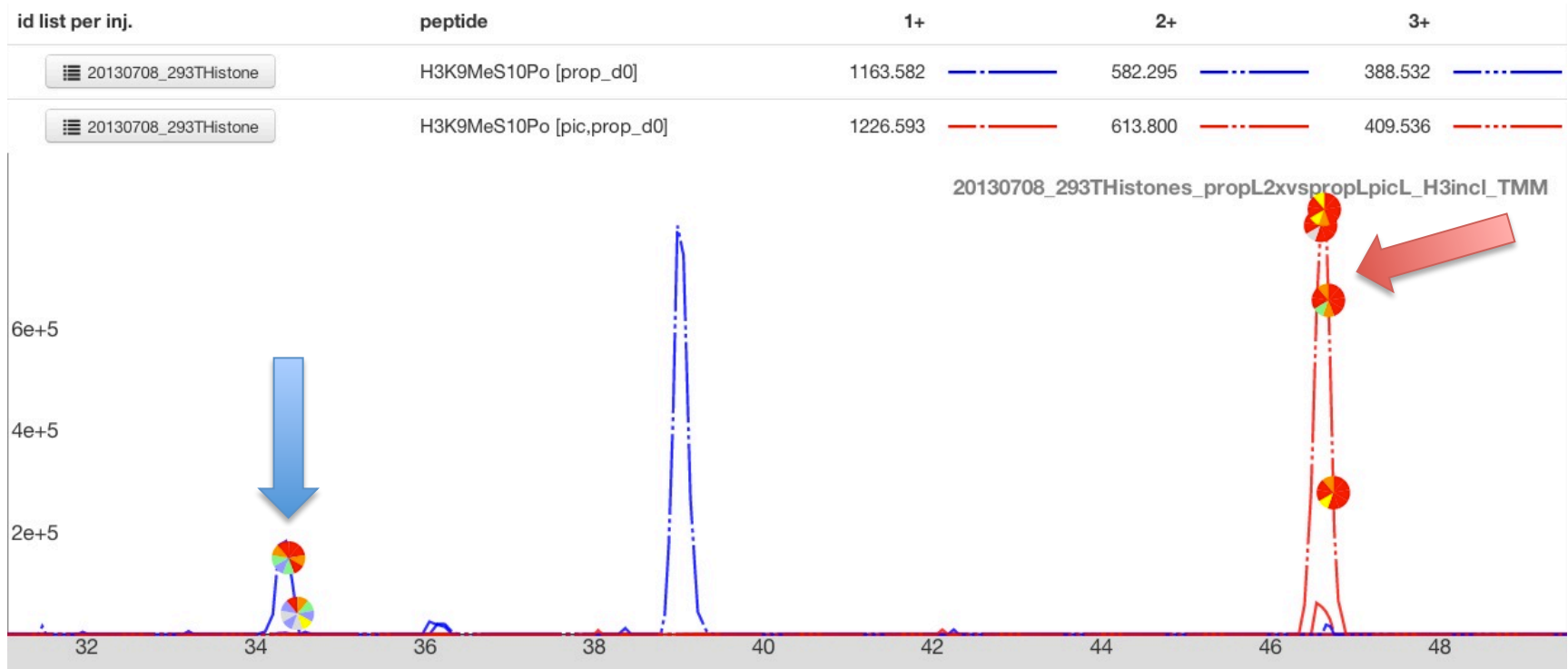
↑
 171Da diagnostic ion

↑
 140Da diagnostic ion

	b++	b		y	y++	
	60.53	120.04	PIC	1027.59	514.30	9
1	159.59	318.18	K	829.45	415.23	8
2	203.11	405.21	Methyl,Propionyl	742.42	371.71	7
			S			
3	253.63	506.26	T	641.37	321.19	6
4	282.14	563.28	G	584.35	292.68	5
5	310.66	620.30	G	527.33	264.17	4
6	402.72	804.43	K	343.21	172.11	3
7	438.23	875.46	Propionyl	272.17	136.59	2
8	486.76	972.51	A	175.12	88.06	1
9	564.81	1128.62	P			
			R			

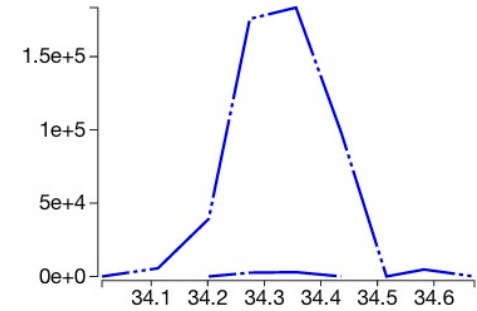
H3_K9-R17:

KMe1SPoTGGKAPR



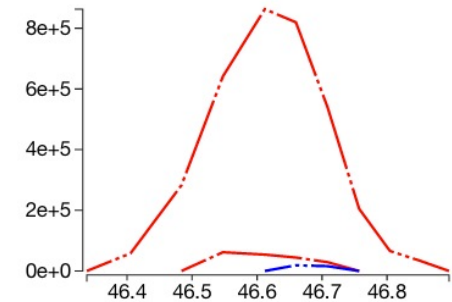
Quanti event: 34.0-34.7min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeS10Po [prop_d0]	1	1163.5820	2.6e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeS10Po [pic,prop_d0]	1	1226.5929	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeS10Po [prop_d0]	2	582.2946	2.4e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeS10Po [pic,prop_d0]	2	613.8001	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeS10Po [prop_d0]	3	388.5322	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeS10Po [pic,prop_d0]	3	409.5358	0.0e+0



Quanti event: 46.1-47.2min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeS10Po [prop_d0]	1	1163.5820	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeS10Po [pic,prop_d0]	1	1226.5929	6.3e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeS10Po [prop_d0]	2	582.2946	1.0e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeS10Po [pic,prop_d0]	2	613.8001	1.2e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeS10Po [prop_d0]	3	388.5322	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeS10Po [pic,prop_d0]	3	409.5358	0.0e+0



H3_K9-R17: Prop-KMe1SPoTGGKAPR MS/MS

Experimental spectrum

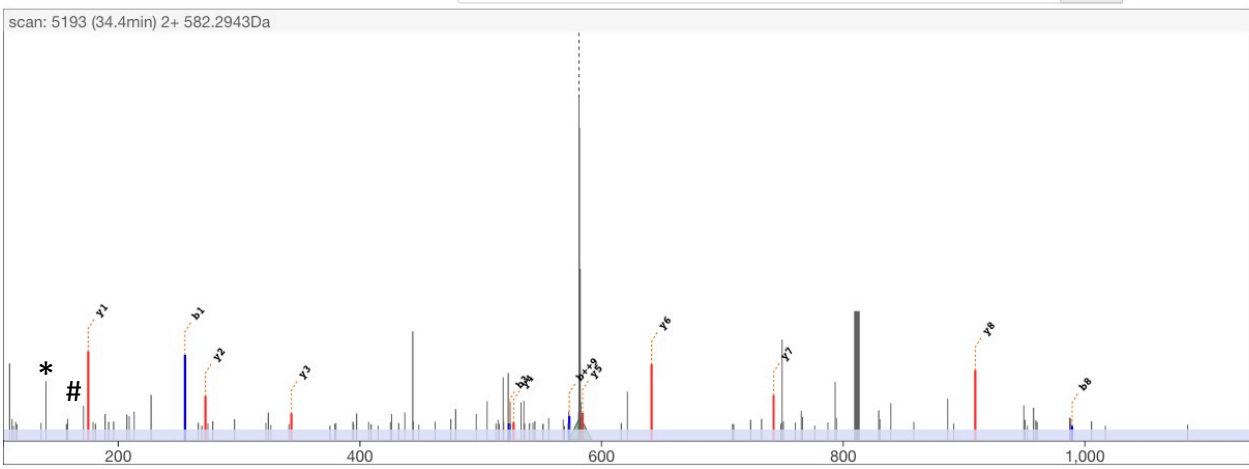
scan 5193
 retention time 34.4min
 precursor m/z 582.2943
 precursor charge 2+

Theoretical

M H²⁺ 582.2946
 MH Δ_{mass} Da -0.0007
 MH Δ_{mass} ppm -0.6

edit peptide

{Propionyl}K(Methyl,Propionyl)S(Phospho)TGGK{Propionyl}APR align



	b++	b		y	y++	
			Propionyl	1107.56	554.28	9
1	128.09	255.17	K	909.42	455.21	8
2	211.59	422.17	Methyl/Propionyl S	742.42	371.71	7
3	262.11	523.22	Phospho T	641.37	321.19	6
4	290.62	580.24	G	584.35	292.68	5
5	319.13	637.26	G	527.33	264.17	4
6	411.19	821.38	K	343.21	172.11	3
7	446.71	892.42	Propionyl A	272.17	136.59	2
8	495.24	989.47	P	175.12	88.06	1
9	573.29	1145.57	R			

Anchor	Current
click on peak	mouse over peak
m/z 909.4161	m/z 811.4410
intensity 2883	intensity 5721
int. rank 8	int. rank 119

Explanation?
 delta mass could be...
 $\Delta_{m/z}$ -97.97504

Tune the seq
 Align anchor peak
 b2,y3,y5++
 match

↑
 y8 – H3PO4

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

Experimental spectrum

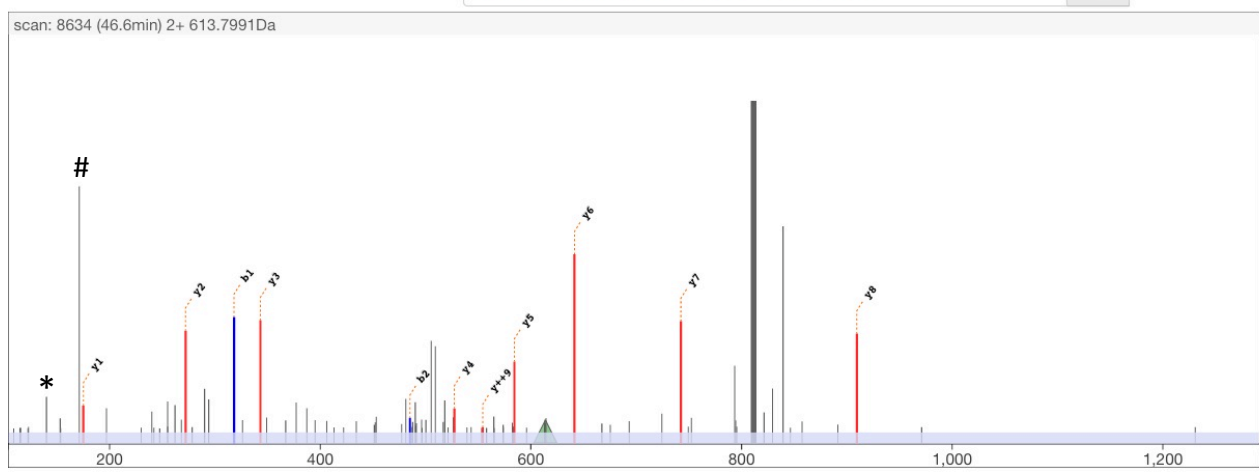
scan 8634
 retention time 46.6min
 precursor m/z 613.7991
 precursor charge 2+

Theoretical

M H²⁺ 613.8001
 MH Δ_{mass} Da -0.0020
 MH Δ_{mass} ppm -1.7

edit peptide

{PIC}K{Methyl,Propionyl}S{Phospho}TGGK{Propionyl}APR align



Anchor		Current	
click on peak		mouse over peak	
m/z	909.4153	m/z	811.4393
intensity	13893	intensity	46635
int. rank	7	int. rank	89

Explanation?
 delta mass could be...
 Δ_{m/z} -97.97601

Tune the seq
 Align anchor peak

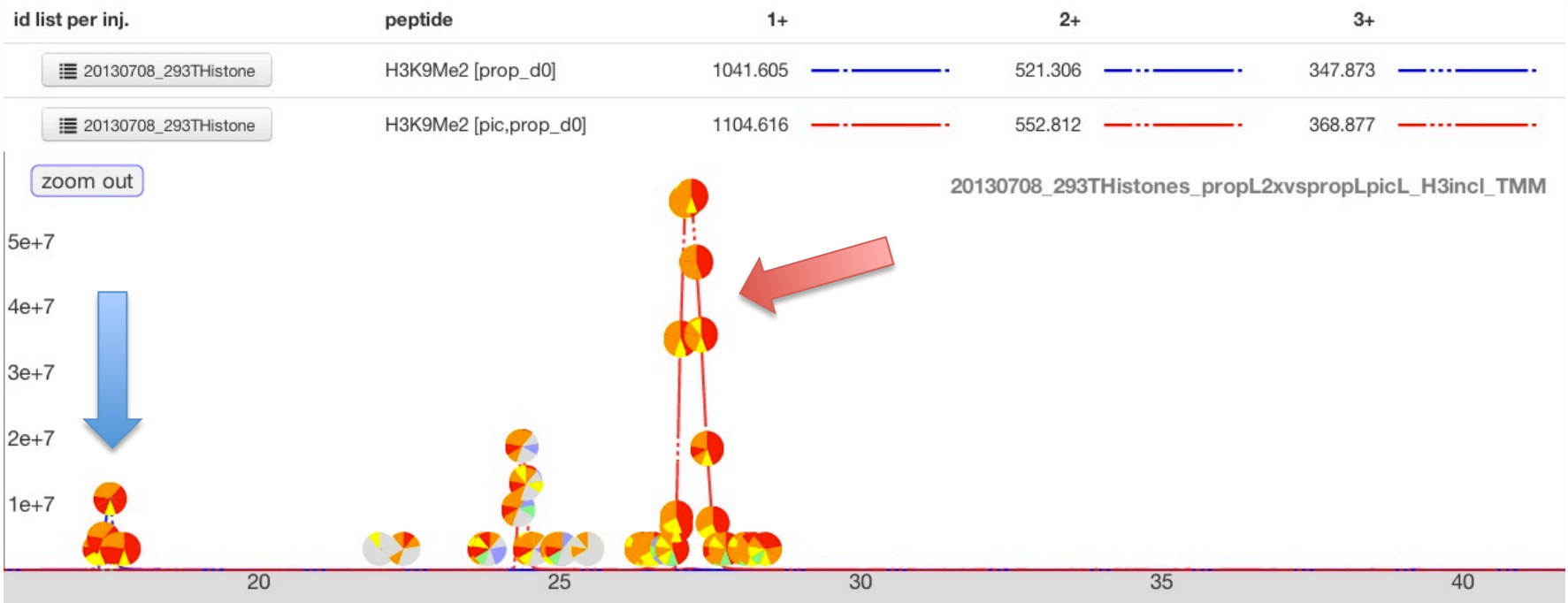
* = 140Da diagnostic ion
 # = 171Da diagnostic ion

↑
 y8 – H3PO4

	b++	b		y	y++	
	60.53	120.04		1107.56	554.28	9
1	159.59	318.18	PIC K {Methyl,Propionyl} S {Phospho} T G G K {Propionyl} A P R	909.42	455.21	8
2	243.09	485.18		742.42	371.71	7
3	293.62	586.23		641.37	321.19	6
4	322.13	643.25		584.35	292.68	5
5	350.64	700.27		527.33	264.17	4
6	442.70	884.39		343.21	172.11	3
7	478.22	955.43		272.17	136.59	2
8	526.74	1052.48		175.12	88.06	1
9	604.79	1208.58				

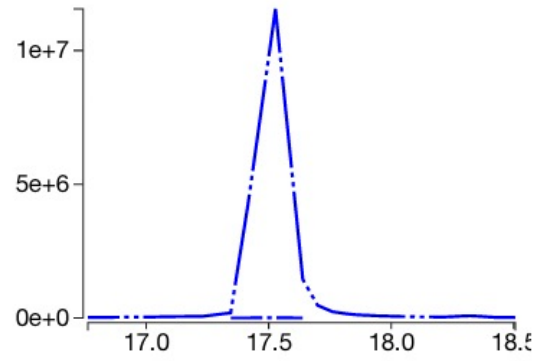
H3_K9-R17:

KMe2STGGKAPR



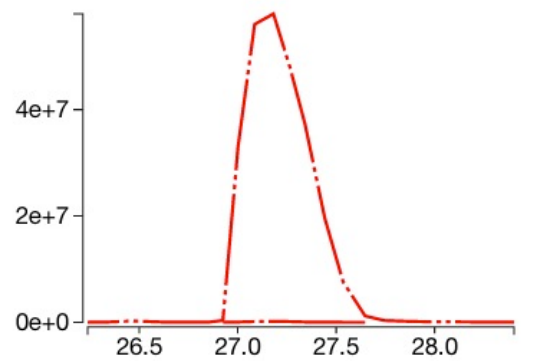
Quanti event: 16.7-18.5min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2 [prop_d0]	1	1041.6051	2.9e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2 [pic,prop_d0]	1	1104.6160	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2 [prop_d0]	2	521.3062	1.2e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2 [pic,prop_d0]	2	552.8116	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2 [prop_d0]	3	347.8732	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2 [pic,prop_d0]	3	368.8769	0.0e+0



Quanti event: 26.2-28.5min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2 [prop_d0]	1	1041.6051	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2 [pic,prop_d0]	1	1104.6160	3.2e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2 [prop_d0]	2	521.3062	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2 [pic,prop_d0]	2	552.8116	1.4e+9
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2 [prop_d0]	3	347.8732	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2 [pic,prop_d0]	3	368.8769	0.0e+0



H3_K9-R17: Prop-KMe2STGGKAPR MS/MS

Experimental spectrum

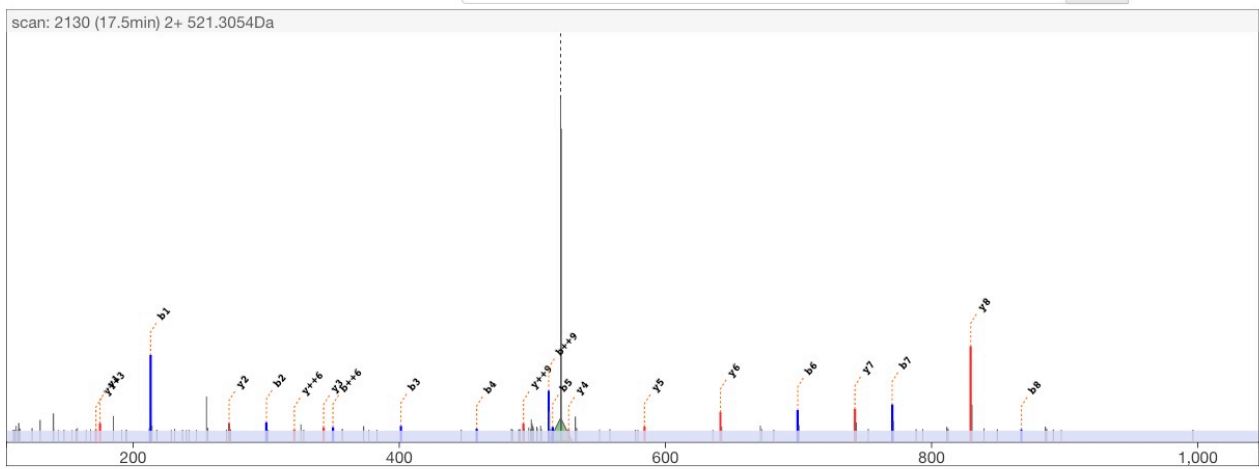
scan 2130
 retention time 17.5min
 precursor m/z 521.3054
 precursor charge 2+

Theoretical

M H²⁺ 521.3062
 MH Δ_{mass} Da -0.0016
 MH Δ_{mass} ppm -1.5

edit peptide

{Propionyl}K{Dimethyl}STGGK{Propionyl}APR



	b++	b		y	y++	
			Propionyl	985.58	493.29	9
1	107.08	213.16	K			
			Dimethyl	829.45	415.23	8
2	150.60	300.19	S	742.42	371.71	7
3	201.12	401.24	T	641.37	321.19	6
4	229.63	458.26	G	584.35	292.68	5
5	258.14	515.28	G	527.33	264.17	4
6	350.21	699.40	K			
			Propionyl	343.21	172.11	3
7	385.72	770.44	A			
8	434.25	867.49	P	272.17	136.59	2
9	512.30	1023.59	R	175.12	88.06	1

Experimental spectrum

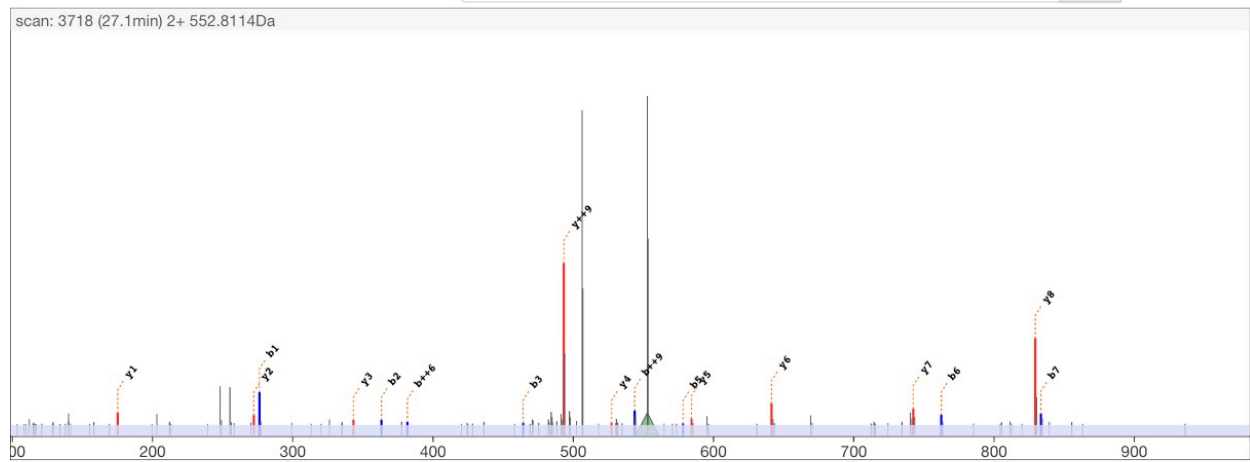
scan 3718
 retention time 27.1min
 precursor m/z 552.8114
 precursor charge 2+

Theoretical

M H²⁺ 552.8116
 MH Δ_{mass} Da -0.0005
 MH Δ_{mass} ppm -0.4

edit peptide

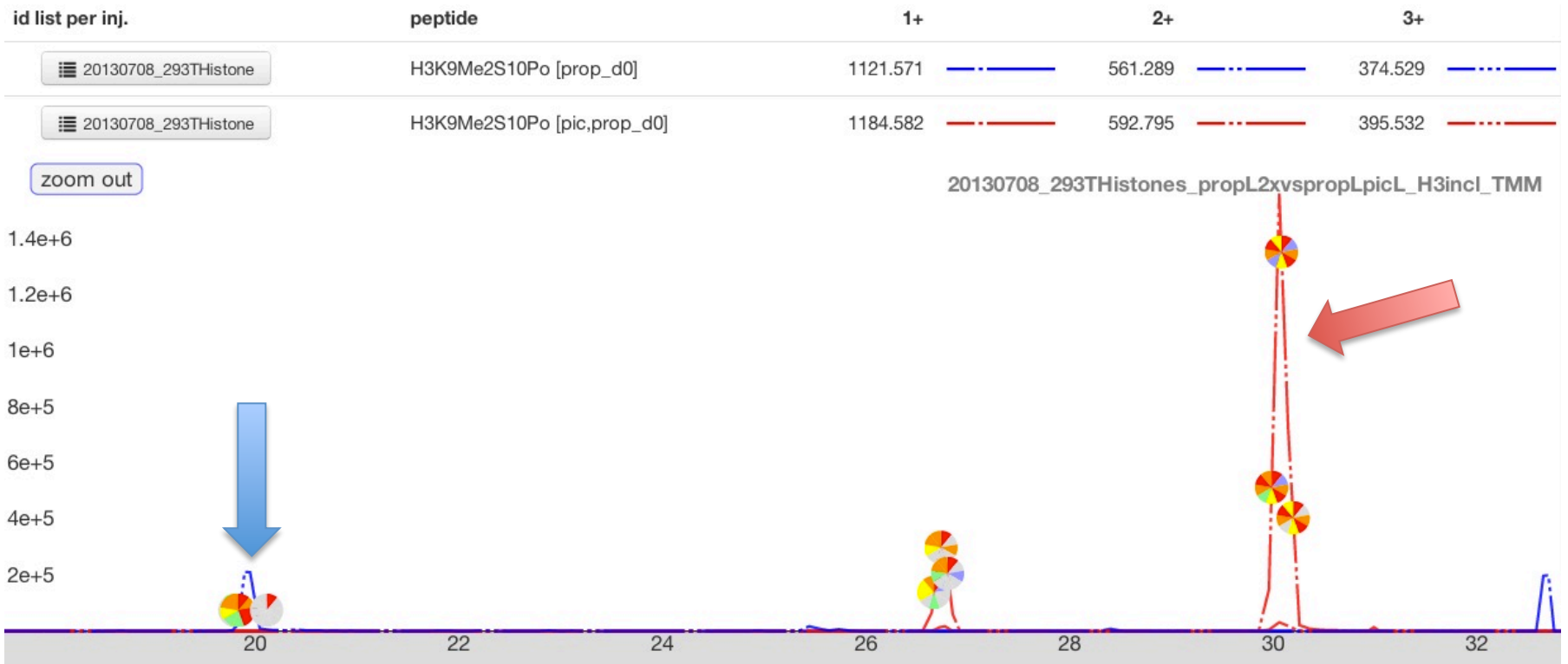
{PIC}K{Dimethyl}STGGK{Propionyl}APR



	b++	b		y	y++	
	60.53	120.04	PIC	985.58	493.29	9
1	138.59	276.17	K	829.45	415.23	8
2	182.10	363.20	Dimethyl	742.42	371.71	7
3	232.63	464.25	S	641.37	321.19	6
4	261.14	521.27	T	584.35	292.68	5
5	289.65	578.29	G	527.33	264.17	4
6	381.71	762.41	G	343.21	172.11	3
7	417.23	833.45	Propionyl	272.17	136.59	2
8	465.76	930.50	K	175.12	88.06	1
9	543.81	1086.61	A			
			P			
			R			

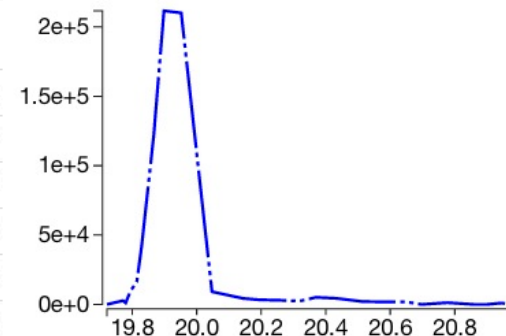
H3_K9-R17:

KMe2SPoTGGKAPR



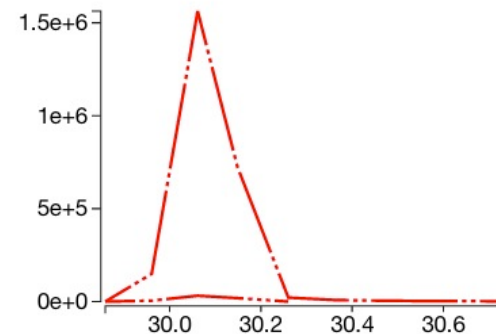
Quanti event: 19.6-21.0min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Po [prop_d0]	1	1121.5715	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Po [pic,prop_d0]	1	1184.5824	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Po [prop_d0]	2	561.2894	2.0e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Po [pic,prop_d0]	2	592.7948	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Po [prop_d0]	3	374.5287	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Po [pic,prop_d0]	3	395.5323	0.0e+0



Quanti event: 29.4-30.8min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Po [prop_d0]	1	1121.5715	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Po [pic,prop_d0]	1	1184.5824	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Po [prop_d0]	2	561.2894	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Po [pic,prop_d0]	2	592.7948	1.4e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Po [prop_d0]	3	374.5287	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Po [pic,prop_d0]	3	395.5323	3.2e+5



H3_K9-R17: Prop-KMe2SPoTGGKAPR MS/MS

Experimental spectrum

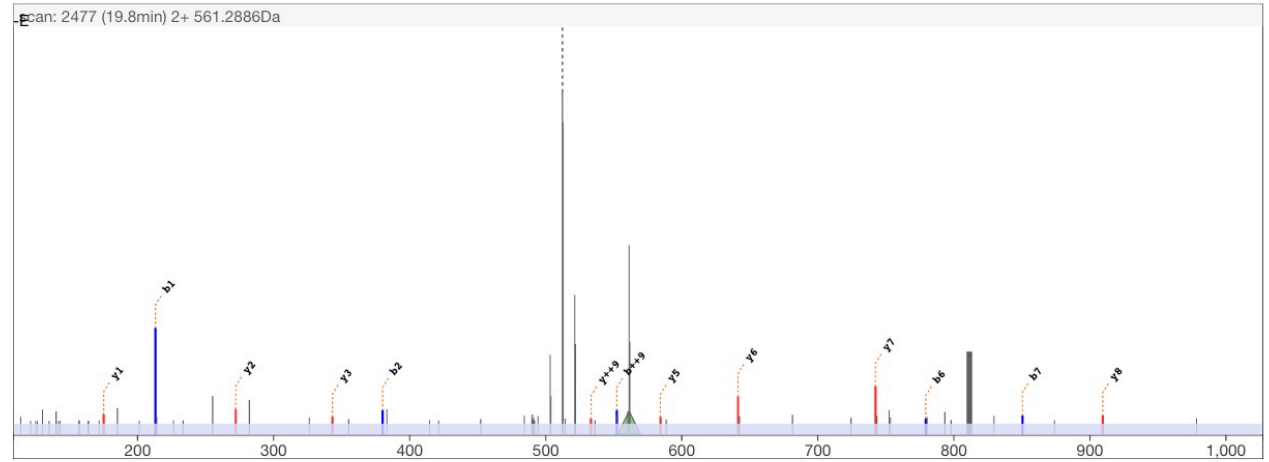
scan 2477
 retention time 19.8min
 precursor m/z 561.2886
 precursor charge 2+

Theoretical

M H²⁺ 561.2894
 MH Δ_{mass} Da -0.0016
 MH Δ_{mass} ppm -1.4

edit peptide

{Propionyl}K{Dimethyl}S{Phospho}TGGK{Propionyl}APR align



	b++	b		y	y++	
			Propionyl	1065.55	533.28	9
1	107.08	213.16	K			
			Dimethyl	909.42	455.21	8
2	190.58	380.16	S			
			Phospho	742.42	371.71	7
3	241.11	481.21	T			
			G	641.37	321.19	6
4	269.62	538.23	G			
			G	584.35	292.68	5
5	298.13	595.25	K			
			Propionyl	527.33	264.17	4
6	390.19	779.37	A			
			K	343.21	172.11	3
7	425.71	850.41	P			
			A	272.17	136.59	2
8	474.23	947.46	R			
			P	175.12	88.06	1
9	552.28	1103.56	R			

Anchor		Current	
click on peak		mouse over peak	
m/z	909.4356	m/z	811.4404
intensity	256	intensity	2255
int. rank	24	int. rank	3

Explanation?
 delta mass could be...
 $\Delta_{m/z}$ -97.99524

Tune the seq
 Align anchor peak

y8 – H3PO4

H3_K9-R17: PIC-KMe2SPoTGGKAPR MS/MS

Experimental spectrum

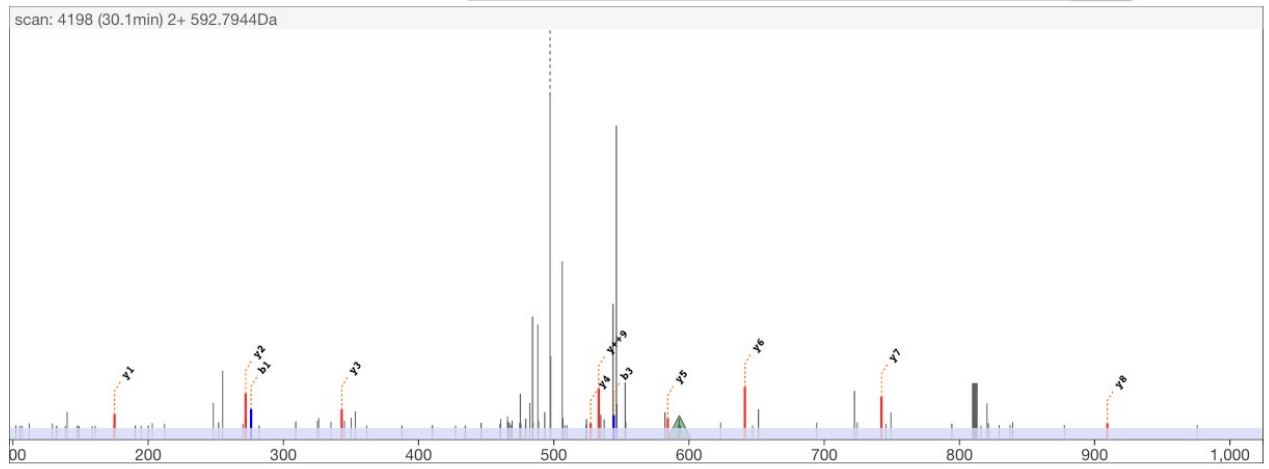
scan 4198
 retention time 30.1min
 precursor m/z 592.7944
 precursor charge 2+

Theoretical

M H²⁺ 592.7948
 MH Δ_{mass} Da -0.0009
 MH Δ_{mass} ppm -0.7

edit peptide

{PIC}K{Dimethyl}S{Phospho}TGGK{Propionyl}APR



Anchor	Current
click on peak	mouse over peak
m/z 909.4088	m/z 811.4411
intensity 2179	intensity 21541
int. rank 50	int. rank 4

Explanation?
 delta mass could be...
 $\Delta_{m/z}$ -97.96765

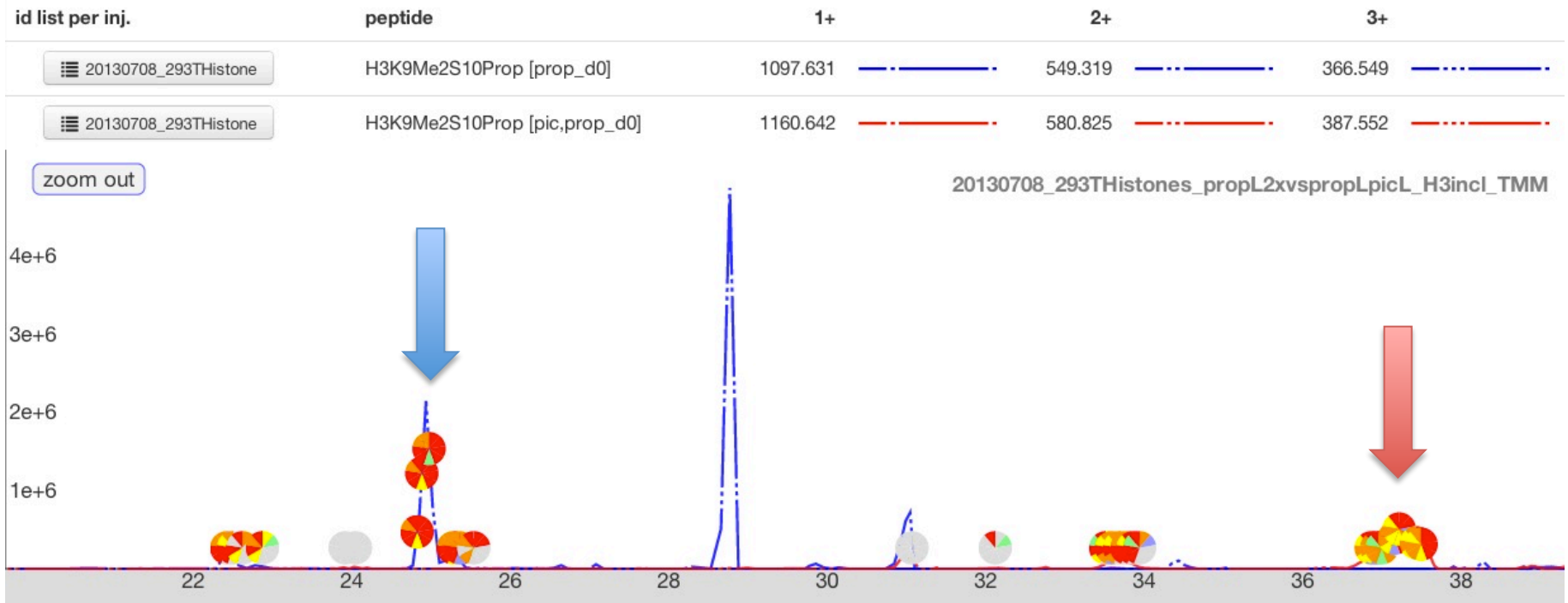
Tune the seq
 Align anchor peak

y8 – H3PO4

	b++	b		y	y++	
	60.53	120.04	PIC	1065.55	533.28	9
1	138.59	276.17	K Dimethyl	909.42	455.21	8
2	222.09	443.17	S Phospho	742.42	371.71	7
3	272.61	544.22	T	641.37	321.19	6
4	301.12	601.24	G	584.35	292.68	5
5	329.63	658.26	G	527.33	264.17	4
6	421.69	842.38	K Propionyl	343.21	172.11	3
7	457.21	913.42	A	272.17	136.59	2
8	505.74	1010.47	P	175.12	88.06	1
9	583.79	1166.57	R			

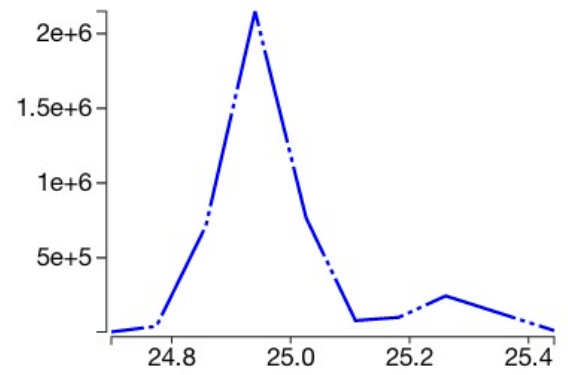
H3_K9-R17:

KMe2SPropTGGKAPR



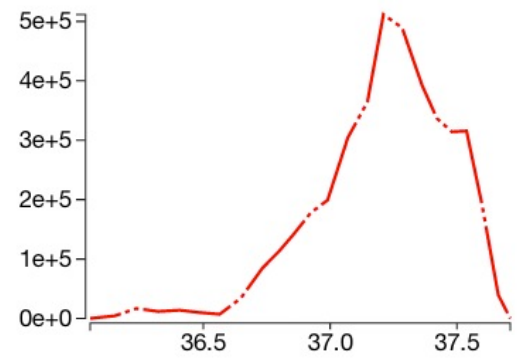
Quanti event: 24.7-25.5min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Prop [prop_d0]	1	1097.6313	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Prop [pic,prop_d0]	1	1160.6422	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Prop [prop_d0]	2	549.3193	2.1e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Prop [pic,prop_d0]	2	580.8248	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Prop [prop_d0]	3	366.5486	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Prop [pic,prop_d0]	3	387.5523	0.0e+0



Quanti event: 35.8-37.8min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Prop [prop_d0]	1	1097.6313	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Prop [pic,prop_d0]	1	1160.6422	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Prop [prop_d0]	2	549.3193	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Prop [pic,prop_d0]	2	580.8248	1.7e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Prop [prop_d0]	3	366.5486	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10Prop [pic,prop_d0]	3	387.5523	0.0e+0



H3_K9-R17: Prop-KMe2SPropTGGKAPR MS/MS

Experimental spectrum

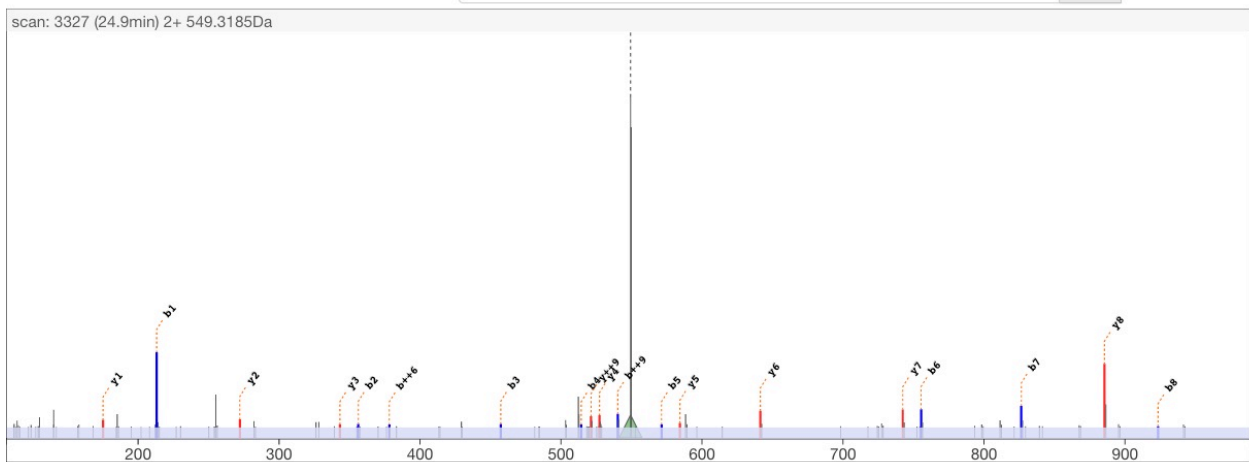
scan 3327
 retention time 24.9min
 precursor m/z 549.3185
 precursor charge 2+

Theoretical

M H²⁺ 549.3193
 MH Δ_{mass} Da -0.0015
 MH Δ_{mass} ppm -1.4

edit peptide

{Propionyl}K{Dimethyl}S{Propionyl}TGGK{Propionyl}APR align



	b++	b		y	y++	
			Propionyl	1041.61	521.31	9
1	107.08	213.16	K	885.48	443.24	8
2	178.61	356.22	S	742.42	371.71	7
3	229.14	457.27	Propionyl	641.37	321.19	6
4	257.65	514.29	T	584.35	292.68	5
5	286.16	571.31	G	527.33	264.17	4
6	378.22	755.43	G	343.21	172.11	3
7	413.74	826.47	Propionyl	272.17	136.59	2
8	462.26	923.52	K	175.12	88.06	1
9	540.31	1079.62	A			
			P			
			R			

H3_K9-R17: PIC-KMe2SPropTGGKAPR MS/MS

Experimental spectrum

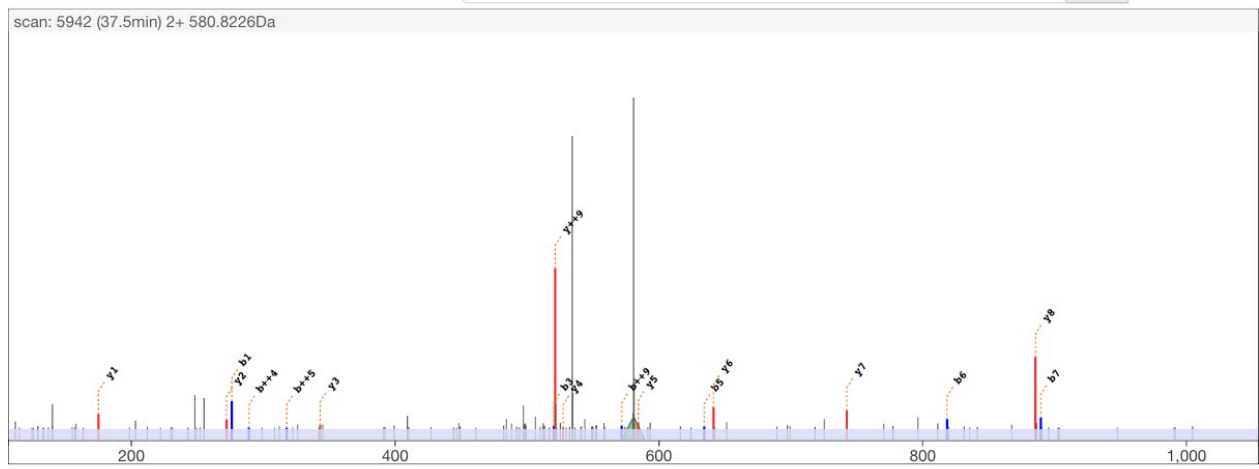
scan 5942
 retention time 37.5min
 precursor m/z 580.8226
 precursor charge 2+

Theoretical

MH²⁺ 580.8248
 MH Δ _{mass} Da -0.0042
 MH Δ _{mass} ppm -3.7

edit peptide

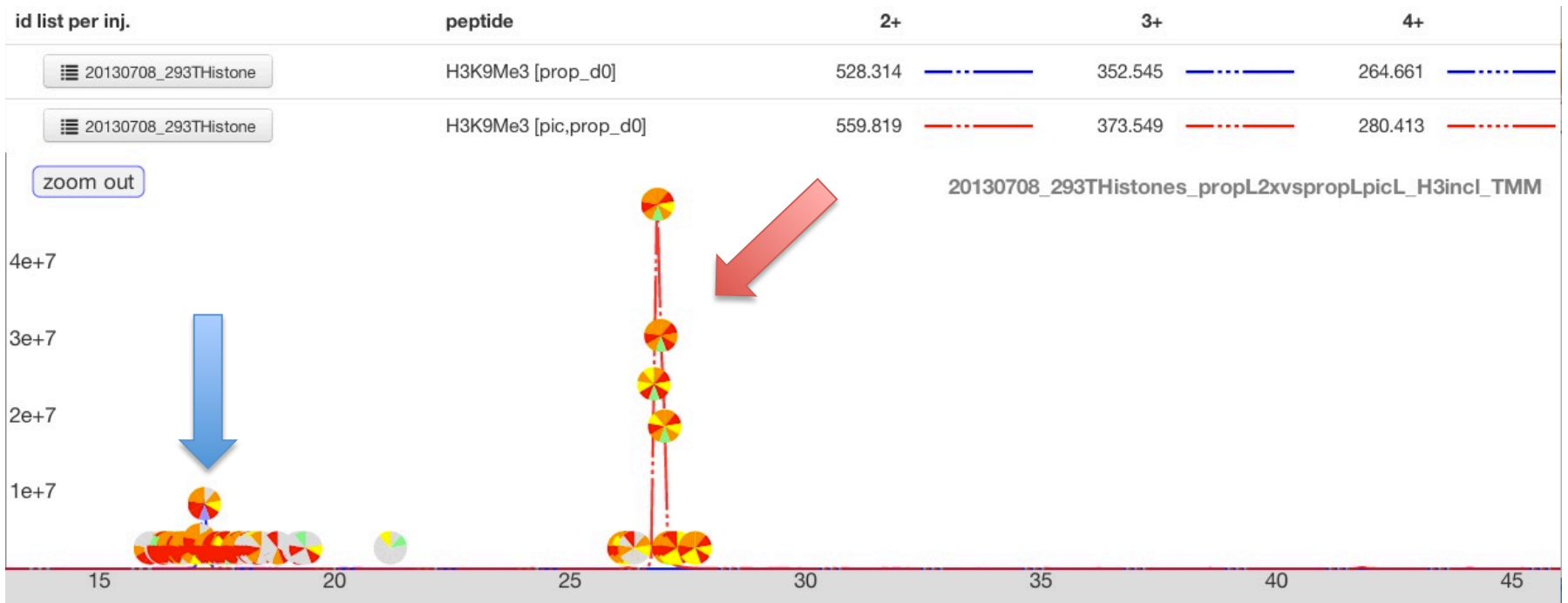
{PIC}K{Dimethyl}S{Propionyl}TGGK{Propionyl}APR align



	b++	b		y	y++	
	60.53	120.04		1041.61	521.31	9
1	138.59	276.17	PIC	885.48	443.24	8
2	210.12	419.23	K	742.42	371.71	7
3	260.64	520.28	Dimethyl	641.37	321.19	6
4	289.15	577.30	S	584.35	292.68	5
5	317.66	634.32	T	527.33	264.17	4
6	409.72	818.44	Propionyl	343.21	172.11	3
7	445.24	889.48	G	272.17	136.59	2
8	493.77	986.53	K	175.12	88.06	1
9	571.82	1142.63	Propionyl			

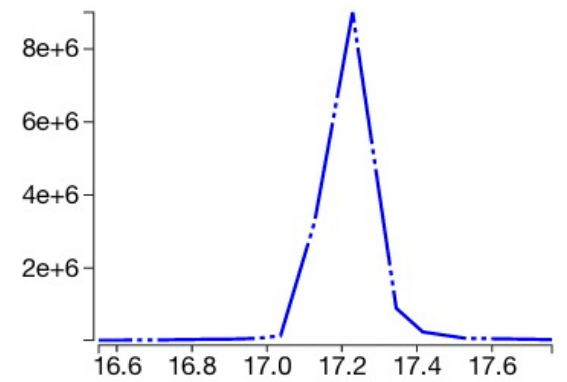
H3_K9-R17:

KMe3STGGKAPR



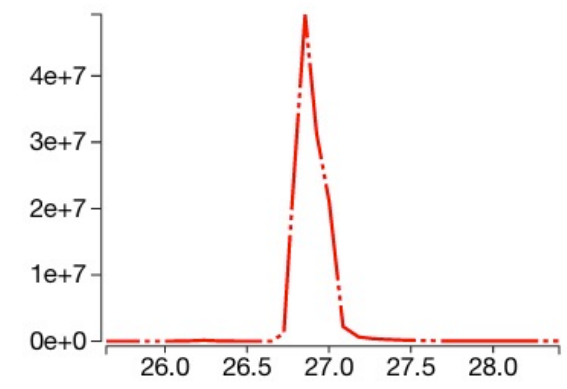
Quanti event: 16.5-17.8min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3 [prop_d0]	2	528.3140	8.7e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3 [pic,prop_d0]	2	559.8195	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3 [prop_d0]	3	352.5451	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3 [pic,prop_d0]	3	373.5487	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3 [prop_d0]	4	264.6607	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3 [pic,prop_d0]	4	280.4134	0.0e+0



Quanti event: 25.6-28.4min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3 [prop_d0]	2	528.3140	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3 [pic,prop_d0]	2	559.8195	5.7e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3 [prop_d0]	3	352.5451	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3 [pic,prop_d0]	3	373.5487	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3 [prop_d0]	4	264.6607	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3 [pic,prop_d0]	4	280.4134	0.0e+0



H3_K9-R17: Prop-KMe3STGGKAPR MS/MS

Experimental spectrum

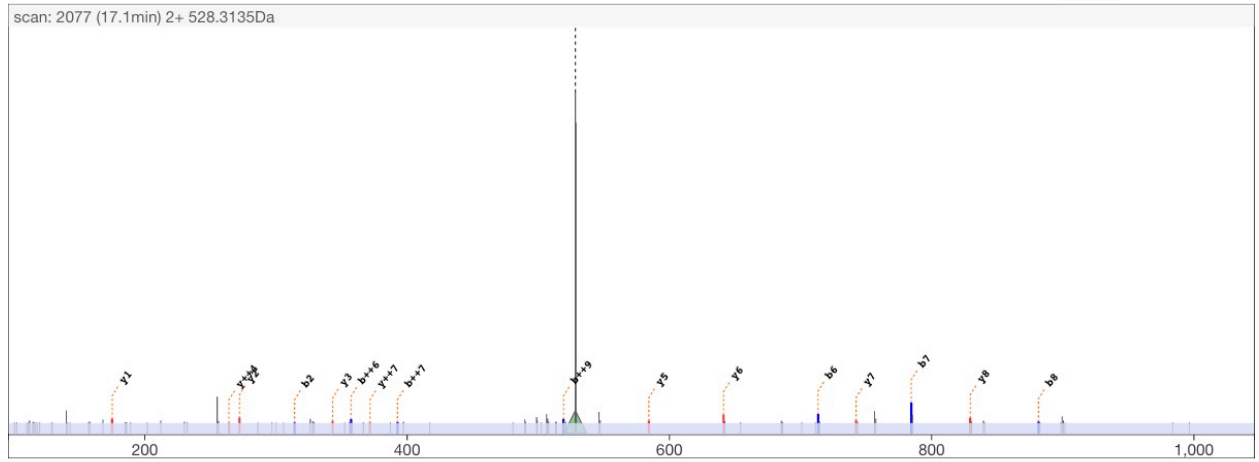
scan 2077
 retention time 17.1min
 precursor m/z 528.3135
 precursor charge 2+

Theoretical

M H²⁺ 528.3140
 MH Δ_{mass} Da -0.0011
 MH Δ_{mass} ppm -1.0

edit peptide

{Propionyl}K{Trimethyl}STGGK{Propionyl}APR align



	b++	b	y	y++	
			999.59	500.30	9
1	114.09	227.18	829.45	415.23	8
2	157.61	314.21	742.42	371.71	7
3	208.13	415.26	641.37	321.19	6
4	236.64	472.28	584.35	292.68	5
5	265.15	529.30	527.33	264.17	4
6	357.21	713.42	343.21	172.11	3
7	392.73	784.46	272.17	136.59	2
8	441.26	881.51	175.12	88.06	1
9	519.31	1037.61			

Experimental spectrum

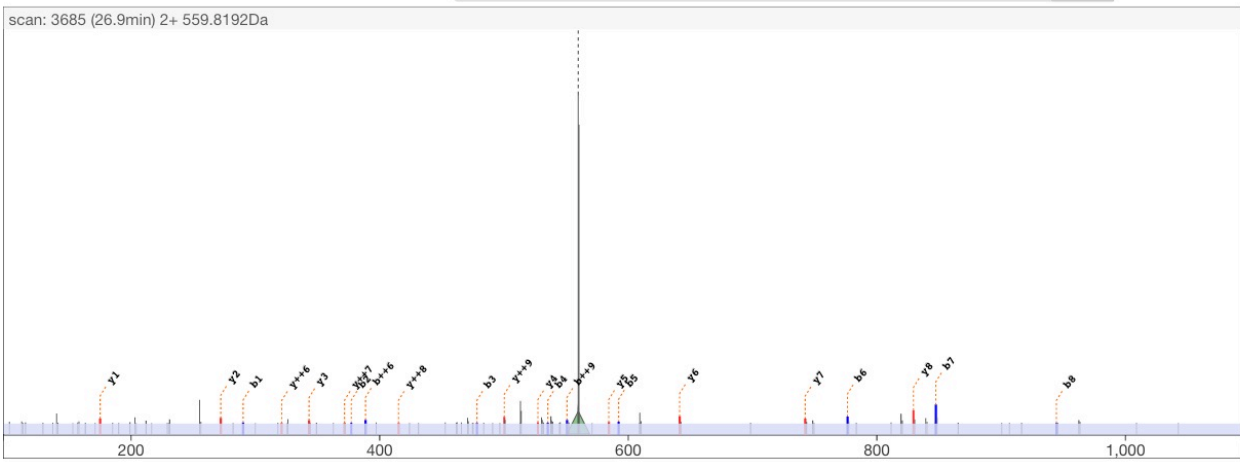
scan 3685
 retention time 26.9min
 precursor m/z 559.8192
 precursor charge 2+

Theoretical

M H²⁺ 559.8195
 MH Δ_{mass} Da -0.0005
 MH Δ_{mass} ppm -0.5

edit peptide

{PIC}K{Trimethyl}STGGK{Propionyl}APR align



	b++	b		y	y++	
	60.53	120.04	PIC	999.59	500.30	9
1	145.60	290.19	K	829.45	415.23	8
2	189.11	377.22	S	742.42	371.71	7
3	239.64	478.27	T	641.37	321.19	6
4	268.15	535.29	G	584.35	292.68	5
5	296.66	592.31	K	527.33	264.17	4
6	388.72	776.43	Propionyl	343.21	172.11	3
7	424.24	847.47	A	272.17	136.59	2
8	472.76	944.52	P	175.12	88.06	1
9	550.81	1100.62	R			

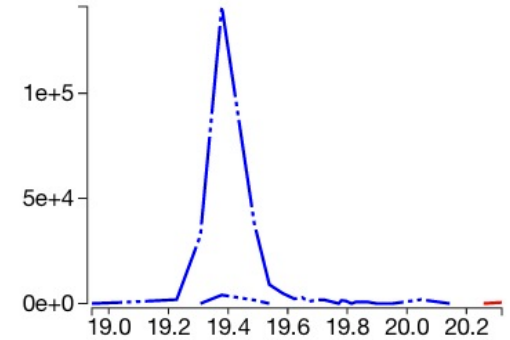
H3_K9-R17:

KMe3SPoTGGKAPR



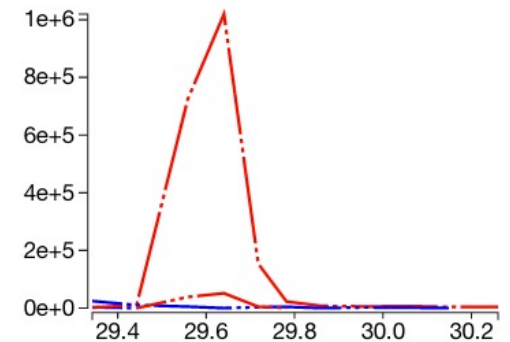
Quanti event: 18.9-20.4min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10Po [prop_d0]	1	1135.5871	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10Po [pic,prop_d0]	1	1198.5980	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10Po [prop_d0]	2	568.2972	1.2e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10Po [pic,prop_d0]	2	599.8026	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10Po [prop_d0]	3	379.2006	3.0e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10Po [pic,prop_d0]	3	400.2042	9.7e+2



Quanti event: 29.3-30.3min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10Po [prop_d0]	1	1135.5871	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10Po [pic,prop_d0]	1	1198.5980	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10Po [prop_d0]	2	568.2972	9.2e+3
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10Po [pic,prop_d0]	2	599.8026	1.0e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10Po [prop_d0]	3	379.2006	2.3e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10Po [pic,prop_d0]	3	400.2042	4.9e+5



H3_K9-R17: Prop-KMe3SPoTGGKAPR MS/MS

Experimental spectrum

scan 2415
 retention time 19.4min
 precursor m/z 568.2967
 precursor charge 2+

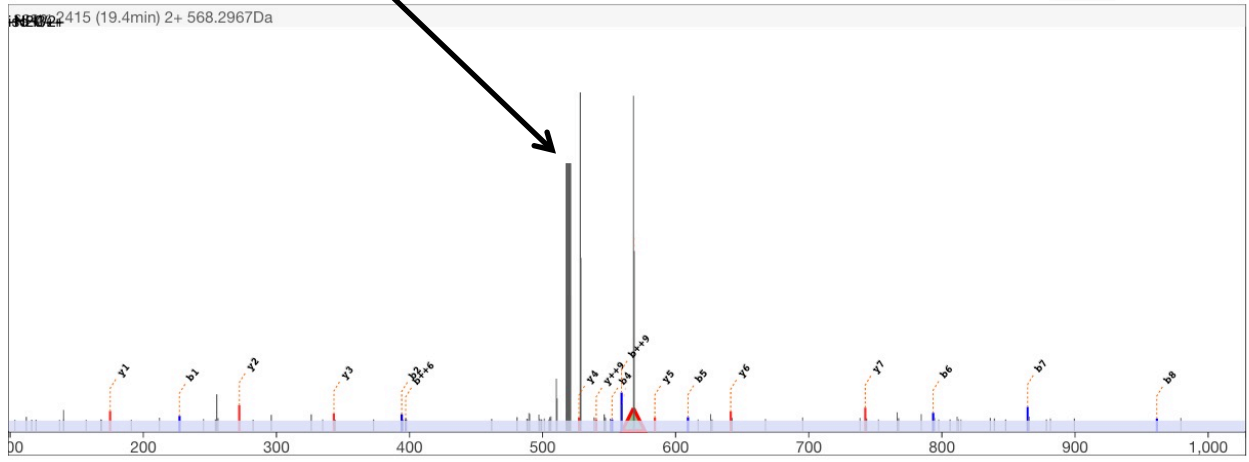
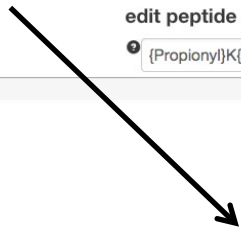
Theoretical

M H²⁺ 568.2972
 MH Δ_{mass} Da -0.0010
 MH Δ_{mass} ppm -0.9

edit peptide

{Propionyl}K{Trimethyl}S{Phospho}TGGK{Propionyl}APR align

precursor - H3PO4



Anchor	Current
click on peak	mouse over peak
m/z 568.2967	m/z 519.3082
intensity NaN	intensity 26844
int. rank	int. rank 79

Explanation?
 delta mass could be...
 $\Delta_{m/z}$ -48.98853

Tune the seq
 Align anchor peak

	b++	b	y	y++	
			1079.56	540.28	9
1	114.09	227.18	909.42	455.21	8
2	197.59	394.17	742.42	371.71	7
3	248.11	495.22	641.37	321.19	6
4	276.63	552.24	584.35	292.68	5
5	305.14	609.26	527.33	264.17	4
6	397.20	793.39	343.21	172.11	3
7	432.71	864.42	272.17	136.59	2
8	481.24	961.48	175.12	88.06	1
9	559.29	1117.58			

Experimental spectrum

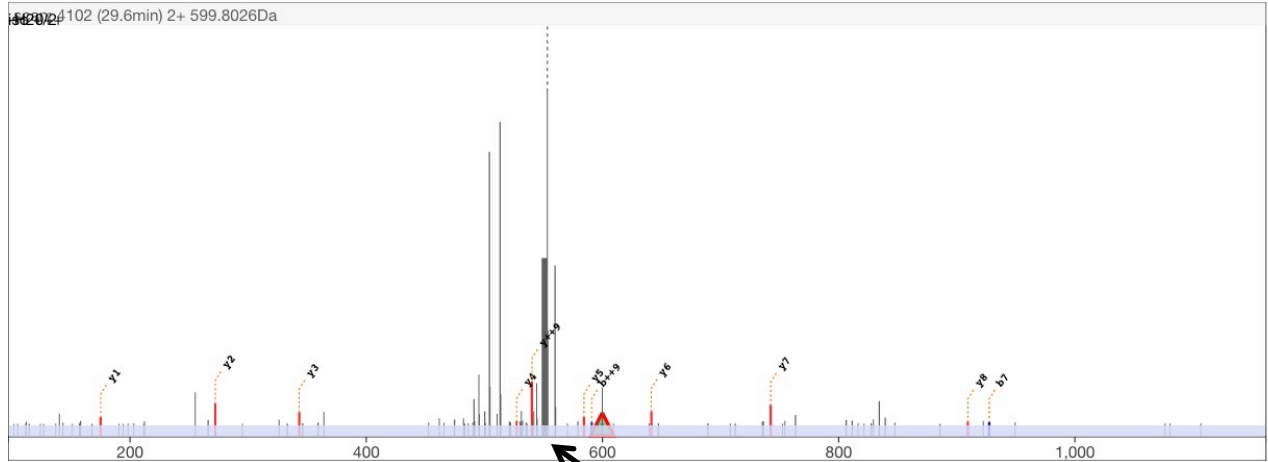
scan 4102
 retention time 29.6min
 precursor m/z 599.8026
 precursor charge 2+

Theoretical

M H²⁺ 599.8026
 MH Δ_{mass} Da -0.0002
 MH Δ_{mass} ppm -0.1

edit peptide

{PIC}K[Trimethyl]S[Phospho]TGGK[Propionyl]APR align



Anchor
 click on peak
 m/z 599.8026
 intensity NaN
 int. rank

Current
 mouse over peak
 m/z 550.8129
 intensity 60500
 int. rank 93

Explanation?
 delta mass could be...
 Δ_{m/z} -48.98969

precursor – H3PO4

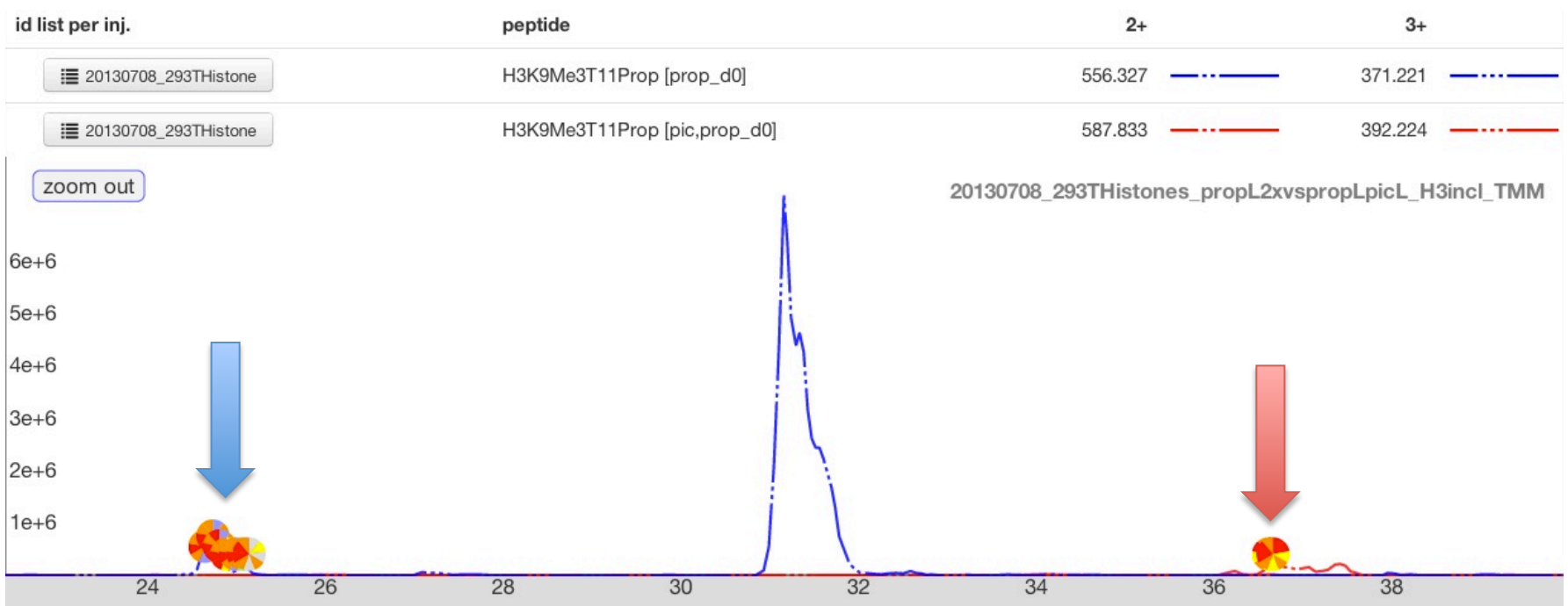
Tune the seq
 Align anchor peak
 b2,y3,y5++
 match

	b++	b		y	y++	
	60.53	120.04	PIC	1079.56	540.28	9
1	145.60	290.19	K Trimethyl	909.42	455.21	8
2	229.10	457.18	S Phospho	742.42	371.71	7
3	279.62	558.23	T	641.37	321.19	6
4	308.13	615.25	G	584.35	292.68	5
5	336.64	672.28	G	527.33	264.17	4
6	428.70	856.40	K Propionyl	343.21	172.11	3
7	464.22	927.43	A	272.17	136.59	2
8	512.75	1024.49	P	175.12	88.06	1
9	590.80	1180.59	R			

H3_K9-R17:

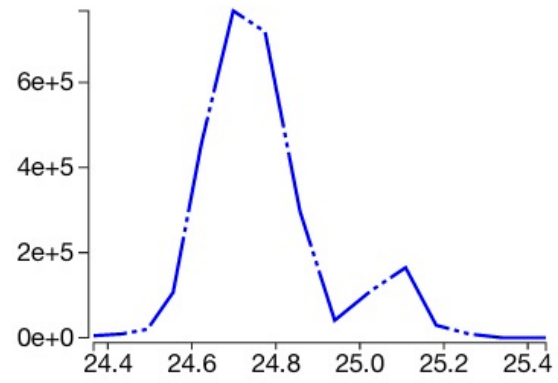
KMe3STPropGGKAPR

T11 seems to be the favourite spot for propionylation on this peptide



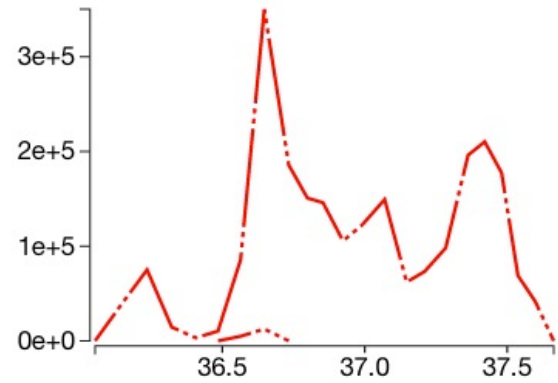
Quanti event: 24.3-25.5min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3T11Prop [prop_d0]	2	556.3271	1.3e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3T11Prop [pic,prop_d0]	2	587.8326	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3T11Prop [prop_d0]	3	371.2205	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3T11Prop [pic,prop_d0]	3	392.2241	0.0e+0



Quanti event: 36.0-37.7min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3T11Prop [prop_d0]	2	556.3271	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3T11Prop [pic,prop_d0]	2	587.8326	1.0e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3T11Prop [prop_d0]	3	371.2205	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3T11Prop [pic,prop_d0]	3	392.2241	8.8e+4



H3_K9-R17: Prop-KMe3SPropTGGKAPR MS/MS

Experimental spectrum

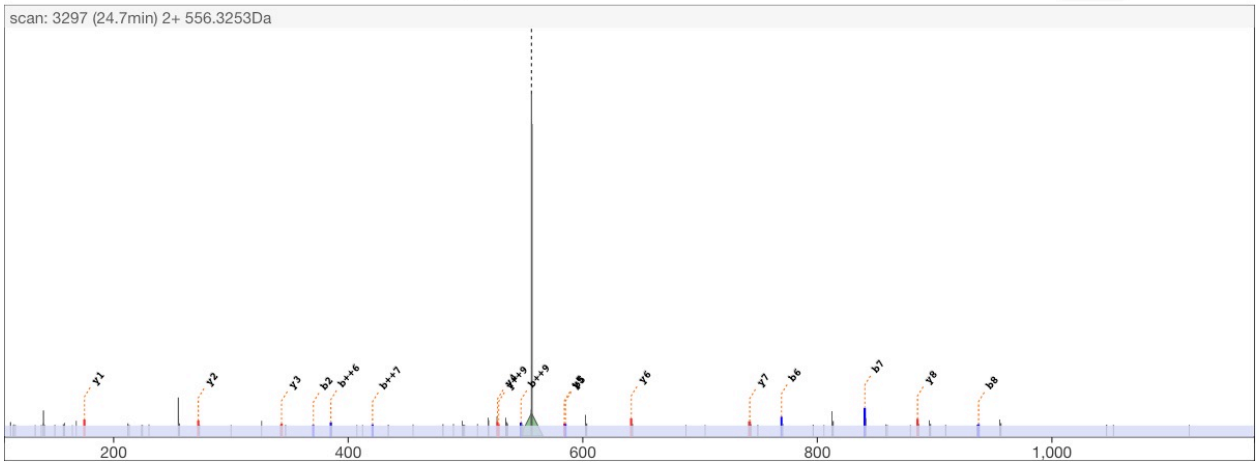
scan 3297
 retention time 24.7min
 precursor m/z 556.3253
 precursor charge 2+

Theoretical

M H²⁺ 556.3271
 MH Δ_{mass} Da -0.0037
 MH Δ_{mass} ppm -3.4

edit peptide

{Propionyl}K{Trimethyl}S{Propionyl}TGGK{Propionyl}APR align



	b++	b		y	y++	
			Propionyl	1055.62	528.31	9
1	114.09	227.18	K			
			Trimethyl	885.48	443.24	8
2	185.62	370.23	S			
			Propionyl	742.42	371.71	7
3	236.14	471.28	T			
4	264.66	528.30	G			
5	293.17	585.32	G			
6	385.23	769.45	K			
			Propionyl	343.21	172.11	3
7	420.74	840.48	A			
8	469.27	937.54	P			
9	547.32	1093.64	R			

H3_K9-R17: PIC-KMe3SPropTGGKAPR MS/MS

Experimental spectrum

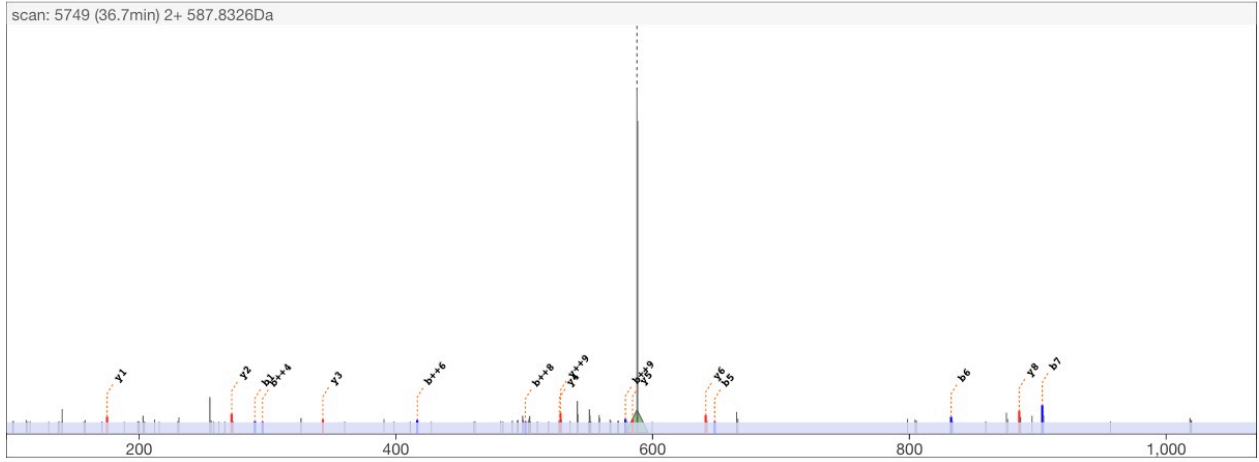
scan 5749
 retention time 36.7min
 precursor m/z 587.8326
 precursor charge 2+

Theoretical

M H²⁺ 587.8326
 MH Δ_{mass} Da 0.0001
 MH Δ_{mass} ppm 0.1

edit peptide

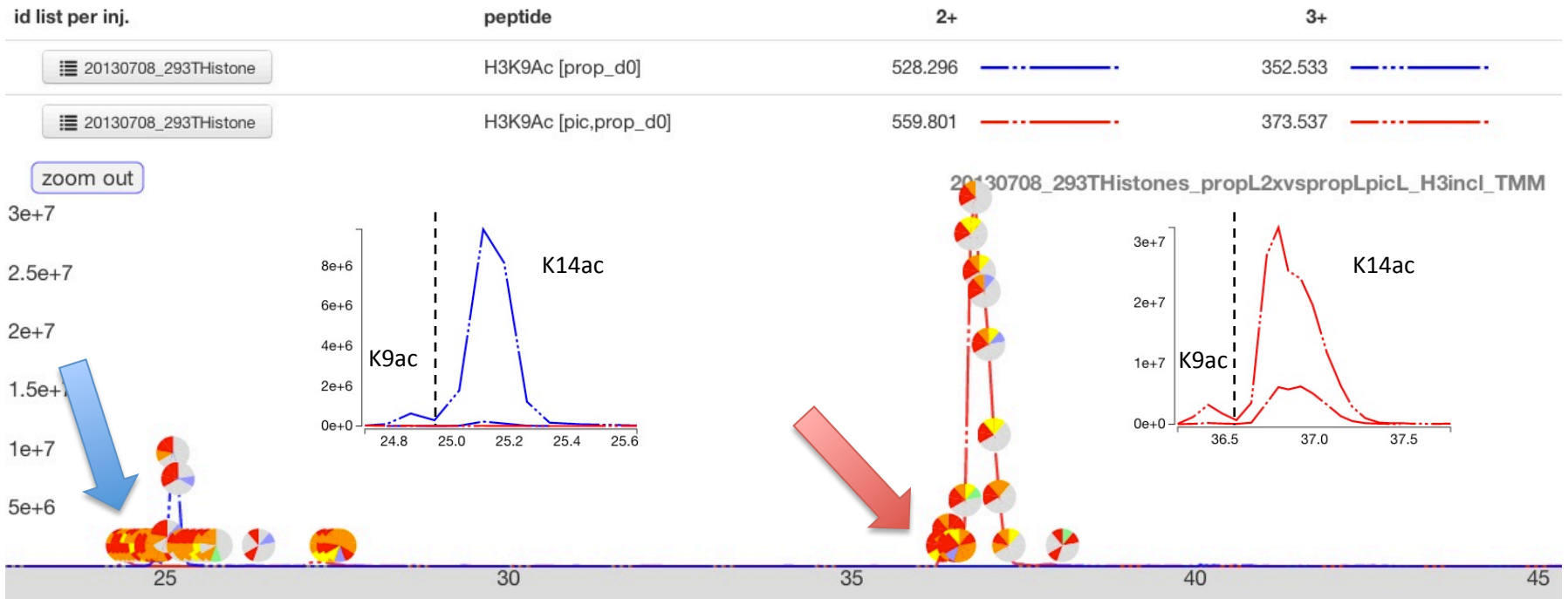
{PIC}K{Trimethyl}S{Propionyl}TGGK{Propionyl}APR



	b++	b		y	y++	
	60.53	120.04	PIC	1055.62	528.31	9
1	145.60	290.19	K	885.48	443.24	8
2	217.13	433.24	S	742.42	371.71	7
3	267.65	534.29	T	641.37	321.19	6
4	296.16	591.31	G	584.35	292.68	5
5	324.67	648.34	G	527.33	264.17	4
6	416.73	832.46	K	343.21	172.11	3
7	452.25	903.49	A	272.17	136.59	2
8	500.78	1000.55	P	175.12	88.06	1
9	578.83	1156.65	R			

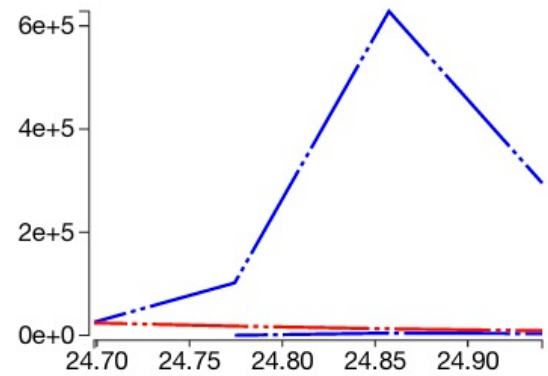
H3_K9-R17: KAcSTGGKAPR

Double-peak of K9ac and K14ac, K9ac elutes earlier from C18 column



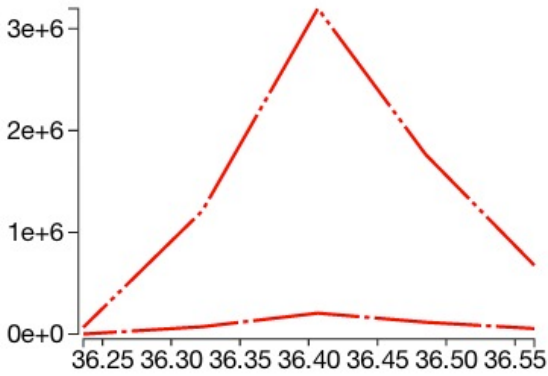
Quanti event: 24.7-25.0min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Ac [prop_d0]	1	1055.5844	3.0e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Ac [pic,prop_d0]	1	1118.5953	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Ac [prop_d0]	2	528.2958	4.4e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Ac [pic,prop_d0]	2	559.8013	2.2e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Ac [prop_d0]	3	352.5330	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Ac [pic,prop_d0]	3	373.5366	0.0e+0



Quanti event: 36.2-36.6min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Ac [prop_d0]	1	1055.5844	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Ac [pic,prop_d0]	1	1118.5953	2.1e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Ac [prop_d0]	2	528.2958	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Ac [pic,prop_d0]	2	559.8013	3.2e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Ac [prop_d0]	3	352.5330	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Ac [pic,prop_d0]	3	373.5366	0.0e+0



Experimental spectrum

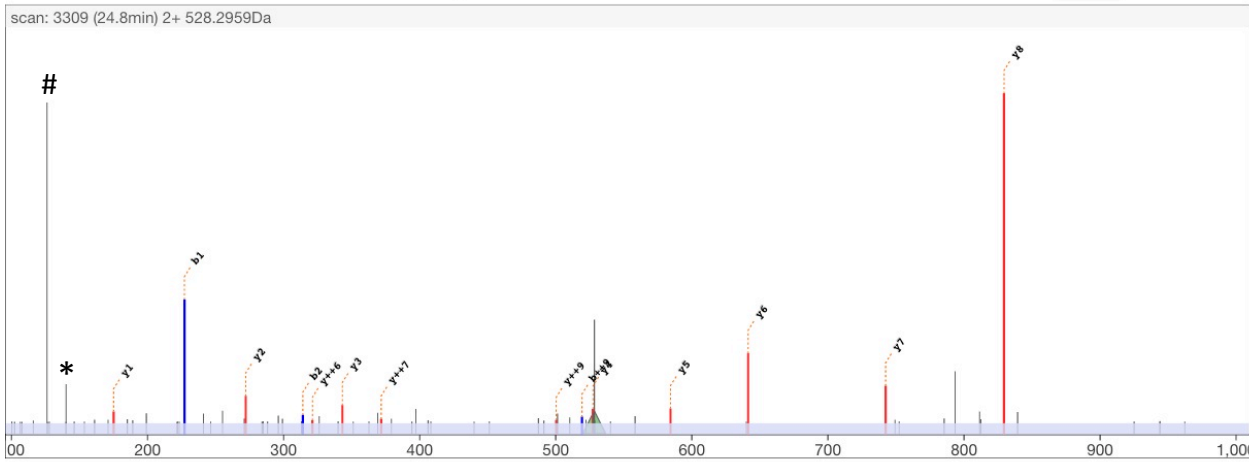
scan 3309
 retention time 24.8min
 precursor m/z 528.2959
 precursor charge 2+

Theoretical

M H²⁺ 528.2958
 MH Δ_{mass} Da 0.0001
 MH Δ_{mass} ppm 0.1

edit peptide

{Propionyl}K{Acetyl}STGGK{Propionyl}APR align



	b++	b		y	y++	
			Propionyl	999.56	500.28	9
1	114.07	227.14	K	829.45	415.23	8
2	157.59	314.17	S	742.42	371.71	7
3	208.11	415.22	T	641.37	321.19	6
4	236.62	472.24	G	584.35	292.68	5
5	265.13	529.26	G	527.33	264.17	4
6	357.20	713.38	K	343.21	172.11	3
7	392.71	784.42	A	272.17	136.59	2
8	441.24	881.47	P	175.12	88.06	1
9	519.29	1037.57	R			

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

Experimental spectrum

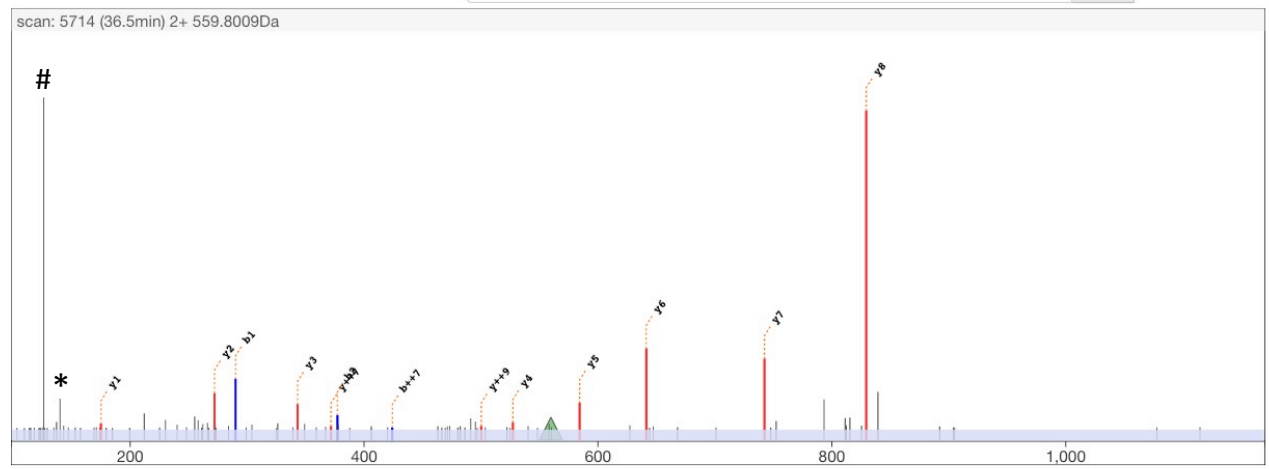
scan 5714
 retention time 36.5min
 precursor m/z 559.8009
 precursor charge 2+

Theoretical

M H²⁺ 559.8013
 MH Δ_{mass} Da -0.0008
 MH Δ_{mass} ppm -0.7

edit peptide

{PIC}K{Acetyl}STGGK{Propionyl}APR

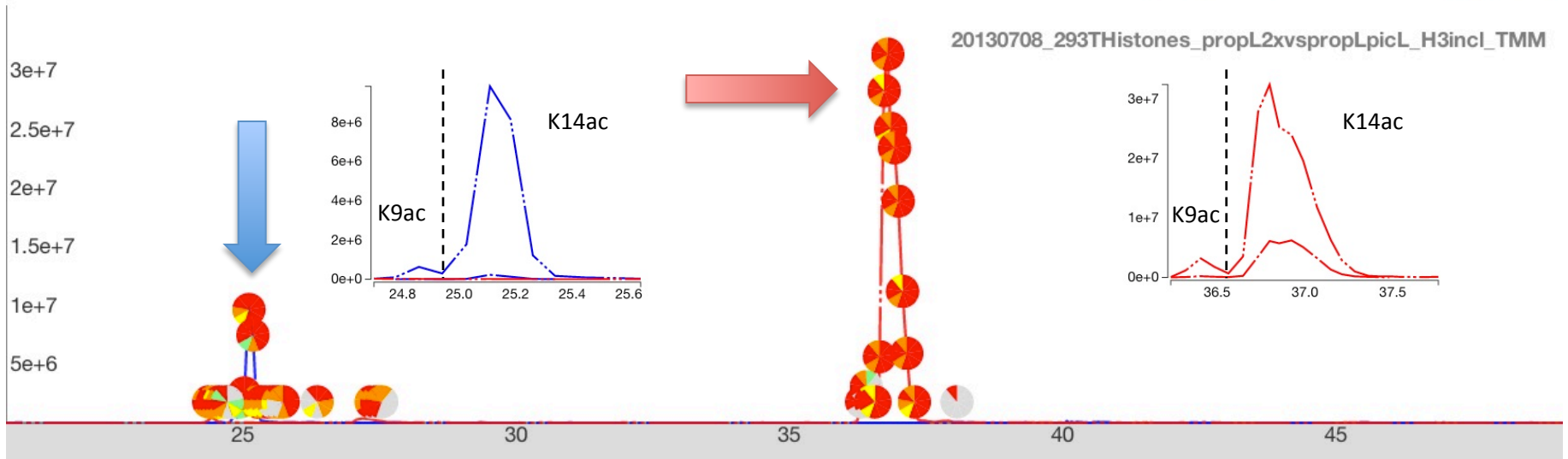


	b++	b		y	y++	
	60.53	120.04	PIC	999.56	500.28	9
1	145.58	290.15	K	829.45	415.23	8
2	189.09	377.18	Acetyl	742.42	371.71	7
3	239.62	478.23	S	641.37	321.19	6
4	268.13	535.25	T	584.35	292.68	5
5	296.64	592.27	G	527.33	264.17	4
6	388.70	776.39	K	343.21	172.11	3
7	424.22	847.43	Propionyl	272.17	136.59	2
8	472.75	944.48	A	175.12	88.06	1
9	550.80	1100.58	P			
			R			

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

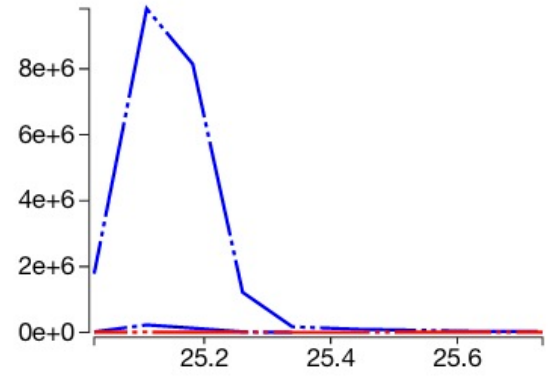
H3_K9-R17: KSTGGKAcAPR

id list per inj.	peptide	2+	3+
20130708_293THistone	H3K14Ac [prop_d0]	528.296	352.533
20130708_293THistone	H3K14Ac [pic,prop_d0]	559.801	373.537



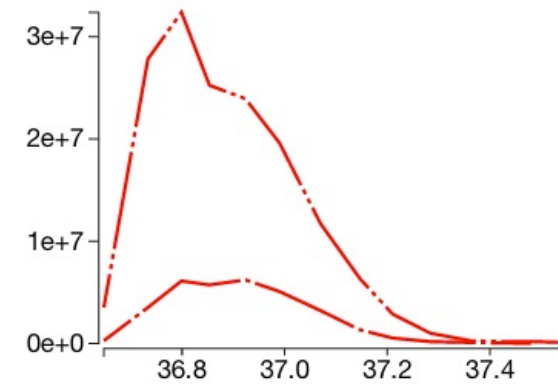
Quanti event: 24.9-25.7min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K14Ac [prop_d0]	1	1055.5844	1.8e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K14Ac [pic,prop_d0]	1	1118.5953	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K14Ac [prop_d0]	2	528.2958	9.5e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K14Ac [pic,prop_d0]	2	559.8013	1.3e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K14Ac [prop_d0]	3	352.5330	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K14Ac [pic,prop_d0]	3	373.5366	0.0e+0



Quanti event: 36.6-37.6min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K14Ac [prop_d0]	1	1055.5844	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K14Ac [pic,prop_d0]	1	1118.5953	1.3e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K14Ac [prop_d0]	2	528.2958	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K14Ac [pic,prop_d0]	2	559.8013	6.3e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K14Ac [prop_d0]	3	352.5330	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K14Ac [pic,prop_d0]	3	373.5366	0.0e+0



Experimental spectrum

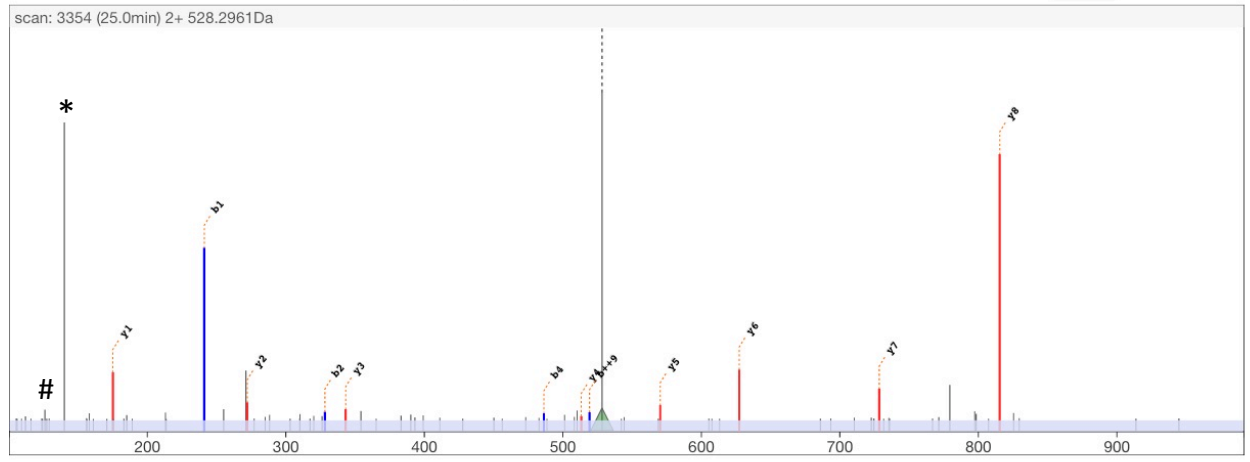
scan 3354
 retention time 25.0min
 precursor m/z 528.2961
 precursor charge 2+

Theoretical

M H²⁺ 528.2958
 MH Δ_{mass} Da 0.0005
 MH Δ_{mass} ppm 0.5

edit peptide

{Propionyl}K{Propionyl}STGGK{Acetyl}APR align



	b++	b	y	y++	
			999.56	500.28	9
1	121.08	241.15	815.44	408.22	8
2	164.60	328.19	728.40	364.71	7
3	215.12	429.23	627.36	314.18	6
4	243.63	486.26	570.34	285.67	5
5	272.14	543.28	513.31	257.16	4
6	357.20	713.38	343.21	172.11	3
7	392.71	784.42	272.17	136.59	2
8	441.24	881.47	175.12	88.06	1
9	519.29	1037.57			

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

Experimental spectrum

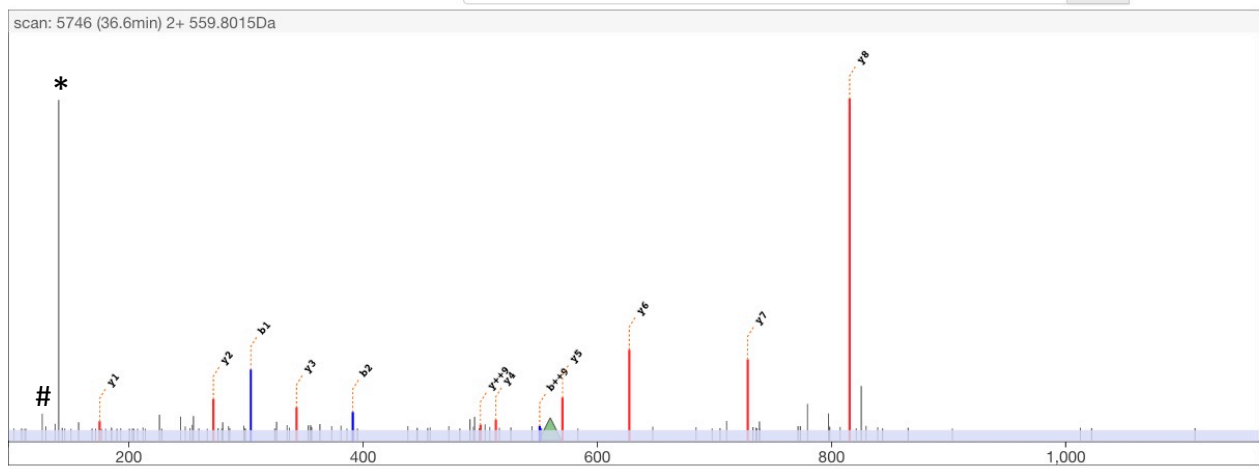
scan 5746
 retention time 36.7min
 precursor m/z 559.8015
 precursor charge 2+

Theoretical

M H²⁺ 559.8013
 MH Δ_{mass} Da 0.0005
 MH Δ_{mass} ppm 0.4

edit peptide

{PIC}K{Propionyl}STGGK{Acetyl}APR align

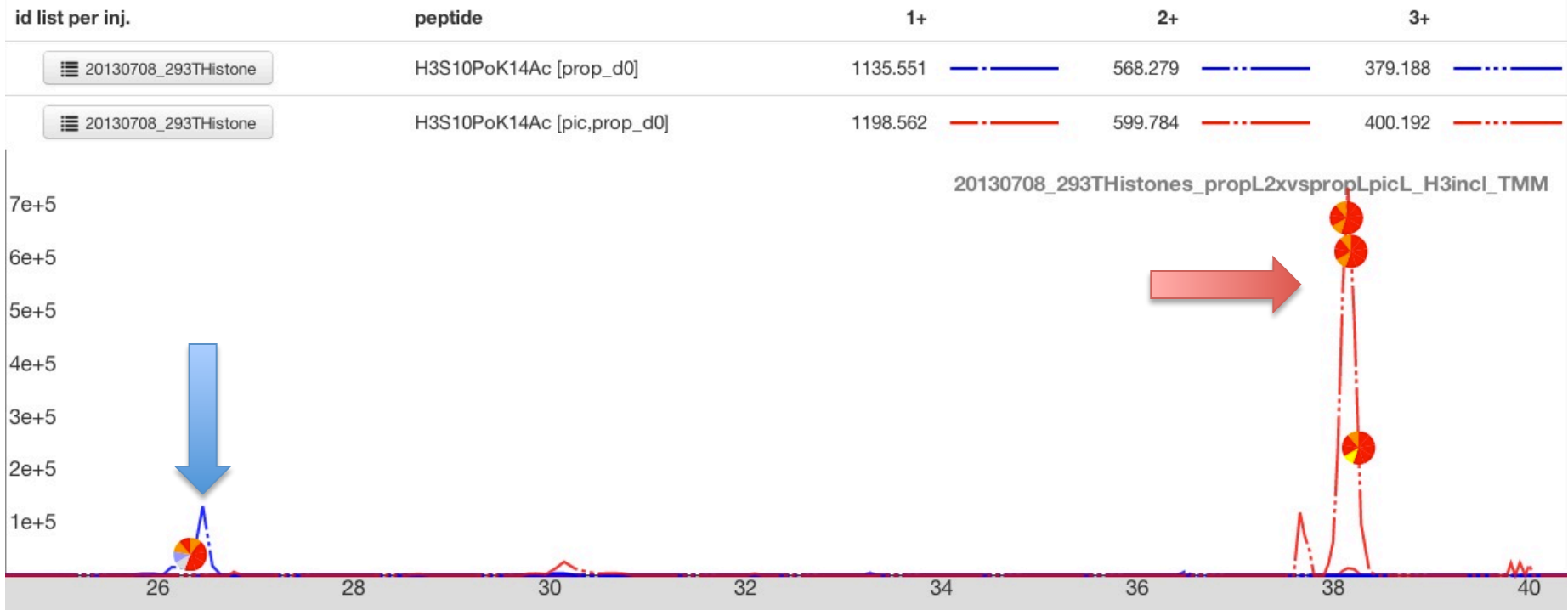


	b++	b		y	y++	
	60.53	120.04	PIC	999.56	500.28	9
1	152.59	304.17	K	815.44	408.22	8
2	196.10	391.20	Propionyl	728.40	364.71	7
3	246.63	492.25	S	627.36	314.18	6
4	275.14	549.27	T	570.34	285.67	5
5	303.65	606.29	G	513.31	257.16	4
6	388.70	776.39	K	343.21	172.11	3
7	424.22	847.43	Acetyl	272.17	136.59	2
8	472.75	944.48	A	175.12	88.06	1
9	550.80	1100.58	P			
			R			

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

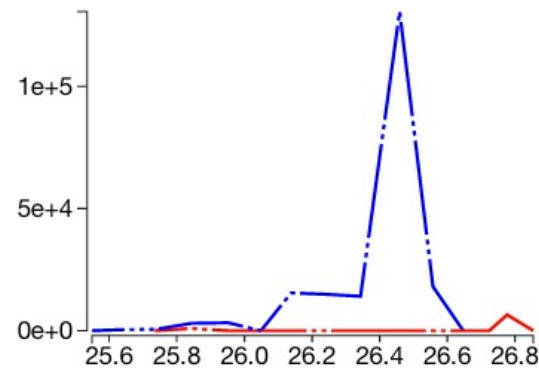
H3_K9-R17:

KSPoTGGKAcAPR



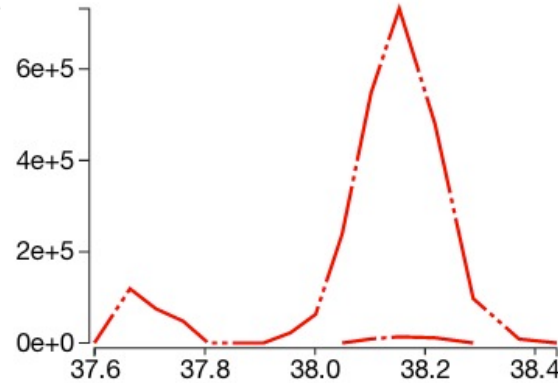
Quanti event: 25.4-27.5min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PoK14Ac [prop_d0]	1	1135.5507	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PoK14Ac [pic,prop_d0]	1	1198.5616	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PoK14Ac [prop_d0]	2	568.2790	1.2e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PoK14Ac [pic,prop_d0]	2	599.7844	3.1e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PoK14Ac [prop_d0]	3	379.1884	4.5e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PoK14Ac [pic,prop_d0]	3	400.1921	0.0e+0



Quanti event: 37.3-38.8min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PoK14Ac [prop_d0]	1	1135.5507	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PoK14Ac [pic,prop_d0]	1	1198.5616	1.2e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PoK14Ac [prop_d0]	2	568.2790	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PoK14Ac [pic,prop_d0]	2	599.7844	8.4e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PoK14Ac [prop_d0]	3	379.1884	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PoK14Ac [pic,prop_d0]	3	400.1921	0.0e+0



H3_K9-R17: Prop-KSPoTGGKAcAPR MS/MS

Experimental spectrum

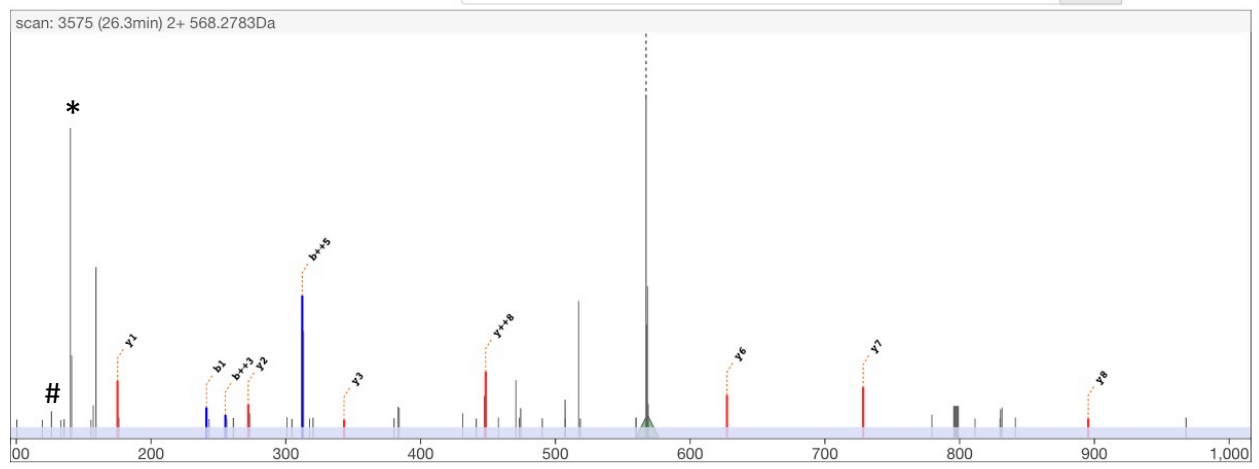
scan 3575
 retention time 26.3min
 precursor m/z 568.2783
 precursor charge 2+

Theoretical

M H²⁺ 568.2790
 MH Δ_{mass} Da -0.0015
 MH Δ_{mass} ppm -1.3

edit peptide

{Propionyl}K{Propionyl}S{Phospho}TGGK{Acetyl}APR align



Anchor	Current
click on peak	mouse over peak
m/z 895.4161	m/z 797.4393
intensity 102	intensity 248
int. rank 42	int. rank 15

Explanation?
 delta mass could be...
 $\Delta_{m/z}$ -97.97681

Tune the seq
 Align anchor peak

	b++	b	y	y++	
			1079.52	540.27	9
1	121.08	241.15	895.40	448.21	8
2	204.58	408.15	728.40	364.71	7
3	255.10	509.20	627.36	314.18	6
4	283.61	566.22	570.34	285.67	5
5	312.13	623.24	513.31	257.16	4
6	397.18	793.35	343.21	172.11	3
7	432.70	864.39	272.17	136.59	2
8	481.22	961.44	175.12	88.06	1
9	559.27	1117.54			

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

y8 - H3PO4

H3_K9-R17: PIC-KSPoTGGKAcAPR MS/MS

Experimental spectrum

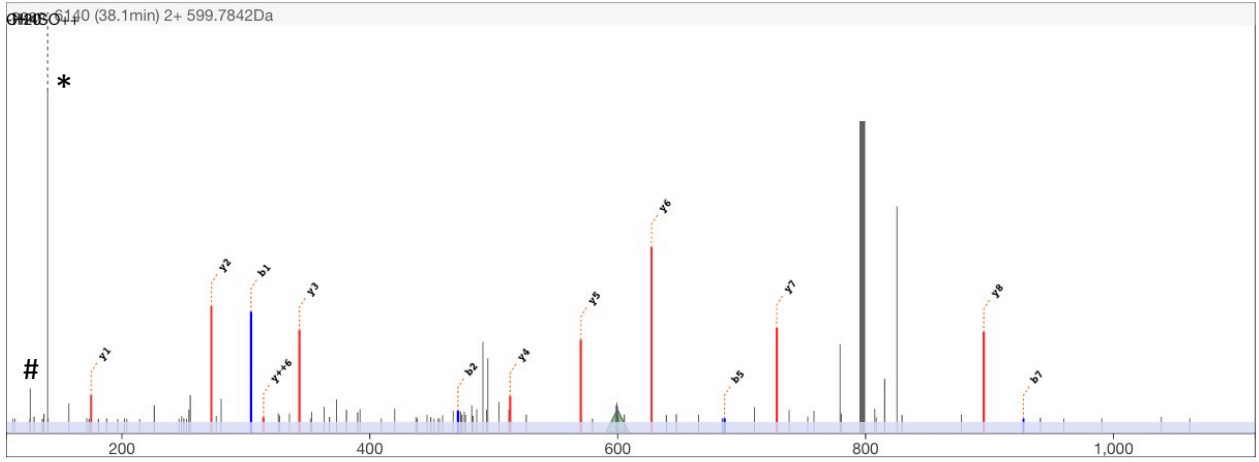
scan 6140
 retention time 38.1min
 precursor m/z 599.7842
 precursor charge 2+

Theoretical

M H²⁺ 599.7844
 MH Δ_{mass} Da -0.0005
 MH Δ_{mass} ppm -0.4

edit peptide

{PIC}K{Propionyl}S{Phospho}TGGK{Acetyl}APR



	b++	b		y	y++	
	60.53	120.04	PIC	1079.52	540.27	9
1	152.59	304.17	K	895.40	448.21	8
2	236.09	471.16	S	728.40	364.71	7
3	286.61	572.21	Phospho	627.36	314.18	6
4	315.12	629.23	T	570.34	285.67	5
5	343.63	686.25	G	513.31	257.16	4
6	428.68	856.36	K	343.21	172.11	3
7	464.20	927.40	Acetyl	272.17	136.59	2
8	512.73	1024.45	A	175.12	88.06	1
9	590.78	1180.55	P			
			R			

Anchor	Current
click on peak	mouse over peak
m/z 895.4010	m/z 797.4262
intensity 11640	intensity 38895
int. rank 6	int. rank 96

Explanation?
 delta mass could be...
 $\Delta_{m/z}$ -97.97479

Tune the seq
 Align anchor peak

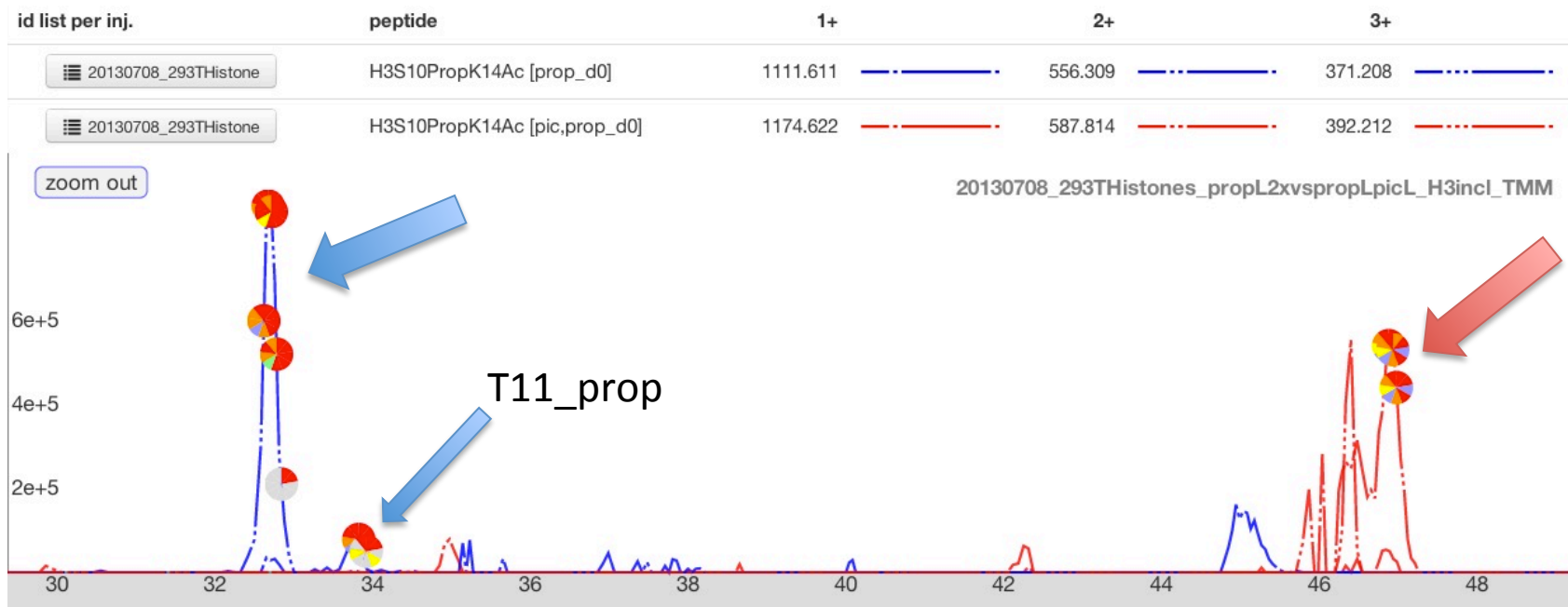


y8 - H3PO4

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

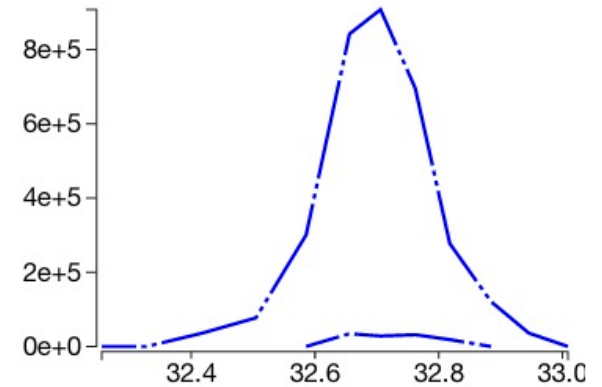
H3_K9-R17:

KS**Prop**TGGK**Ac**APR



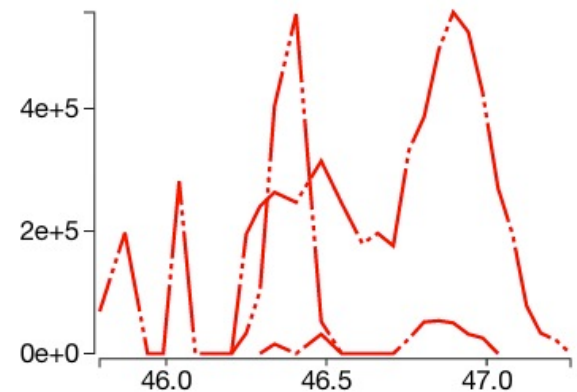
Quanti event: 32.2-33.2min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PropK14Ac [prop_d0]	1	1111.6106	3.9e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PropK14Ac [pic,prop_d0]	1	1174.6215	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PropK14Ac [prop_d0]	2	556.3089	1.2e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PropK14Ac [pic,prop_d0]	2	587.8144	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PropK14Ac [prop_d0]	3	371.2084	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PropK14Ac [pic,prop_d0]	3	392.2120	0.0e+0



Quanti event: 45.7-47.3min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PropK14Ac [prop_d0]	1	1111.6106	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PropK14Ac [pic,prop_d0]	1	1174.6215	8.4e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PropK14Ac [prop_d0]	2	556.3089	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PropK14Ac [pic,prop_d0]	2	587.8144	1.8e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PropK14Ac [prop_d0]	3	371.2084	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3S10PropK14Ac [pic,prop_d0]	3	392.2120	4.4e+6



Experimental spectrum

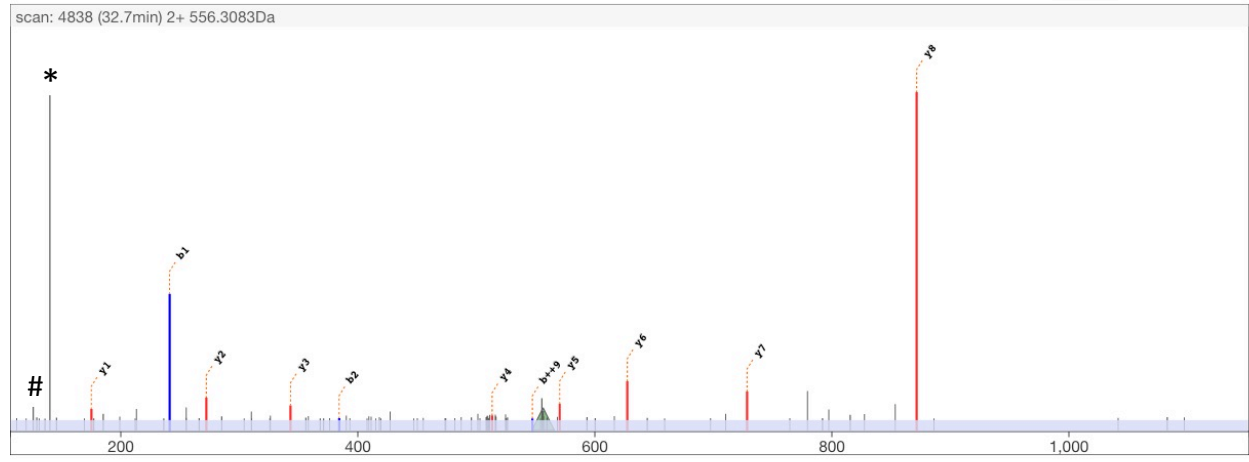
scan 4838
 retention time 32.7min
 precursor m/z 556.3083
 precursor charge 2+

Theoretical

M H²⁺ 556.3089
 MH Δ_{mass} Da -0.0012
 MH Δ_{mass} ppm -1.1

edit peptide

{Propionyl}K{Propionyl}S{Propionyl}TGGK{Acetyl}APR



	b++	b	y	y++	
			1055.58	528.30	9
1	121.08	241.15	871.46	436.24	8
2	192.61	384.21	728.40	364.71	7
3	243.13	485.26	627.36	314.18	6
4	271.64	542.28	570.34	285.67	5
5	300.16	599.30	513.31	257.16	4
6	385.21	769.41	343.21	172.11	3
7	420.73	840.45	272.17	136.59	2
8	469.25	937.50	175.12	88.06	1
9	547.30	1093.60			

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

Experimental spectrum

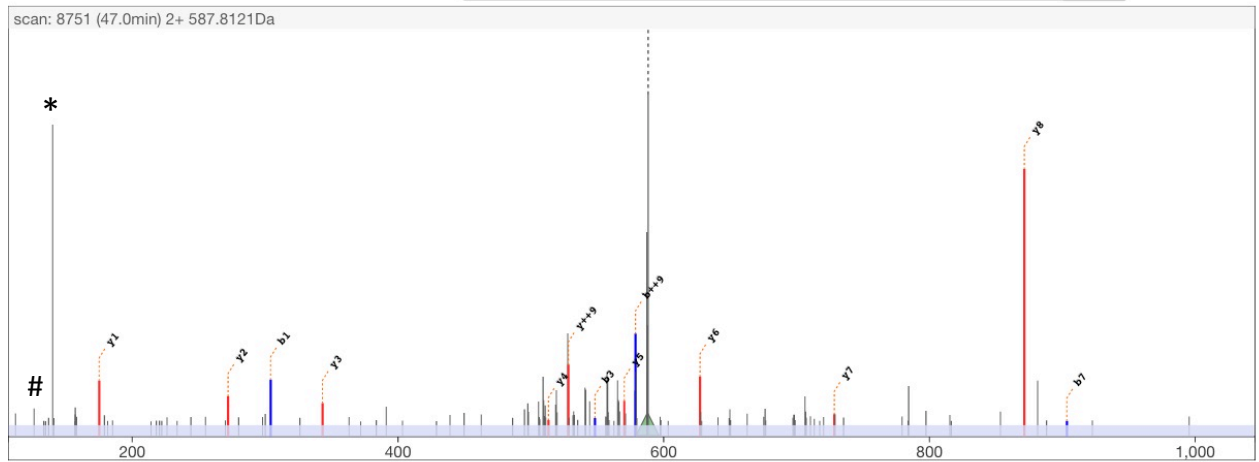
scan 8751
 retention time 47.0min
 precursor m/z 587.8121
 precursor charge 2+

Theoretical

M H²⁺ 587.8144
 MH Δ_{mass} Da -0.0045
 MH Δ_{mass} ppm -3.8

edit peptide

{PIC}K{Propionyl}S{Propionyl}TGGK{Acetyl}APR align

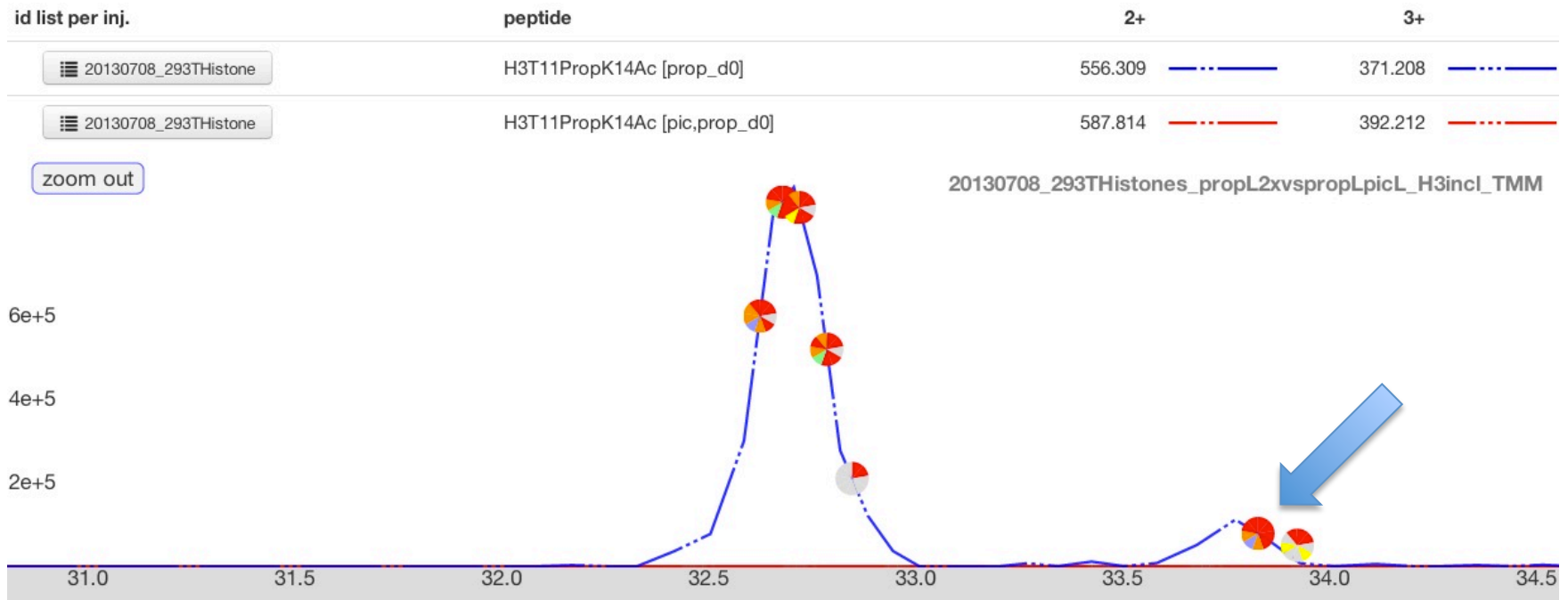


	b++	b		y	y++	
	60.53	120.04	PIC	1055.58	528.30	9
1	152.59	304.17	K	871.46	436.24	8
2	224.12	447.22	S	728.40	364.71	7
3	274.64	548.27	Propionyl	627.36	314.18	6
4	303.15	605.29	T	570.34	285.67	5
5	331.66	662.31	G	513.31	257.16	4
6	416.71	832.42	G	343.21	172.11	3
7	452.23	903.46	K	272.17	136.59	2
8	500.76	1000.51	Acetyl	175.12	88.06	1
9	578.81	1156.61	A			
			P			
			R			

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

H3_K9-R17:

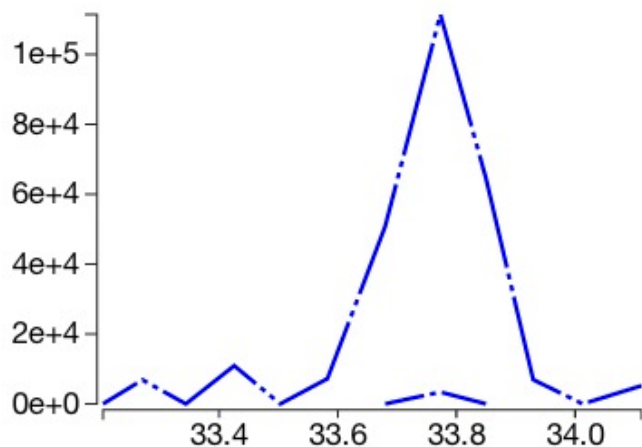
KSTPropGGKAcAPR



Quanti event: 33.1-34.2min



injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3T11PropK14Ac [prop_d0]	1	1111.6106	1.7e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3T11PropK14Ac [pic,prop_d0]	1	1174.6215	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3T11PropK14Ac [prop_d0]	2	556.3089	1.3e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3T11PropK14Ac [pic,prop_d0]	2	587.8144	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3T11PropK14Ac [prop_d0]	3	371.2084	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3T11PropK14Ac [pic,prop_d0]	3	392.2120	0.0e+0



No peaks detected for PIC-labeling.

H3_K9-R17: Prop-KSTPropGGKAcAPR MS/MS

Experimental spectrum

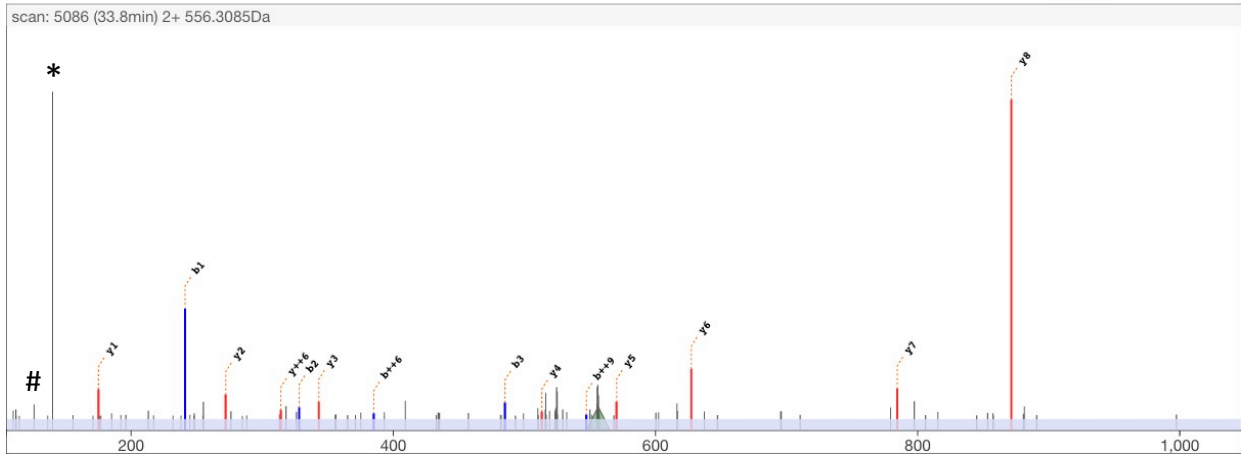
scan 5086
 retention time 33.8min
 precursor m/z 556.3085
 precursor charge 2+

Theoretical

M H²⁺ 556.3089
 MH Δ_{mass} Da -0.0009
 MH Δ_{mass} ppm -0.8

edit peptide

{Propionyl}K{Propionyl}ST{Propionyl}GGK{Acetyl}APR

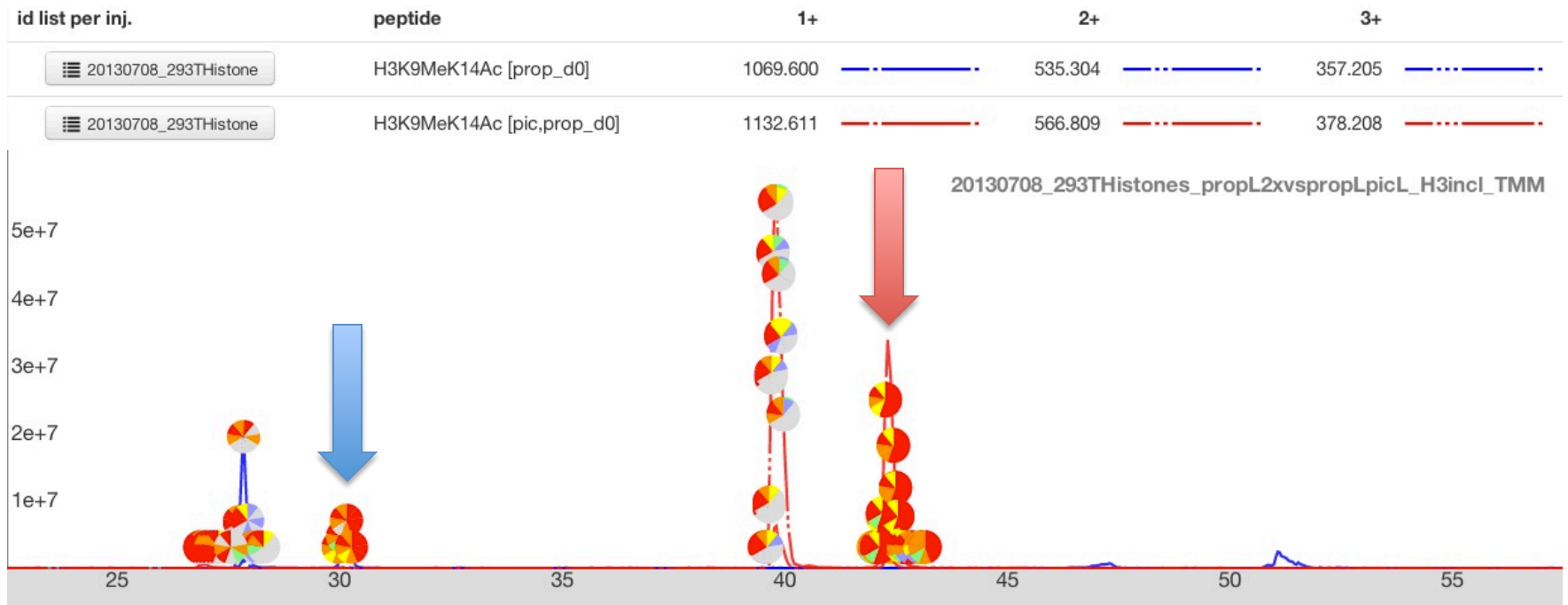


	b++	b		y	y++	
			Propionyl	1055.58	528.30	9
1	121.08	241.15	K	871.46	436.24	8
2	164.60	328.19	Propionyl	784.43	392.72	7
3	243.13	485.26	S	627.36	314.18	6
4	271.64	542.28	T	570.34	285.67	5
5	300.16	599.30	Propionyl	513.31	257.16	4
6	385.21	769.41	G	343.21	172.11	3
7	420.73	840.45	K	272.17	136.59	2
8	469.25	937.50	Acetyl	175.12	88.06	1
9	547.30	1093.60	A			
			P			
			R			

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

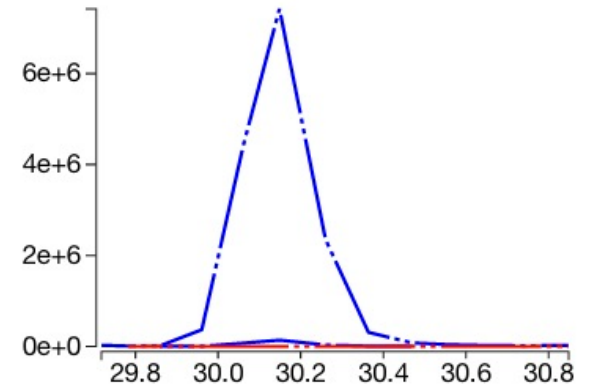
H3_K9-R17:

KMe1STGGKAcAPR



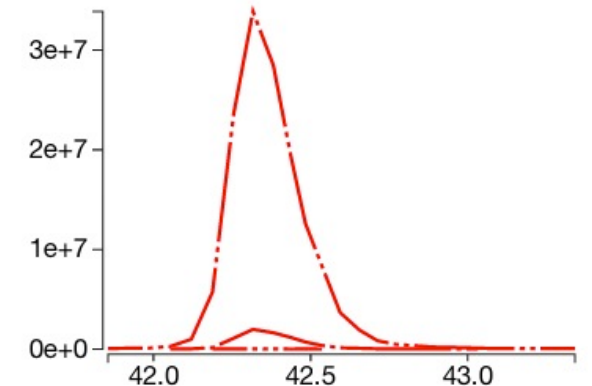
Quanti event: 29.7-30.9min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeK14Ac [prop_d0]	1	1069.6000	1.5e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeK14Ac [pic,prop_d0]	1	1132.6109	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeK14Ac [prop_d0]	2	535.3037	9.0e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeK14Ac [pic,prop_d0]	2	566.8091	4.1e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeK14Ac [prop_d0]	3	357.2049	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeK14Ac [pic,prop_d0]	3	378.2085	0.0e+0



Quanti event: 41.8-43.4min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeK14Ac [prop_d0]	1	1069.6000	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeK14Ac [pic,prop_d0]	1	1132.6109	2.6e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeK14Ac [prop_d0]	2	535.3037	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeK14Ac [pic,prop_d0]	2	566.8091	5.0e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeK14Ac [prop_d0]	3	357.2049	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeK14Ac [pic,prop_d0]	3	378.2085	3.5e+5



H3_K9-R17: Prop-KMe1STGGKAcAPR MS/MS

Experimental spectrum

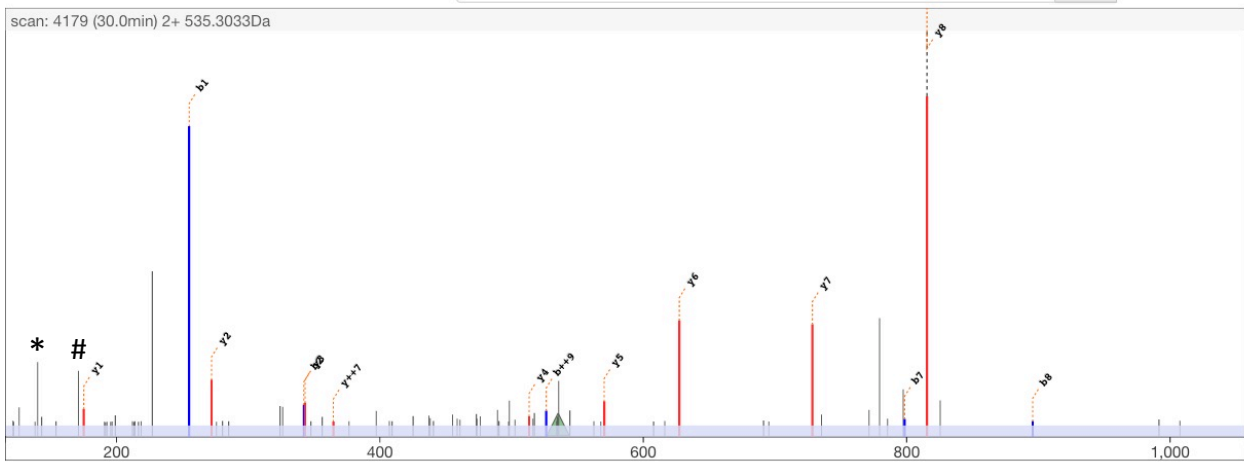
scan 4179
 retention time 30.0min
 precursor m/z 535.3033
 precursor charge 2+

Theoretical

M H²⁺ 535.3037
 MH Δ_{mass} Da -0.0006
 MH Δ_{mass} ppm -0.6

edit peptide

{Propionyl}K{Methyl,Propionyl}STGGK{Acetyl}APR align



	b++	b		y	y++	
			Propionyl	1013.57	507.29	9
1	128.09	255.17	K	815.44	408.22	8
2	171.60	342.20	Methyl,Propionyl	728.40	364.71	7
3	222.13	443.25	S	627.36	314.18	6
4	250.64	500.27	T	570.34	285.67	5
5	279.15	557.29	G	513.31	257.16	4
6	364.20	727.40	K	343.21	172.11	3
7	399.72	798.44	Acetyl	272.17	136.59	2
8	448.25	895.49	A	175.12	88.06	1
9	526.30	1051.59	P			
			R			

* = 126Da diagnostic ion

= 171Da diagnostic ion

Experimental spectrum

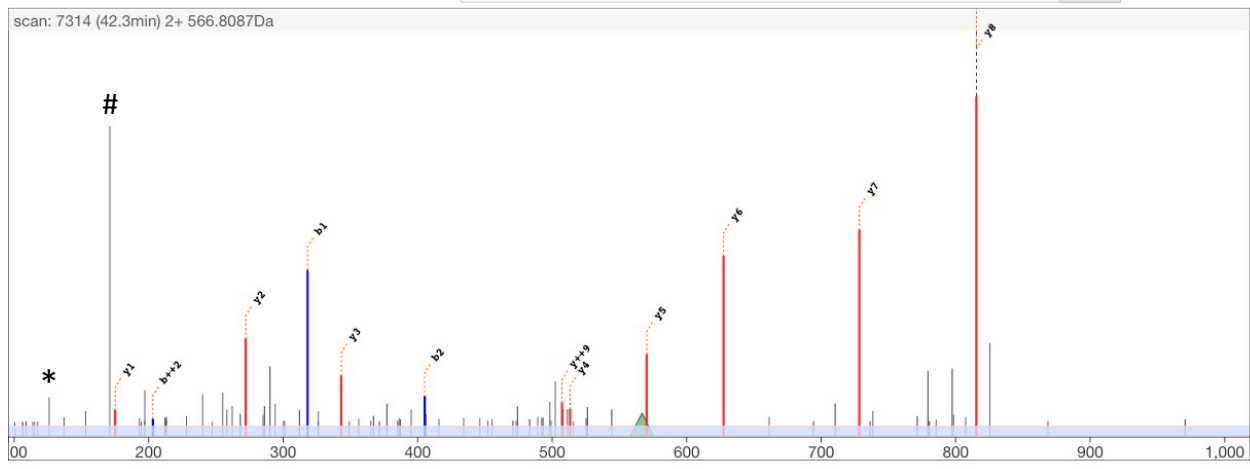
scan 7314
 retention time 42.3min
 precursor m/z 566.8087
 precursor charge 2+

Theoretical

M H²⁺ 566.8091
 MH Δ_{mass} Da -0.0008
 MH Δ_{mass} ppm -0.7

edit peptide

{PIC}K{Methyl,Propionyl}STGGK{Acetyl}APR align



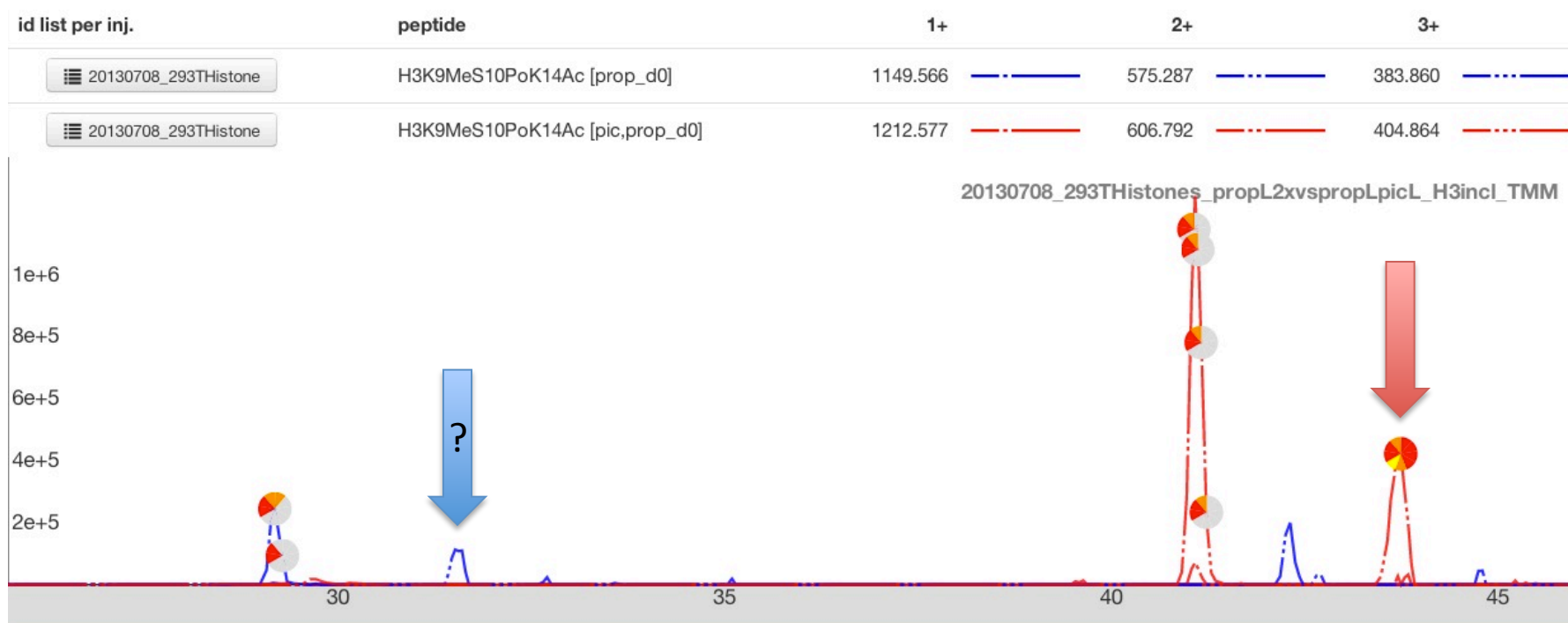
	b++	b		y	y++	
	60.53	120.04	PIC	1013.57	507.29	9
1	159.59	318.18	K	815.44	408.22	8
2	203.11	405.21	Methyl,Propionyl	728.40	364.71	7
3	253.63	506.26	S	627.36	314.18	6
4	282.14	563.28	T	570.34	285.67	5
5	310.66	620.30	G	513.31	257.16	4
6	395.71	790.41	K	343.21	172.11	3
7	431.23	861.45	Acetyl	272.17	136.59	2
8	479.75	958.50	A	175.12	88.06	1
9	557.80	1114.60	P			
			R			

* = 126Da diagnostic ion
 # = 171Da diagnostic ion

H3_K9-R17:

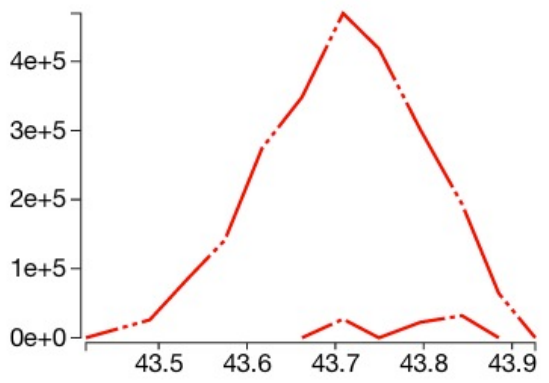
KMe1SPoTGGKAcAPR

No MS2 for Prop-labeling detected in peak with correct retention-time shift.



Quanti event: 43.2-44.1min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeS10PoK14Ac [prop_d0]	1	1149.5664	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeS10PoK14Ac [pic,prop_d0]	1	1212.5773	2.2e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeS10PoK14Ac [prop_d0]	2	575.2868	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeS10PoK14Ac [pic,prop_d0]	2	606.7923	6.2e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeS10PoK14Ac [prop_d0]	3	383.8603	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeS10PoK14Ac [pic,prop_d0]	3	404.8639	0.0e+0



No peaks identified for Prop-labeling.

Experimental spectrum

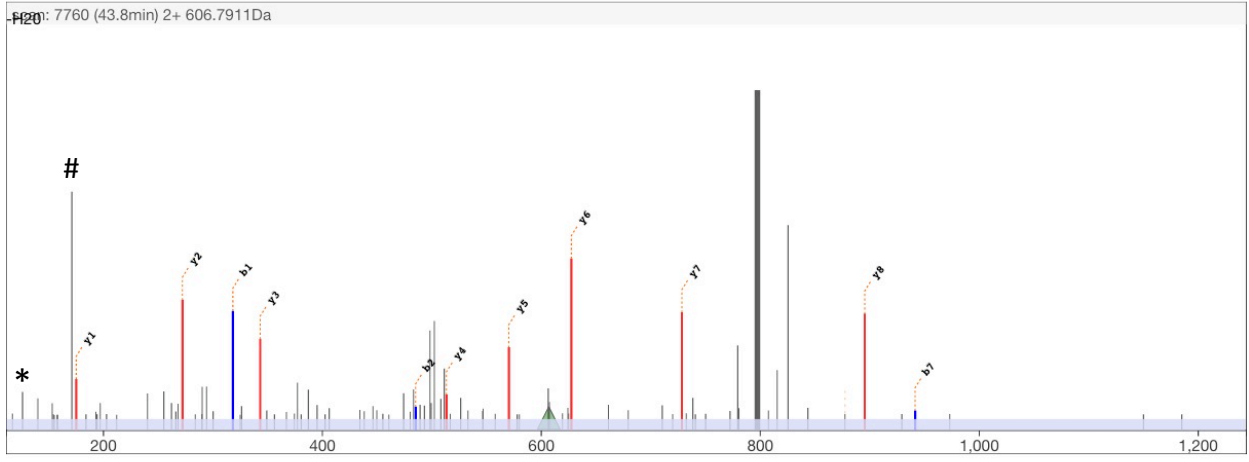
scan 7760
 retention time 43.7min
 precursor m/z 606.7911
 precursor charge 2+

Theoretical

M H²⁺ 606.7923
 MH Δ_{mass} Da -0.0023
 MH Δ_{mass} ppm -1.9

edit peptide

{PIC}K{Methyl,Propionyl}S{Phospho}TGGK{Acetyl}APR



	b++	b		y	y++
	60.53	120.04	PIC	1093.54	547.27
1	159.59	318.18	K	895.40	448.21
2	243.09	485.18	Methyl,Propionyl	728.40	364.71
3	293.62	586.23	S	627.36	314.18
4	322.13	643.25	Phospho	570.34	285.67
5	350.64	700.27	T	513.31	257.16
6	435.69	870.38	G	343.21	172.11
7	471.21	941.41	K	272.17	136.59
8	519.74	1038.47	Acetyl	175.12	88.06
9	597.79	1194.57	A		
			P		
			R		

Anchor	Current
click on peak	mouse over peak
m/z 895.4007	m/z 797.4244
intensity 7984	intensity 24889
int. rank 7	int. rank 0

Explanation?
 delta mass could be...
 Δ_{m/z} -97.97626

Tune the seq
 Align anchor peak

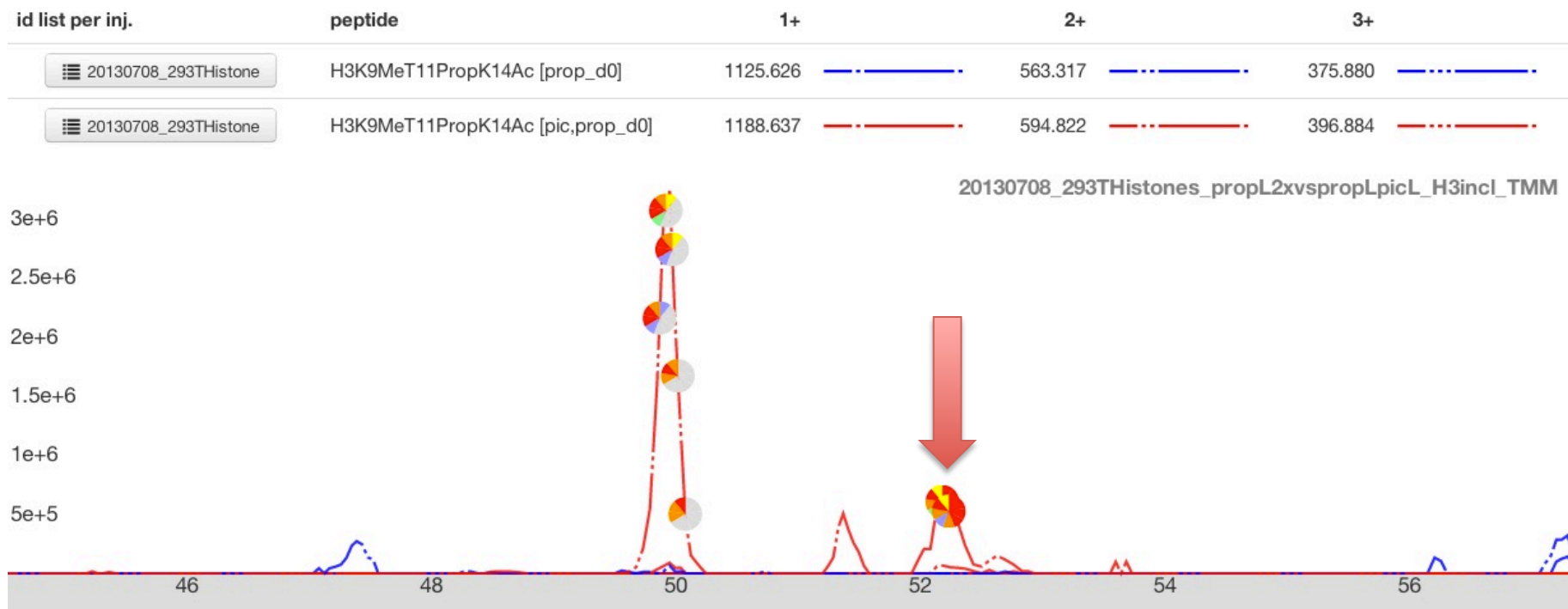
↑
 y8 - H3PO4

* = 126Da diagnostic ion
 # = 171Da diagnostic ion

H3_K9-R17:

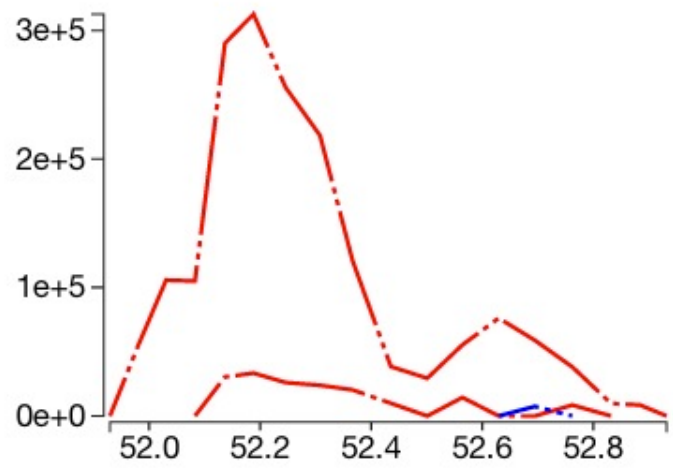
KMe**1**Sor**T****Prop**GG**K**Ac**APR**

Peak contains overlapping spectra for either PTM. T11prop shown, no MS2 found for Prop-labeling.



Quanti event: 51.9-53.1min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeT11PropK14Ac [prop_d0]	1	1125.6263	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeT11PropK14Ac [pic,prop_d0]	1	1188.6372	5.9e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeT11PropK14Ac [prop_d0]	2	563.3168	3.0e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeT11PropK14Ac [pic,prop_d0]	2	594.8222	6.2e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeT11PropK14Ac [prop_d0]	3	375.8803	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9MeT11PropK14Ac [pic,prop_d0]	3	396.8839	0.0e+0



No peak identified for Prop-labeling.

Experimental spectrum

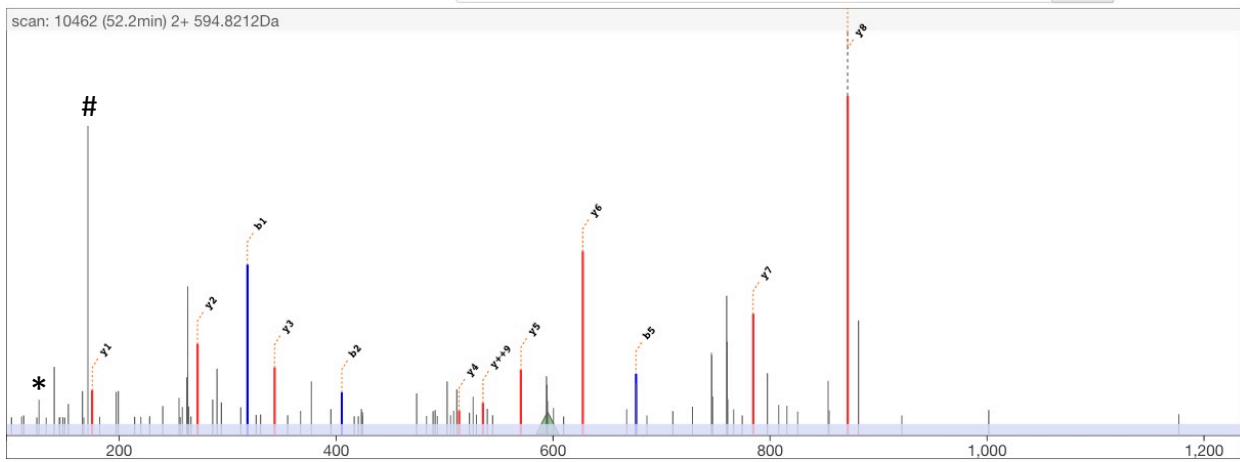
scan 10462
 retention time 52.2min
 precursor m/z 594.8212
 precursor charge 2+

Theoretical

M H²⁺ 594.8222
 MH Δ_{mass} Da -0.0021
 MH Δ_{mass} ppm -1.8

edit peptide

{PIC}K{Methyl,Propionyl}ST{Propionyl}GGK{Acetyl}APR align



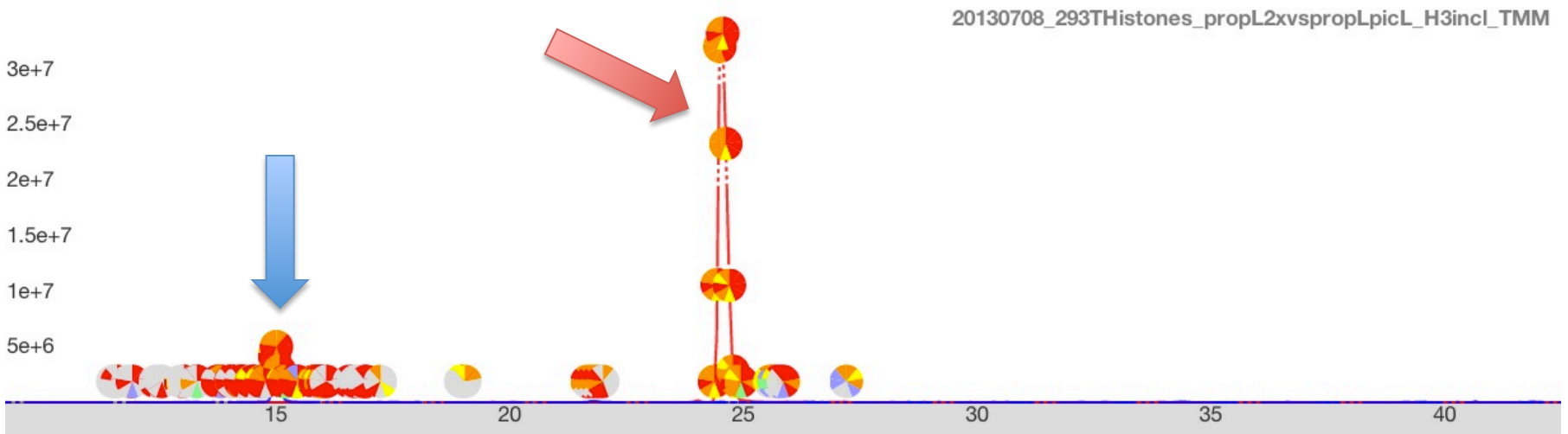
	b++	b		y	y++	
	60.53	120.04	PIC	1069.60	535.30	9
1	159.59	318.18	K	871.46	436.24	8
2	203.11	405.21	Methyl,Propionyl	784.43	392.72	7
3	281.65	562.29	S	627.36	314.18	6
4	310.16	619.31	T	570.34	285.67	5
5	338.67	676.33	Propionyl	513.31	257.16	4
6	423.72	846.44	G	343.21	172.11	3
7	459.24	917.47	K	272.17	136.59	2
8	507.77	1014.53	Acetyl	175.12	88.06	1
9	585.82	1170.63	A			
			P			
			R			

* = 126Da diagnostic ion
 # = 171Da diagnostic ion

H3_K9-R17:

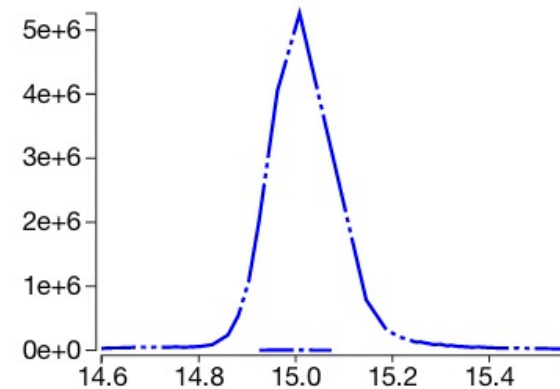
KMe2STGGKAcAPR

id list per inj.	peptide	1+	2+	3+
☰ 20130708_293THistone	H3K9Me2K14Ac [prop_d0]	1027.589	514.298	343.201
☰ 20130708_293THistone	H3K9Me2K14Ac [pic]	1090.600	545.804	364.205



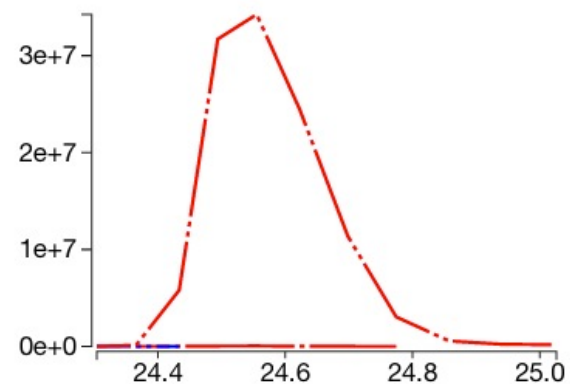
Quanti event: 14.6-15.6min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2K14Ac [prop_d0]	1	1027.5895	6.4e+3
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2K14Ac [pic]	1	1090.6004	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2K14Ac [prop_d0]	2	514.2984	5.2e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2K14Ac [pic]	2	545.8038	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2K14Ac [prop_d0]	3	343.2013	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2K14Ac [pic]	3	364.2050	0.0e+0



Quanti event: 24.3-25.0min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2K14Ac [prop_d0]	1	1027.5895	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2K14Ac [pic]	1	1090.6004	4.1e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2K14Ac [prop_d0]	2	514.2984	1.2e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2K14Ac [pic]	2	545.8038	4.5e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2K14Ac [prop_d0]	3	343.2013	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2K14Ac [pic]	3	364.2050	0.0e+0



Experimental spectrum

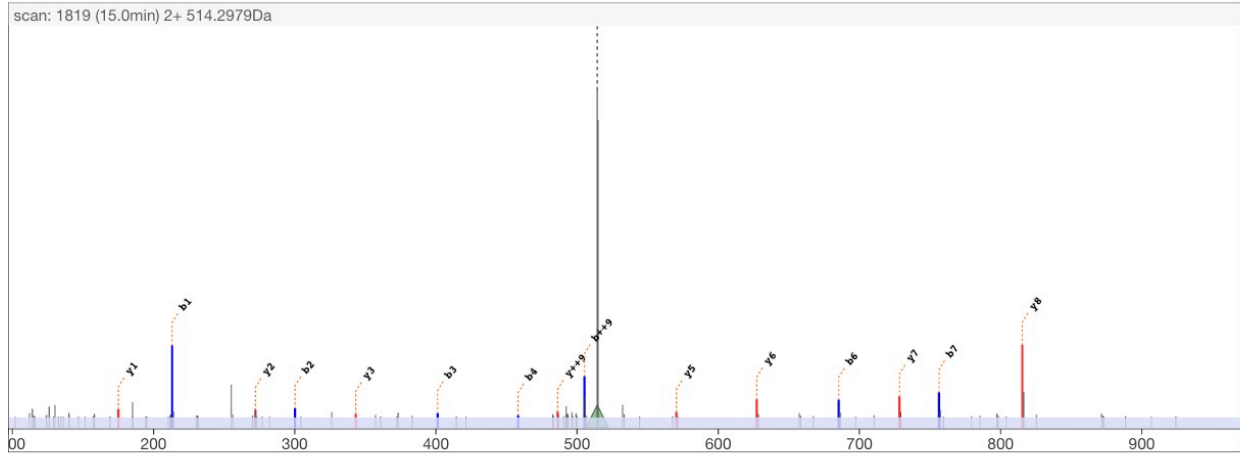
scan 1819
 retention time 15.0min
 precursor m/z 514.2979
 precursor charge 2+

Theoretical

M H²⁺ 514.2984
 MH Δ_{mass} Da -0.0009
 MH Δ_{mass} ppm -0.9

edit peptide

{Propionyl}K{Dimethyl}STGGK{Acetyl}APR align



	b++	b	y	y++	
1	107.08	213.16	971.56	486.29	9
2	150.60	300.19	815.44	408.22	8
3	201.12	401.24	728.40	364.71	7
4	229.63	458.26	627.36	314.18	6
5	258.14	515.28	570.34	285.67	5
6	343.20	685.39	513.31	257.16	4
7	378.72	756.43	343.21	172.11	3
8	427.24	853.48	272.17	136.59	2
9	505.29	1009.58	175.12	88.06	1

Propionyl
 K
 Dimethyl
 S
 T
 G
 K
 Acetyl
 A
 P
 R

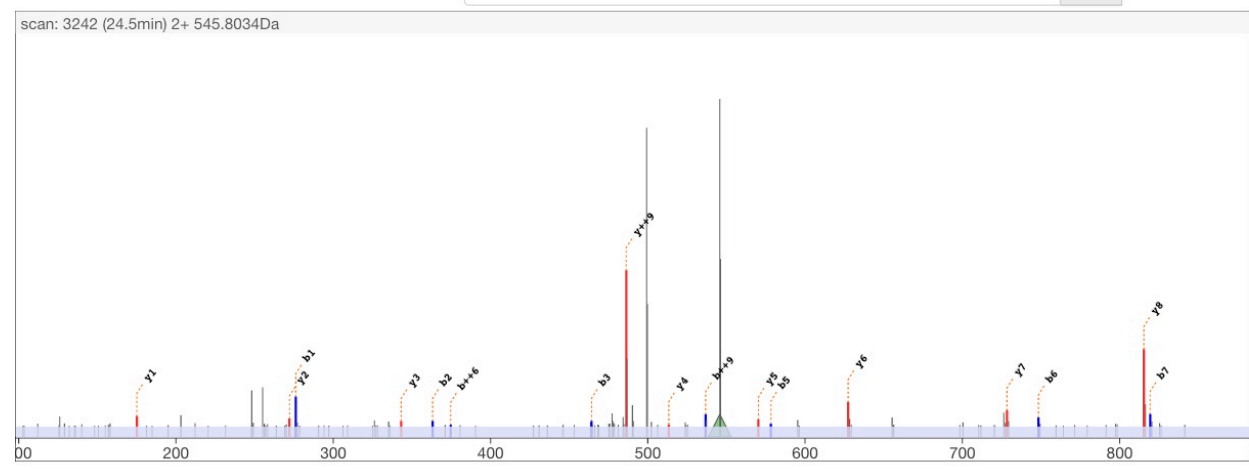
Experimental spectrum

scan 3242
 retention time 24.5min
 precursor m/z 545.8034
 precursor charge 2+

Theoretical

M H²⁺ 545.8038
 MH Δ_{mass} Da -0.0008
 MH Δ_{mass} ppm -0.8

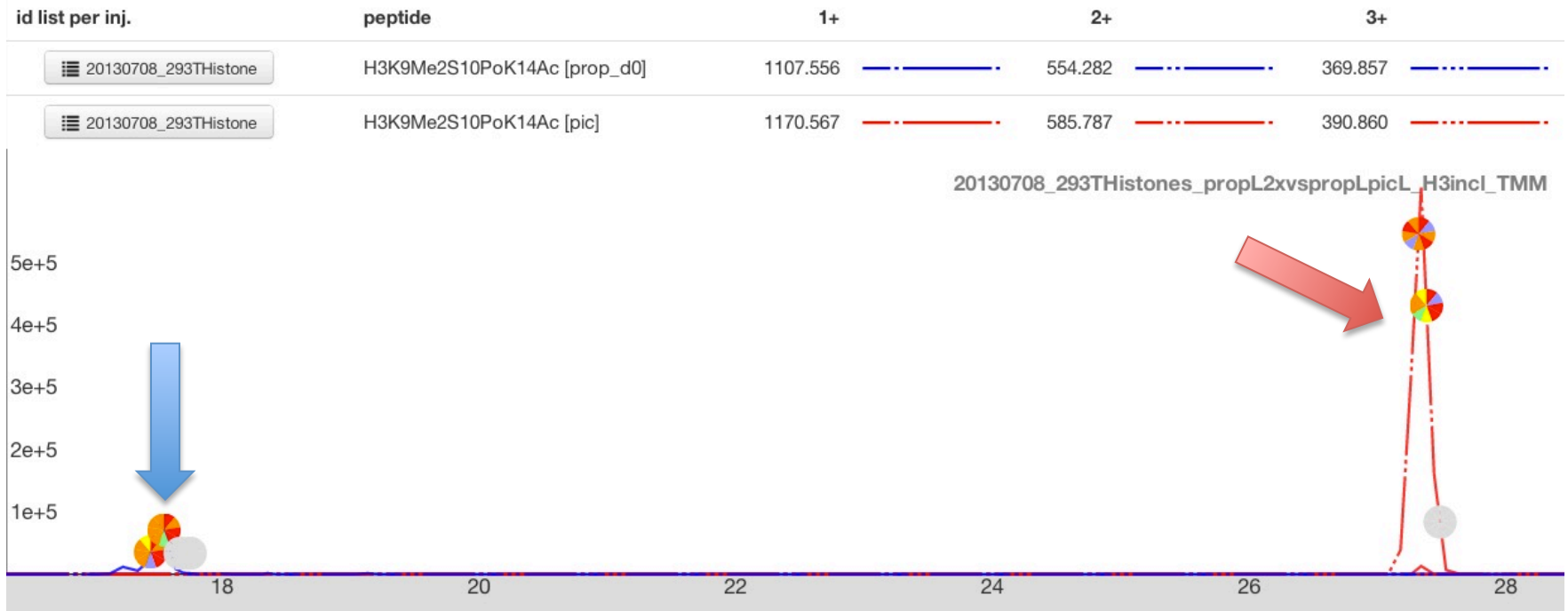
edit peptide



	b++	b		y	y++	
	60.53	120.04	PIC	971.56	486.29	9
1	138.59	276.17	K	815.44	408.22	8
2	182.10	363.20	S	728.40	364.71	7
3	232.63	464.25	T	627.36	314.18	6
4	261.14	521.27	G	570.34	285.67	5
5	289.65	578.29	G	513.31	257.16	4
6	374.70	748.40	K	343.21	172.11	3
7	410.22	819.44	Acetyl	272.17	136.59	2
8	458.75	916.49	A	175.12	88.06	1
9	536.80	1072.59	P			
			R			

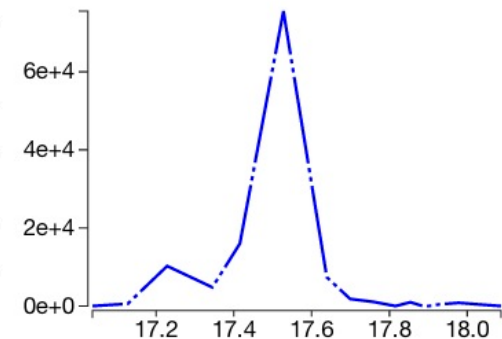
H3_K9-R17:

KMe2SPoTGGKAcAPR



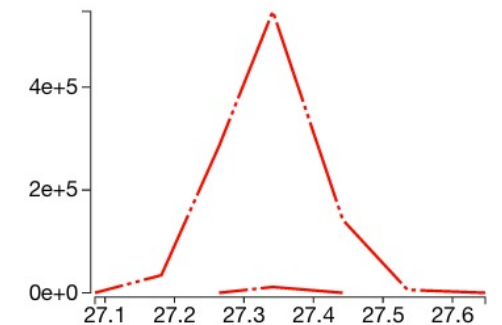
Quanti event: 16.6-18.2min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PoK14Ac [prop_d0]	1	1107.5558	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PoK14Ac [pic]	1	1170.5667	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PoK14Ac [prop_d0]	2	554.2815	7.5e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PoK14Ac [pic]	2	585.7870	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PoK14Ac [prop_d0]	3	369.8568	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PoK14Ac [pic]	3	390.8604	0.0e+0



Quanti event: 26.7-28.1min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PoK14Ac [prop_d0]	1	1107.5558	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PoK14Ac [pic]	1	1170.5667	6.1e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PoK14Ac [prop_d0]	2	554.2815	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PoK14Ac [pic]	2	585.7870	5.3e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PoK14Ac [prop_d0]	3	369.8568	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PoK14Ac [pic]	3	390.8604	0.0e+0



Experimental spectrum

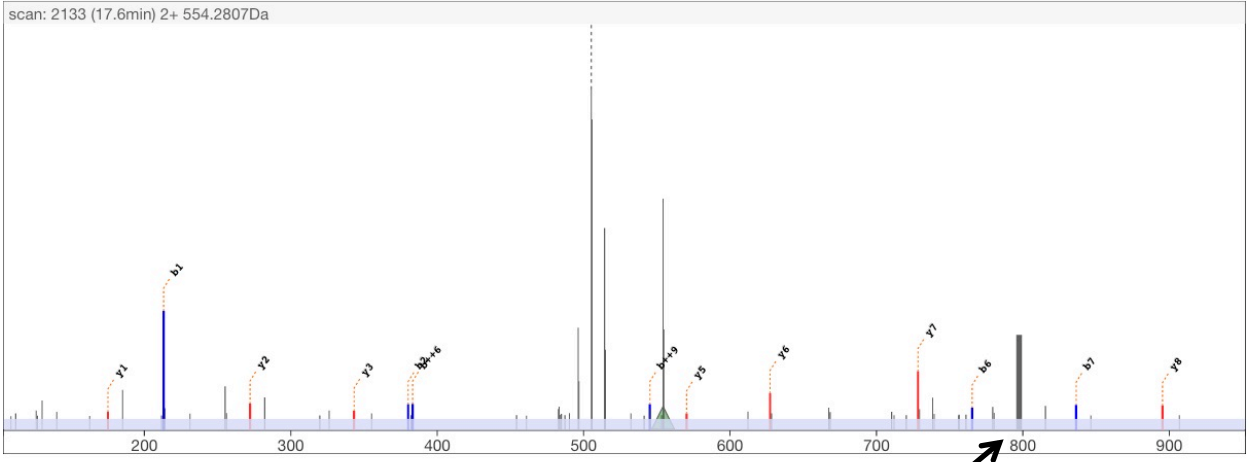
scan 2133
 retention time 17.5min
 precursor m/z 554.2807
 precursor charge 2+

Theoretical

M H²⁺ 554.2815
 MH Δ_{mass} Da -0.0017
 MH Δ_{mass} ppm -1.5

edit peptide

{Propionyl}K{Dimethyl}S{Phospho}TGGK{Acetyl}APR align



Anchor	Current
click on peak	mouse over peak
m/z 895.4067	m/z 797.4252
intensity 405	intensity 2514
int. rank 16	int. rank 64

Explanation?
 delta mass could be...
 Δ_{m/z} -97.98145

Tune the seq
 Align anchor peak

y8 – H3PO4

	b++	b	y	y++	
			1051.53	526.27	9
1	107.08	213.16	895.40	448.21	8
2	190.58	380.16	728.40	364.71	7
3	241.11	481.21	627.36	314.18	6
4	269.62	538.23	570.34	285.67	5
5	298.13	595.25	513.31	257.16	4
6	383.18	765.35	343.21	172.11	3
7	418.70	836.39	272.17	136.59	2
8	467.23	933.44	175.12	88.06	1
9	545.28	1089.55			

Propionyl
 K
 Dimethyl
 S
 Phospho
 T
 G
 G
 K
 Acetyl
 A
 P
 R

Experimental spectrum

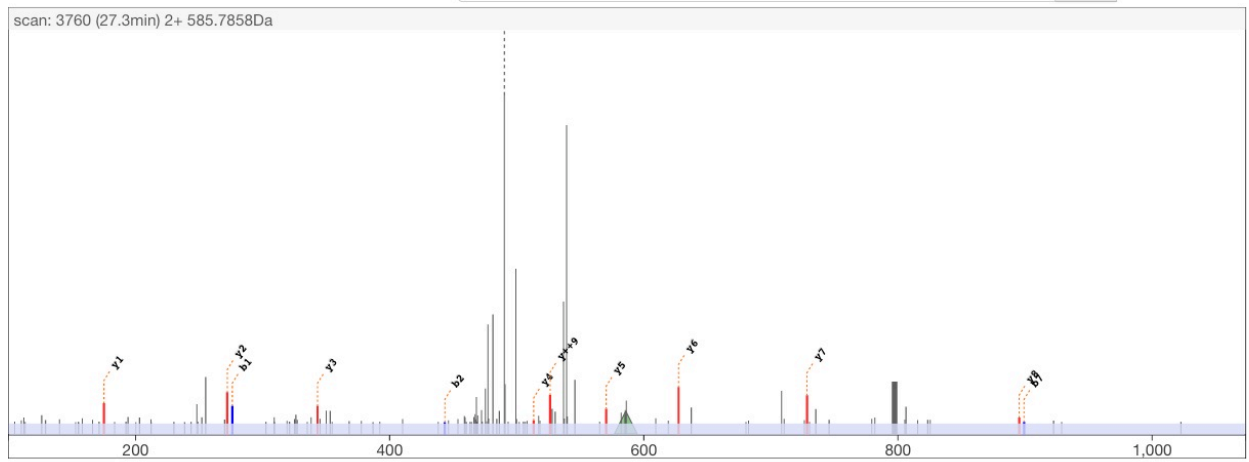
scan 3760
 retention time 27.3min
 precursor m/z 585.7858
 precursor charge 2+

Theoretical

M H²⁺ 585.7870
 MH Δ_{mass} Da -0.0024
 MH Δ_{mass} ppm -2.1

edit peptide

{PIC}K{Dimethyl}S{Phospho}TGGK{Acetyl}APR



Anchor		Current	
click on peak		mouse over peak	
m/z	895.4056	m/z	797.4261
intensity	799	intensity	5590
int. rank	40	int. rank	3

Explanation?
 delta mass could be...
 $\Delta_{m/z}$ -97.97949

Tune the seq
 Align anchor peak

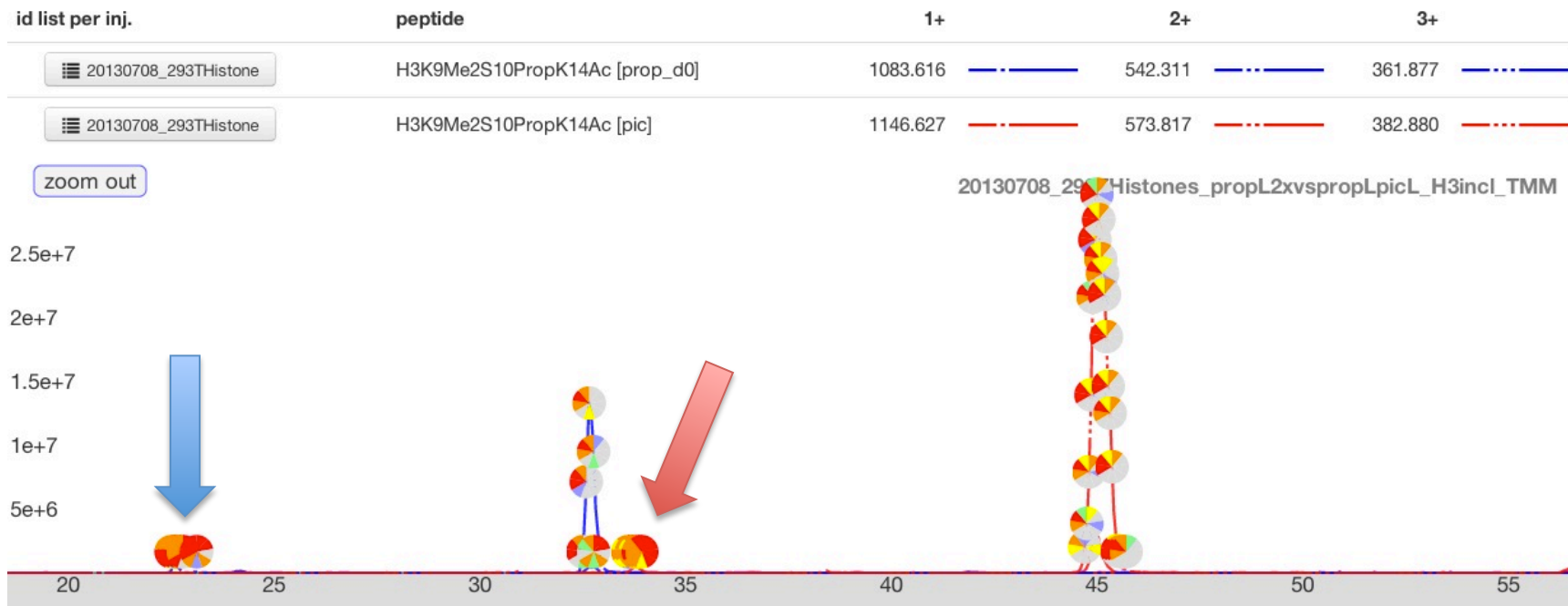
y8 – H3PO4

	b++	b		y	y++	
	60.53	120.04	PIC	1051.53	526.27	9
1	138.59	276.17	K	895.40	448.21	8
2	222.09	443.17	S	728.40	364.71	7
3	272.61	544.22	Phospho	627.36	314.18	6
4	301.12	601.24	T	570.34	285.67	5
5	329.63	658.26	G	513.31	257.16	4
6	414.69	828.37	K	343.21	172.11	3
7	450.20	899.40	Acetyl	272.17	136.59	2
8	498.73	996.46	A	175.12	88.06	1
9	576.78	1152.56	P			
			R			

H3_K9-R17:

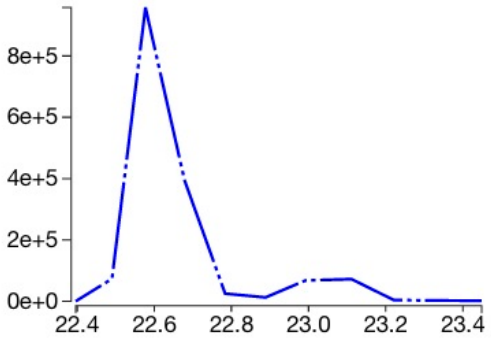
KMe2SorTPropGGKAcAPR

Peak contains overlapping spectra for either PTM. S10prop shown.



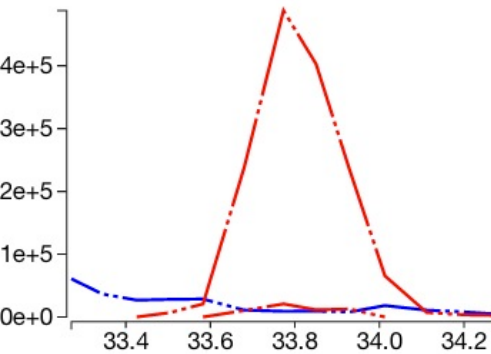
Quanti event: 22.2-23.5min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PropK14Ac [prop_d0]	1	1083.6157	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PropK14Ac [pic]	1	1146.6266	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PropK14Ac [prop_d0]	2	542.3115	9.5e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PropK14Ac [pic]	2	573.8169	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PropK14Ac [prop_d0]	3	361.8767	0.0e+0



Quanti event: 33.2-34.3min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PropK14Ac [prop_d0]	1	1083.6157	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PropK14Ac [pic]	1	1146.6266	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PropK14Ac [prop_d0]	2	542.3115	1.1e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PropK14Ac [pic]	2	573.8169	7.4e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PropK14Ac [prop_d0]	3	361.8767	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me2S10PropK14Ac [pic]	3	382.8804	2.8e+5



H3_K9-R17: Prop-KMe2SPropTGGKAcAPR MS/MS

Experimental spectrum

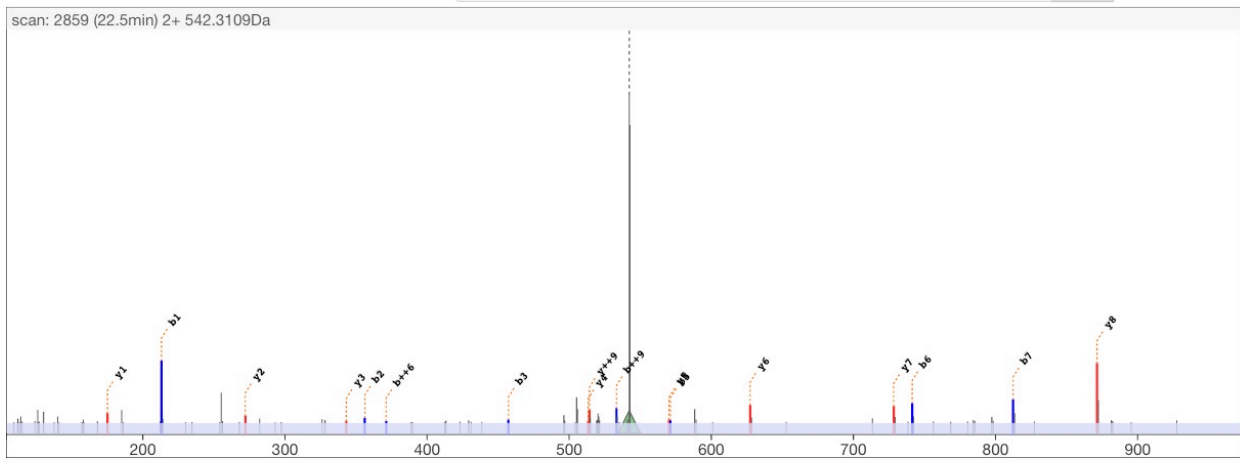
scan 2859
 retention time 22.5min
 precursor m/z 542.3109
 precursor charge 2+

Theoretical

M H²⁺ 542.3115
 MH Δ_{mass} Da -0.0013
 MH Δ_{mass} ppm -1.2

edit peptide

{Propionyl}K{Dimethyl}S{Propionyl}TGGK{Acetyl}APR align



	b++	b	y	y++	
			1027.59	514.30	9
1	107.08	213.16	871.46	436.24	8
2	178.61	356.22	728.40	364.71	7
3	229.14	457.27	627.36	314.18	6
4	257.65	514.29	570.34	285.67	5
5	286.16	571.31	513.31	257.16	4
6	371.21	741.41	343.21	172.11	3
7	406.73	812.45	272.17	136.59	2
8	455.26	909.50	175.12	88.06	1
9	533.31	1065.61			

Propionyl
 K
 Dimethyl
 S
 Propionyl
 T
 G
 K
 Acetyl
 A
 P
 R

Experimental spectrum

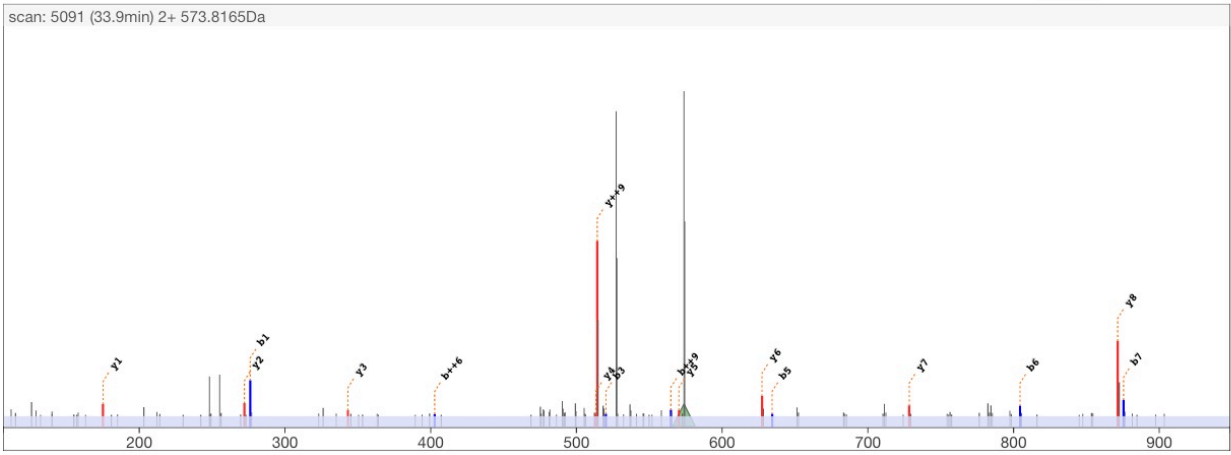
scan 5091
 retention time 33.9min
 precursor m/z 573.8165
 precursor charge 2+

Theoretical

M H²⁺ 573.8169
 MH Δ_{mass} Da -0.0008
 MH Δ_{mass} ppm -0.7

edit peptide

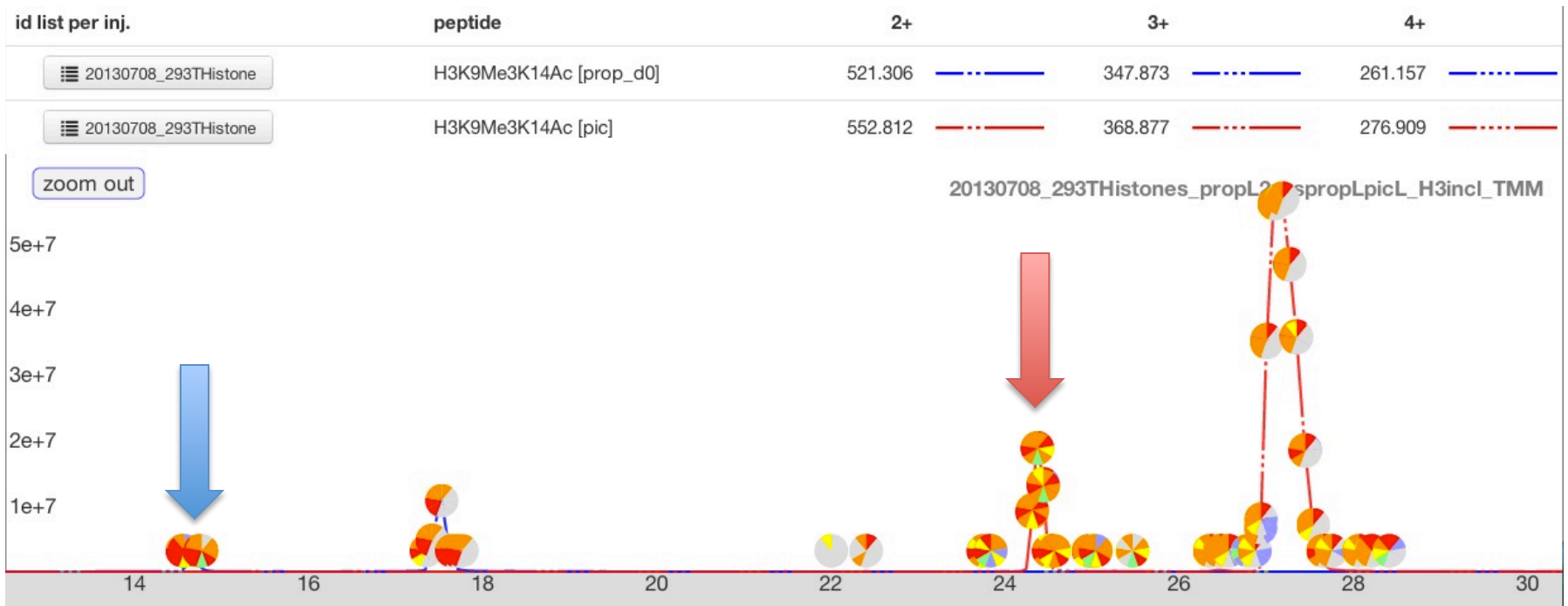
{PIC}K{Dimethyl}S{Propionyl}TGGK{Acetyl}APR align



	b++	b		y	y++	
	60.53	120.04	PIC	1027.59	514.30	9
1	138.59	276.17	K	871.46	436.24	8
2	210.12	419.23	Dimethyl S	728.40	364.71	7
3	260.64	520.28	Propionyl T	627.36	314.18	6
4	289.15	577.30	G	570.34	285.67	5
5	317.66	634.32	G	513.31	257.16	4
6	402.72	804.43	K	343.21	172.11	3
7	438.23	875.46	Acetyl A	272.17	136.59	2
8	486.76	972.51	P	175.12	88.06	1
9	564.81	1128.62	R			

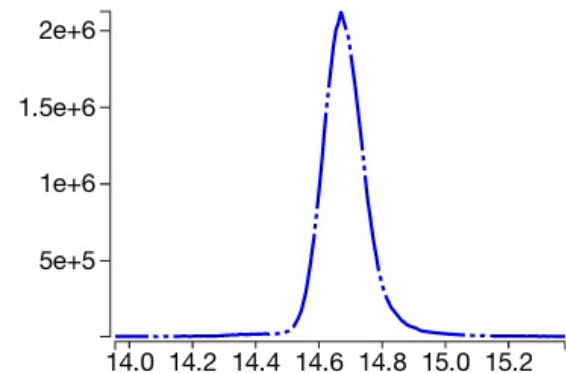
H3_K9-R17:

KMe3STGGKAcAPR



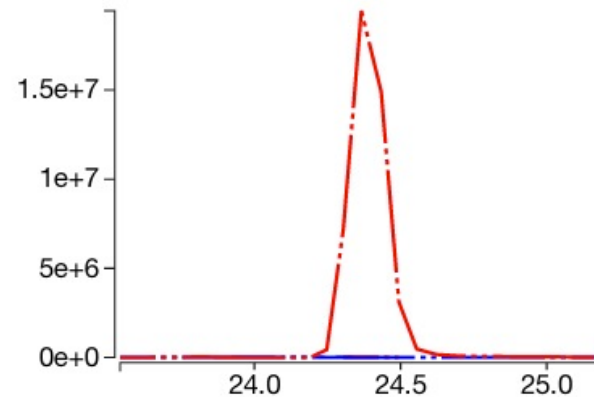
Quanti event: 13.6-15.6min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3K14Ac [prop_d0]	1	1041.6051	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3K14Ac [pic]	1	1104.6160	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3K14Ac [prop_d0]	2	521.3062	2.1e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3K14Ac [pic]	2	552.8116	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3K14Ac [prop_d0]	3	347.8732	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3K14Ac [pic]	3	368.8769	0.0e+0



Quanti event: 23.5-25.2min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3K14Ac [prop_d0]	1	1041.6051	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3K14Ac [pic]	1	1104.6160	3.6e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3K14Ac [prop_d0]	2	521.3062	2.0e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3K14Ac [pic]	2	552.8116	1.8e+8
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3K14Ac [prop_d0]	3	347.8732	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3K14Ac [pic]	3	368.8769	0.0e+0



Experimental spectrum

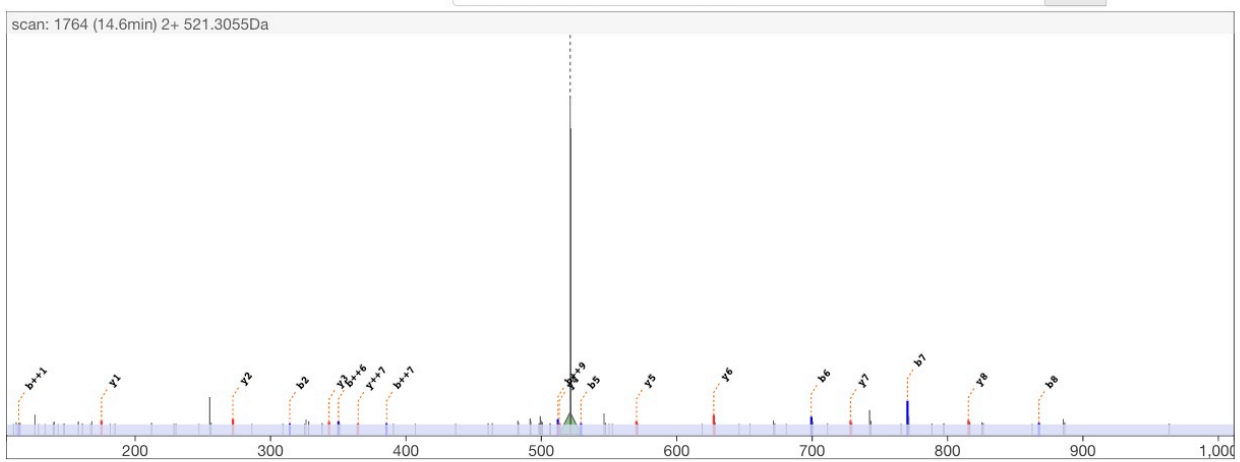
scan 1764
 retention time 14.6min
 precursor m/z 521.3055
 precursor charge 2+

Theoretical

M H²⁺ 521.3062
 MH Δ_{mass} Da -0.0013
 MH Δ_{mass} ppm -1.3

edit peptide

{Propionyl}K{Trimethyl}STGGK{Acetyl}APR align



	b++	b		y	y++	
			Propionyl	985.58	493.29	9
1	114.09	227.18	K	815.44	408.22	8
2	157.61	314.21	S	728.40	364.71	7
3	208.13	415.26	T	627.36	314.18	6
4	236.64	472.28	G	570.34	285.67	5
5	265.15	529.30	G	513.31	257.16	4
6	350.21	699.40	K	343.21	172.11	3
7	385.72	770.44	Acetyl	272.17	136.59	2
8	434.25	867.49	A	175.12	88.06	1
9	512.30	1023.59	P			
			R			

Experimental spectrum

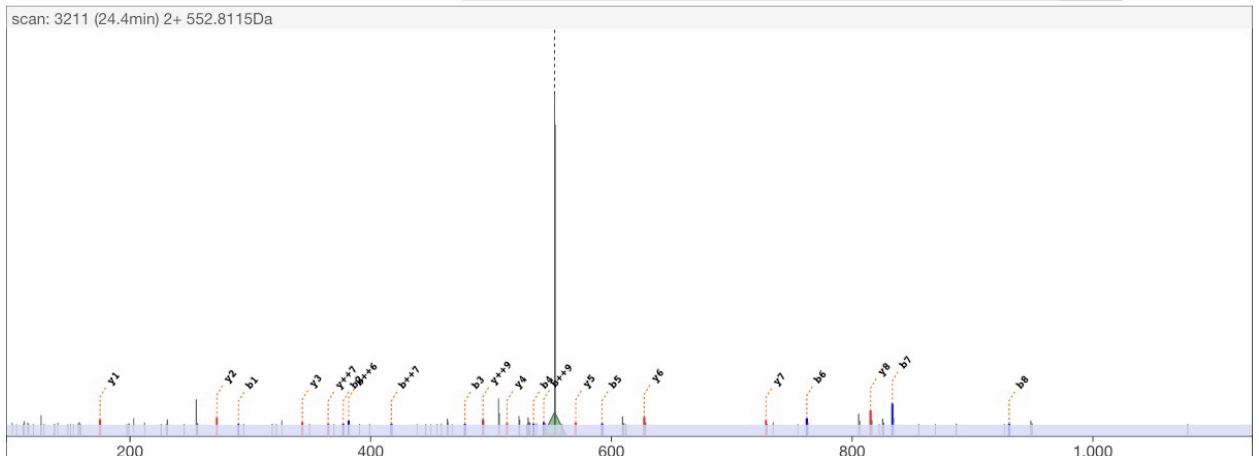
scan 3211
 retention time 24.4min
 precursor m/z 552.8115
 precursor charge 2+

Theoretical

M H²⁺ 552.8116
 MH Δ_{mass} Da -0.0004
 MH Δ_{mass} ppm -0.3

edit peptide

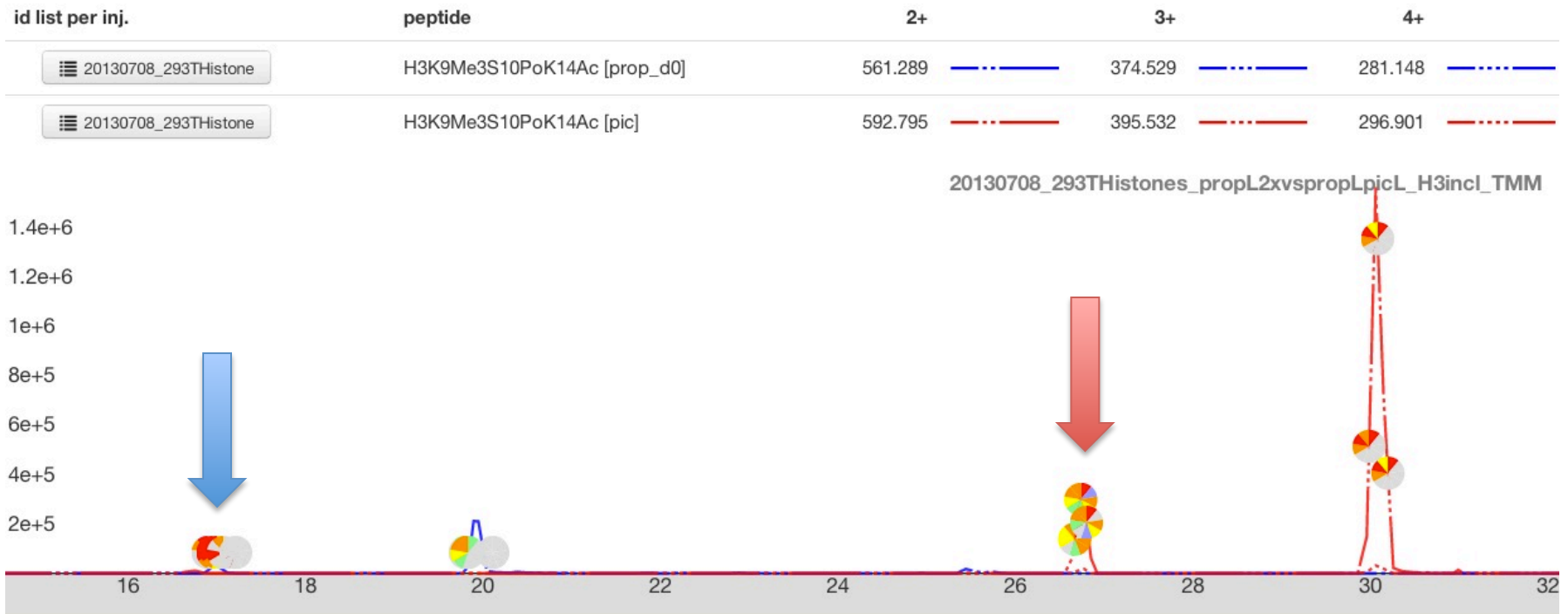
{PIC}K{Trimethyl}STGGK{Acetyl}APR



	b++	b		y	y++	
	60.53	120.04	PIC	985.58	493.29	9
1	145.60	290.19	K Trimethyl	815.44	408.22	8
2	189.11	377.22	S	728.40	364.71	7
3	239.64	478.27	T	627.36	314.18	6
4	268.15	535.29	G	570.34	285.67	5
5	296.66	592.31	K Acetyl	513.31	257.16	4
6	381.71	762.41	A	343.21	172.11	3
7	417.23	833.45	P	272.17	136.59	2
8	465.76	930.50	R	175.12	88.06	1
9	543.81	1086.61				

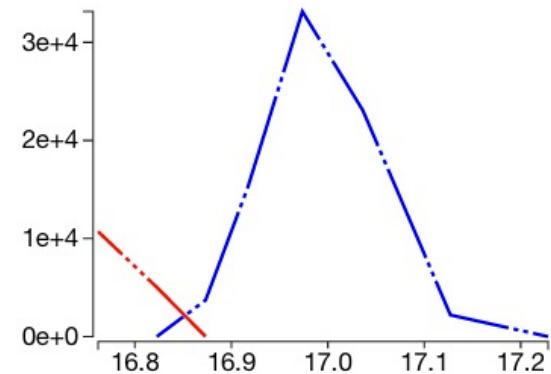
H3_K9-R17:

KMe3SPoTGGKAcAPR



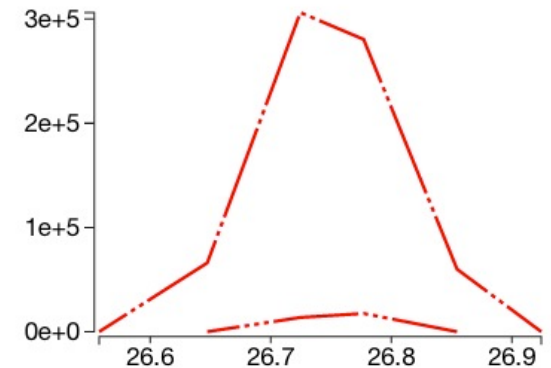
Quanti event: 16.7-17.4min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PoK14Ac [prop_d0]	2	561.2894	2.9e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PoK14Ac [pic]	2	592.7948	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PoK14Ac [prop_d0]	3	374.5287	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PoK14Ac [pic]	3	395.5323	3.6e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PoK14Ac [prop_d0]	4	281.1483	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PoK14Ac [pic]	4	296.9010	0.0e+0



Quanti event: 26.3-27.3min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PoK14Ac [prop_d0]	2	561.2894	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PoK14Ac [pic]	2	592.7948	2.9e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PoK14Ac [prop_d0]	3	374.5287	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PoK14Ac [pic]	3	395.5323	1.2e+5
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PoK14Ac [prop_d0]	4	281.1483	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PoK14Ac [pic]	4	296.9010	0.0e+0



Experimental spectrum

scan 2063
 retention time 17.0min
 precursor m/z 561.2885
 precursor charge 2+

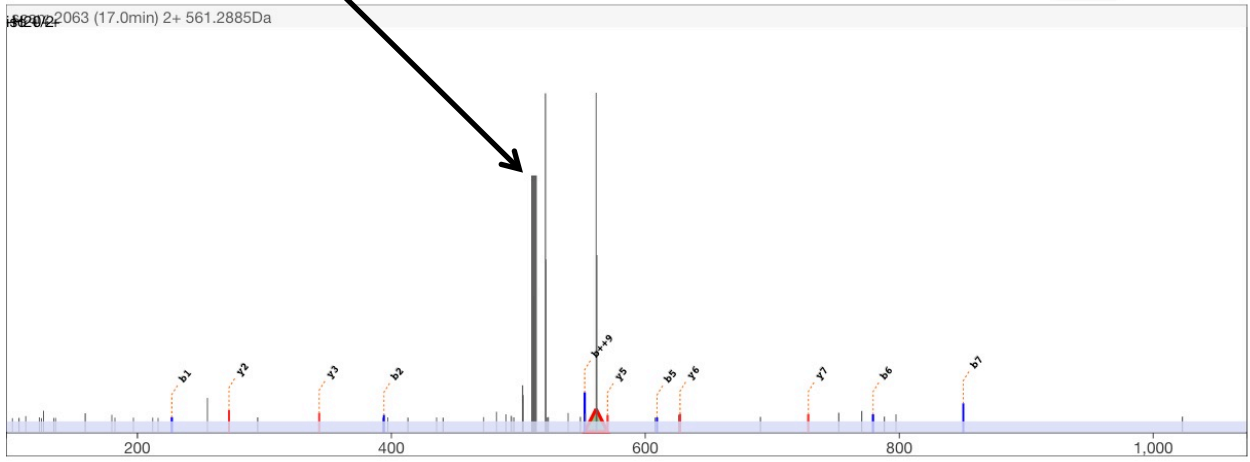
Theoretical

M H²⁺ 561.2894
 MH Δ_{mass} Da -0.0018
 MH Δ_{mass} ppm -1.6

precursor – H3PO4

edit peptide

{Propionyl}K{Trimethyl}S{Phospho}TGGK{Acetyl}APR align



Anchor	Current
click on peak	mouse over peak
m/z 561.2885	m/z 512.2998
intensity NaN	intensity 6090
int. rank	int. rank 52

Explanation?
 delta mass could be...
 $\Delta_{m/z}$ -48.98865

Tune the seq
 Align anchor peak

	b++	b		y	y++	
			Propionyl	1065.55	533.28	9
1	114.09	227.18	K	895.40	448.21	8
			Trimethyl			
2	197.59	394.17	S	728.40	364.71	7
			Phospho			
3	248.11	495.22	T	627.36	314.18	6
			G			
4	276.63	552.24	G	570.34	285.67	5
			G			
5	305.14	609.26	K	513.31	257.16	4
			Acetyl			
6	390.19	779.37	A	343.21	172.11	3
			P			
7	425.71	850.41	R	272.17	136.59	2
8	474.23	947.46		175.12	88.06	1
9	552.28	1103.56				

Experimental spectrum

scan 3644
 retention time 26.7min
 precursor m/z 592.7941
 precursor charge 2+

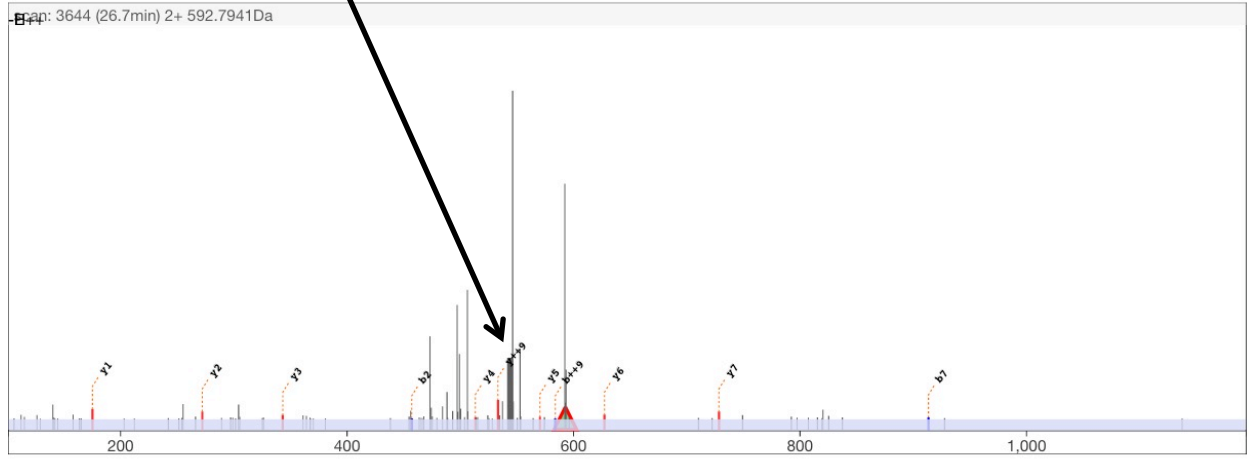
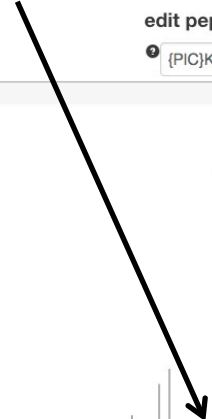
Theoretical

MH²⁺ 592.7948
 MH Δ_{mass} Da -0.0015
 MH Δ_{mass} ppm -1.3

edit peptide

{PIC}K[Trimethyl]S[Phospho]TGGK[Acetyl]APR

precursor – H3PO4



Anchor
 click on peak
 m/z 592.7941
 intensity NaN
 int. rank

Current
 mouse over peak
 m/z 543.8055
 intensity 15927
 int. rank 90

Explanation?
 delta mass could be...
 Δ_{m/z} -48.98853

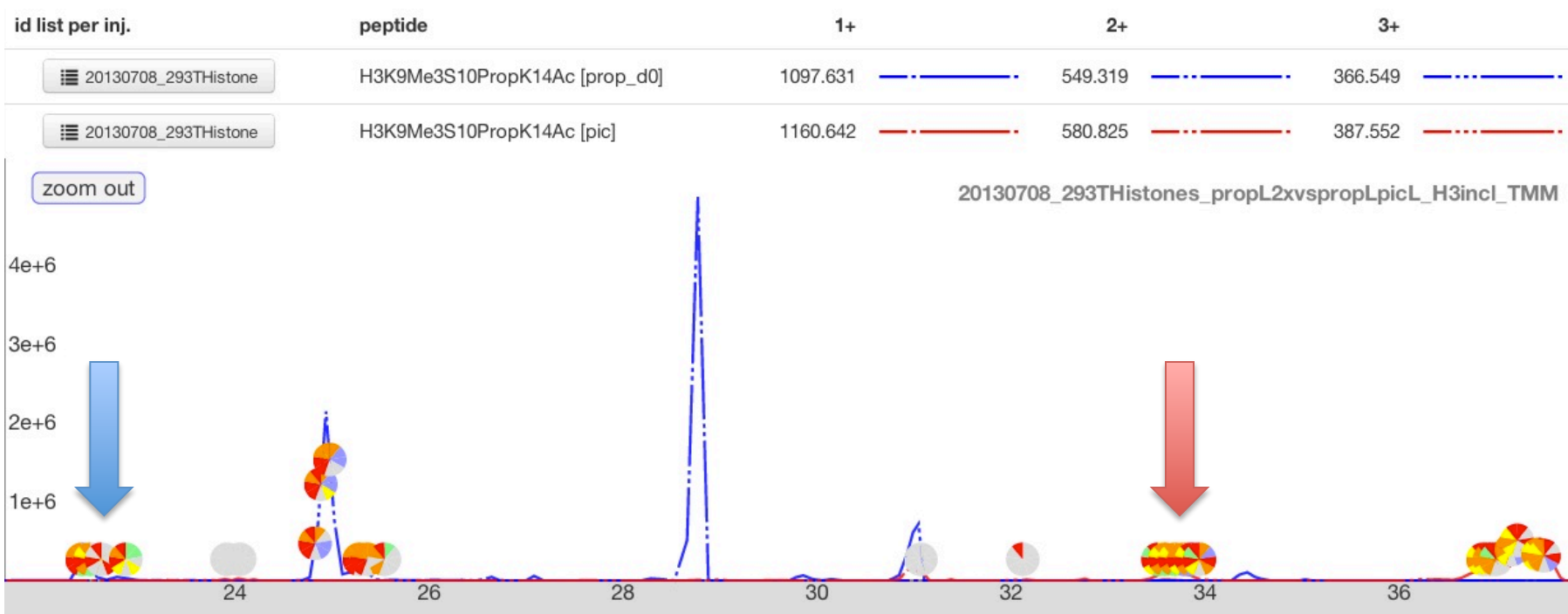
Tune the seq
 Align anchor peak

	b++	b		y	y++	
	60.53	120.04	PIC K Trimethyl S Phospho T G G K Acetyl A P R	1065.55	533.28	9
1	145.60	290.19		895.40	448.21	8
2	229.10	457.18		728.40	364.71	7
3	279.62	558.23		627.36	314.18	6
4	308.13	615.25		570.34	285.67	5
5	336.64	672.28		513.31	257.16	4
6	421.69	842.38		343.21	172.11	3
7	457.21	913.42		272.17	136.59	2
8	505.74	1010.47		175.12	88.06	1
9	583.79	1166.57				

H3_K9-R17:

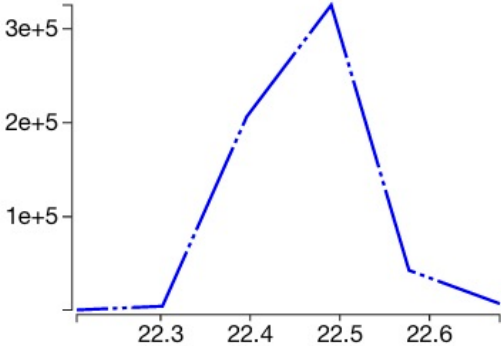
KMe3SorTPropGGKAcAPR

Peaks contain overlapping spectra for either PTM. S10prop shown.



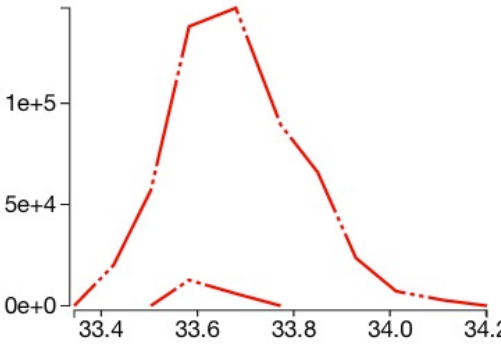
Quanti event: 22.2-22.7min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PropK14Ac [prop_d0]	1	1097.6313	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PropK14Ac [pic]	1	1160.6422	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PropK14Ac [prop_d0]	2	549.3193	3.2e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PropK14Ac [pic]	2	580.8248	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PropK14Ac [prop_d0]	3	366.5486	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PropK14Ac [pic]	3	387.5523	0.0e+0



Quanti event: 33.3-34.2min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PropK14Ac [prop_d0]	1	1097.6313	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PropK14Ac [pic]	1	1160.6422	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PropK14Ac [prop_d0]	2	549.3193	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PropK14Ac [pic]	2	580.8248	2.9e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PropK14Ac [prop_d0]	3	366.5486	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9Me3S10PropK14Ac [pic]	3	387.5523	1.0e+5



H3_K9-R17: Prop-KMe3SPropTGGKAcAPR MS/MS

Experimental spectrum

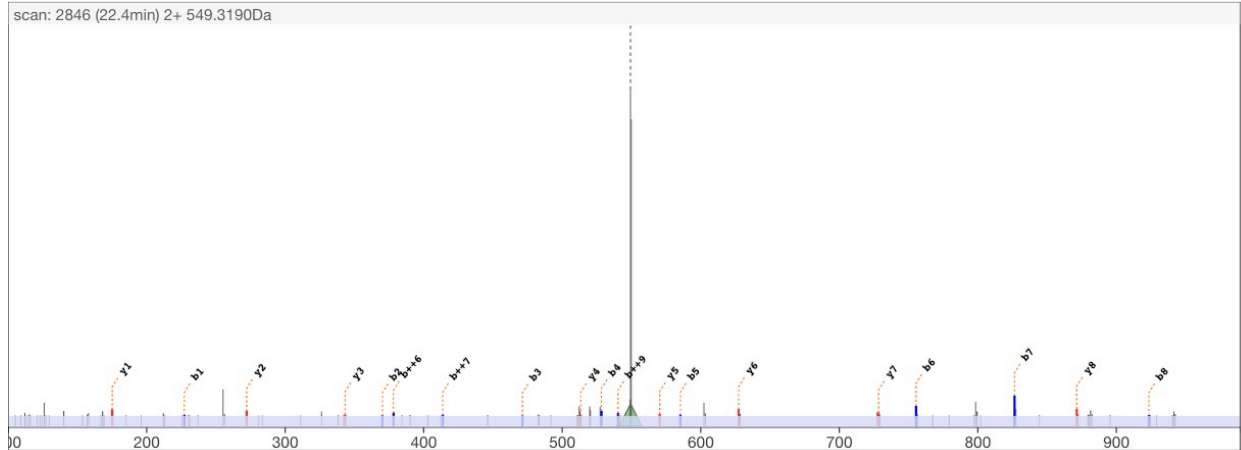
scan 2846
 retention time 22.4min
 precursor m/z 549.3190
 precursor charge 2+

Theoretical

M H²⁺ 549.3193
 MH Δ _{mass} Da -0.0006
 MH Δ _{mass} ppm -0.5

edit peptide

{Propionyl}K{Trimethyl}S{Propionyl}TGGK{Acetyl}APR align



	b++	b		y	y++	
			Propionyl	1041.61	521.31	9
1	114.09	227.18	K			
			Trimethyl	871.46	436.24	8
2	185.62	370.23	S			
			Propionyl	728.40	364.71	7
3	236.14	471.28	T			
			G	627.36	314.18	6
4	264.66	528.30	G			
			G	570.34	285.67	5
5	293.17	585.32	K			
			Acetyl	513.31	257.16	4
6	378.22	755.43	A			
			K	343.21	172.11	3
7	413.74	826.47	A			
			P	272.17	136.59	2
8	462.26	923.52	P			
			R	175.12	88.06	1
9	540.31	1079.62				

Experimental spectrum

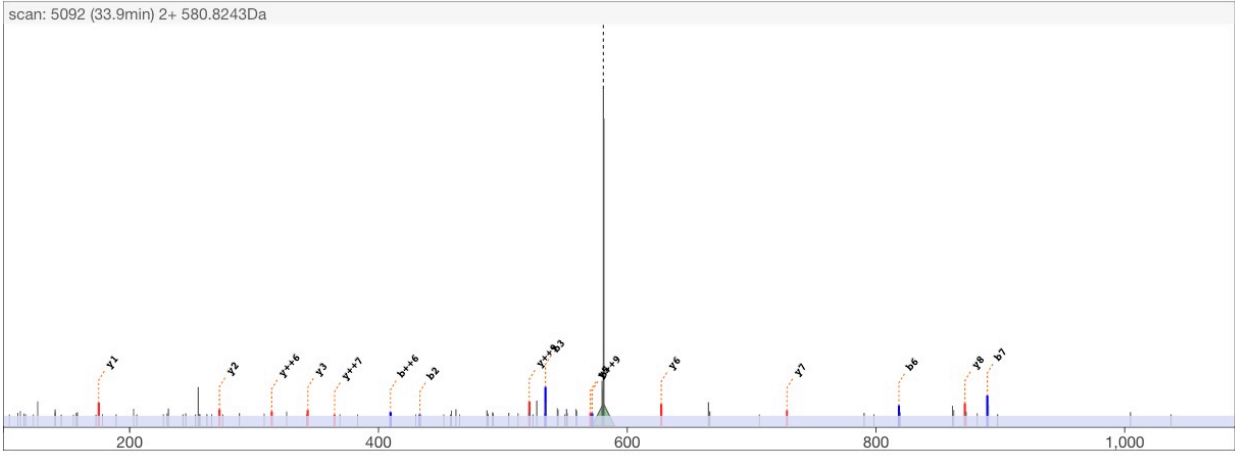
scan 5092
 retention time 33.9min
 precursor m/z 580.8243
 precursor charge 2+

Theoretical

M H²⁺ 580.8248
 MH Δ_{mass} Da -0.0010
 MH Δ_{mass} ppm -0.8

edit peptide

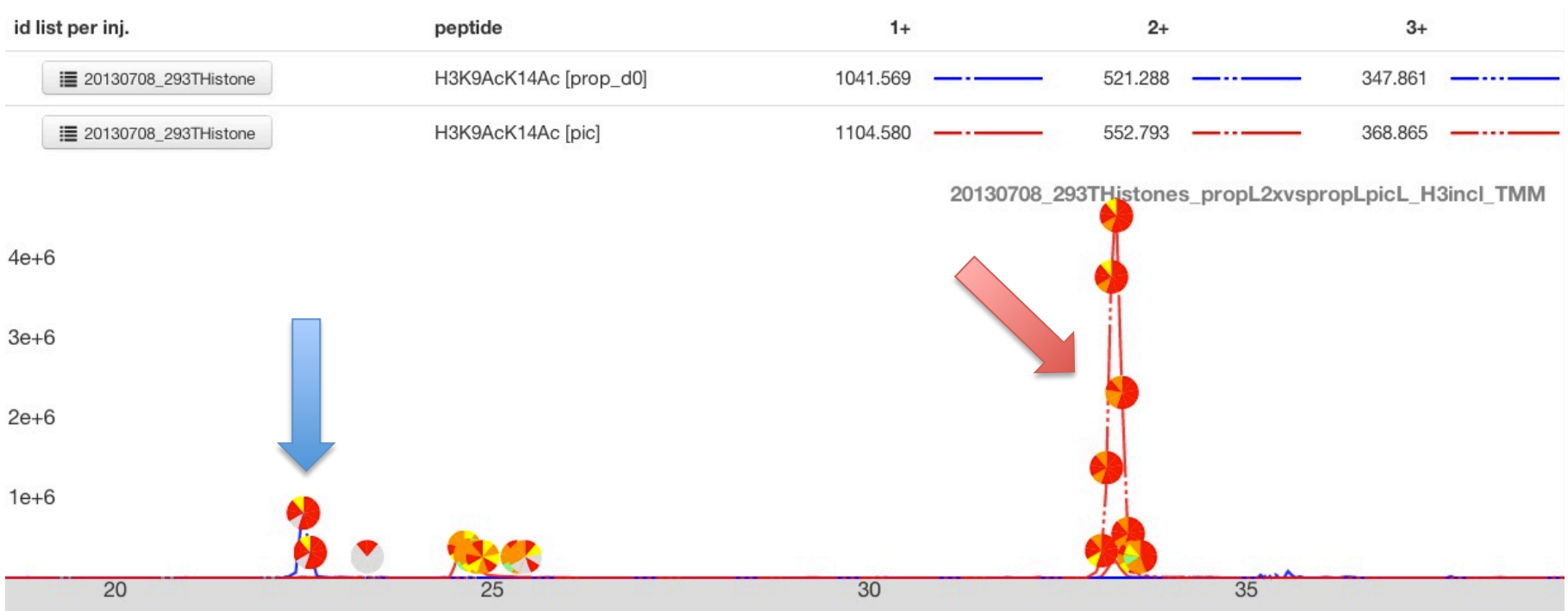
{PIC}K{Trimethyl}S{Propionyl}TGGK{Acetyl}APR align



	b++	b		y	y++	
	60.53	120.04	PIC	1041.61	521.31	9
1	145.60	290.19	K	871.46	436.24	8
2	217.13	433.24	Trimethyl S	728.40	364.71	7
3	267.65	534.29	Propionyl T	627.36	314.18	6
4	296.16	591.31	G	570.34	285.67	5
5	324.67	648.34	G	513.31	257.16	4
6	409.72	818.44	K	343.21	172.11	3
7	445.24	889.48	Acetyl A	272.17	136.59	2
8	493.77	986.53	P	175.12	88.06	1
9	571.82	1142.63	R			

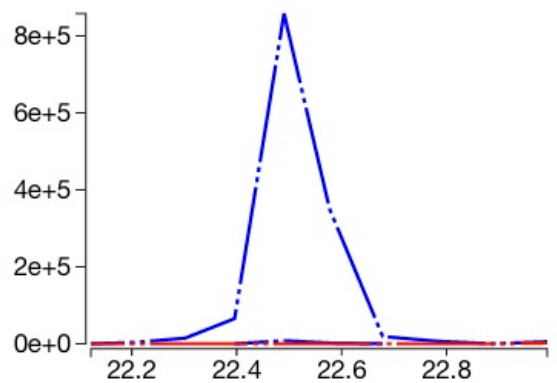
H3_K9-R17:

KAcSTGGKAcAPR



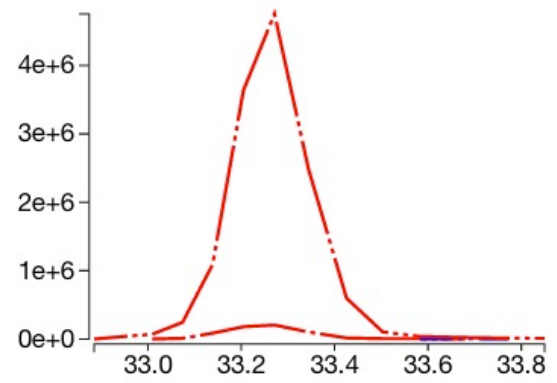
Quanti event: 22.1-23.0min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9AcK14Ac [prop_d0]	1	1041.5687	5.5e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9AcK14Ac [pic]	1	1104.5796	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9AcK14Ac [prop_d0]	2	521.2880	7.3e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9AcK14Ac [pic]	2	552.7935	6.4e+3
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9AcK14Ac [prop_d0]	3	347.8611	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9AcK14Ac [pic]	3	368.8647	0.0e+0



Quanti event: 32.6-33.9min

injection	peptide	charge	m/z	auc
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9AcK14Ac [prop_d0]	1	1041.5687	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9AcK14Ac [pic]	1	1104.5796	2.6e+6
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9AcK14Ac [prop_d0]	2	521.2880	4.4e+4
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9AcK14Ac [pic]	2	552.7935	5.5e+7
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9AcK14Ac [prop_d0]	3	347.8611	0.0e+0
20130708_293THistones_propL2xvspropLpicL_H3incl_TMM	H3K9AcK14Ac [pic]	3	368.8647	0.0e+0



Experimental spectrum

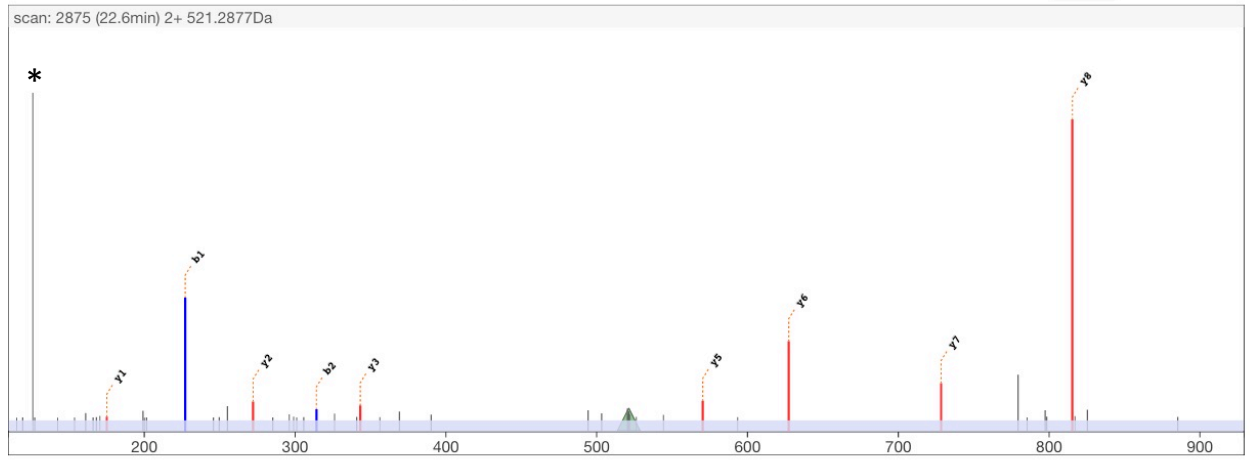
scan 2875
 retention time 22.6min
 precursor m/z 521.2877
 precursor charge 2+

Theoretical

M H²⁺ 521.2880
 MH Δ_{mass} Da -0.0006
 MH Δ_{mass} ppm -0.5

edit peptide

{Propionyl}K{Acetyl}STGGK{Acetyl}APR align



	b++	b		y	y++	
			Propionyl	985.54	493.27	9
1	114.07	227.14	K	815.44	408.22	8
2	157.59	314.17	Acetyl	728.40	364.71	7
3	208.11	415.22	S	627.36	314.18	6
4	236.62	472.24	T	570.34	285.67	5
5	265.13	529.26	G	513.31	257.16	4
6	350.19	699.37	Acetyl	343.21	172.11	3
7	385.71	770.40	K	272.17	136.59	2
8	434.23	867.46	A	175.12	88.06	1
9	512.28	1023.56	P			
			R			

* = 126Da diagnostic ion

Experimental spectrum

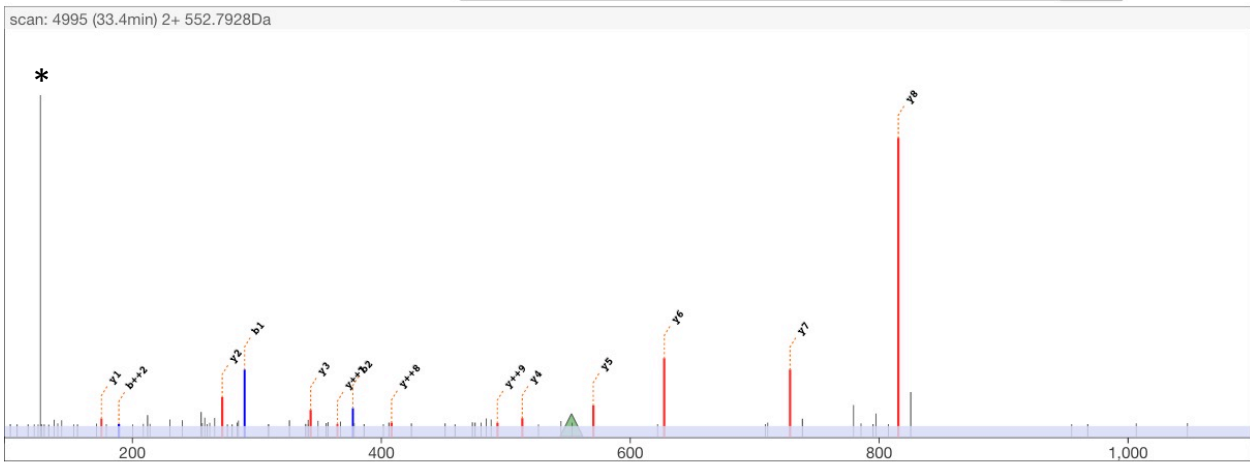
scan 4995
 retention time 33.4min
 precursor m/z 552.7928
 precursor charge 2+

Theoretical

M H²⁺ 552.7935
 MH Δ_{mass} Da -0.0013
 MH Δ_{mass} ppm -1.2

edit peptide

{PIC}K(Acetyl)STGGK(Acetyl)APR align



	b++	b		y	y++	
	60.53	120.04	PIC	985.54	493.27	9
1	145.58	290.15	K	815.44	408.22	8
2	189.09	377.18	Acetyl	728.40	364.71	7
3	239.62	478.23	S	627.36	314.18	6
4	268.13	535.25	T	570.34	285.67	5
5	296.64	592.27	G	513.31	257.16	4
6	381.69	762.38	G	343.21	172.11	3
7	417.21	833.42	Acetyl	272.17	136.59	2
8	465.74	930.47	K	175.12	88.06	1
9	543.79	1086.57	A			
			P			
			R			

* = 126Da diagnostic ion