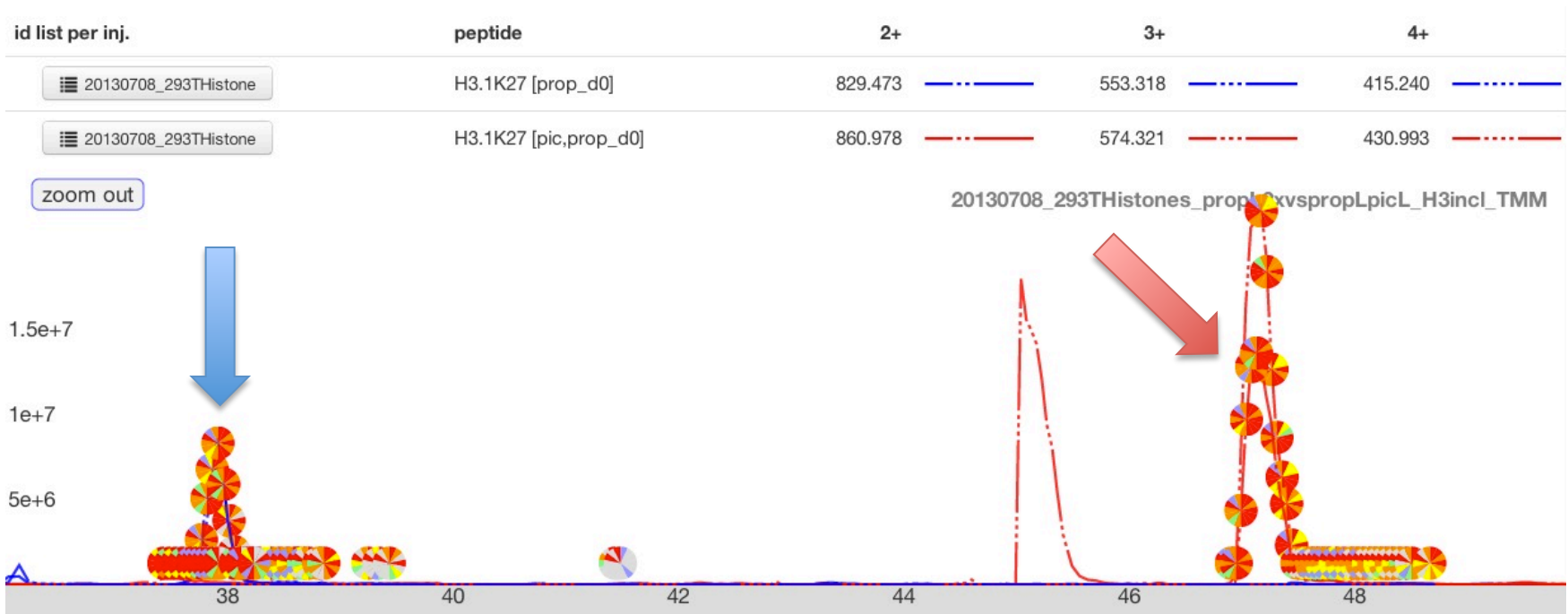


H3.1_K27-R40

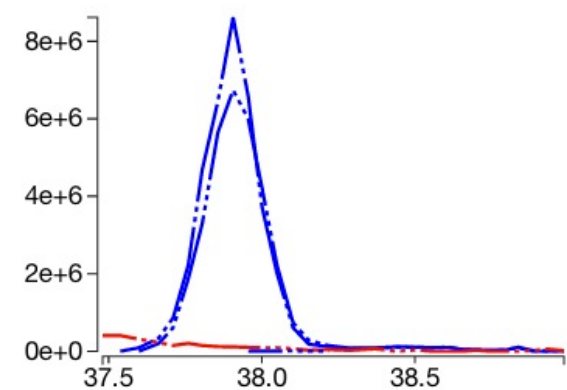
KSAPATGGVKKPHR

H3.1_K27-R40: KSAPATGGVKKPHR



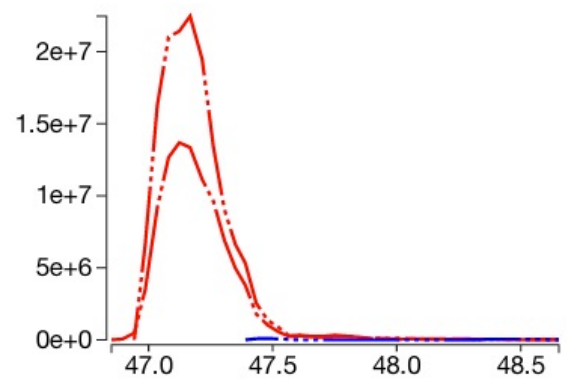
Quanti event: 37.5-39.1min

| injection | peptide | charge | m/z | auc |
|-----------------------------------------------------|-----------------------|--------|----------|--------|
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27 [prop_d0] | 2 | 829.4728 | 1.1e+8 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27 [pic,prop_d0] | 2 | 860.9783 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27 [prop_d0] | 3 | 553.3177 | 9.7e+7 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27 [pic,prop_d0] | 3 | 574.3213 | 8.4e+6 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27 [prop_d0] | 4 | 415.2401 | 8.4e+4 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27 [pic,prop_d0] | 4 | 430.9928 | 0.0e+0 |



Quanti event: 46.8-48.7min

| injection | peptide | charge | m/z | auc |
|-----------------------------------------------------|-----------------------|--------|----------|--------|
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27 [prop_d0] | 2 | 829.4728 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27 [pic,prop_d0] | 2 | 860.9783 | 2.6e+8 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27 [prop_d0] | 3 | 553.3177 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27 [pic,prop_d0] | 3 | 574.3213 | 4.0e+8 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27 [prop_d0] | 4 | 415.2401 | 1.5e+6 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27 [pic,prop_d0] | 4 | 430.9928 | 0.0e+0 |



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

Experimental spectrum

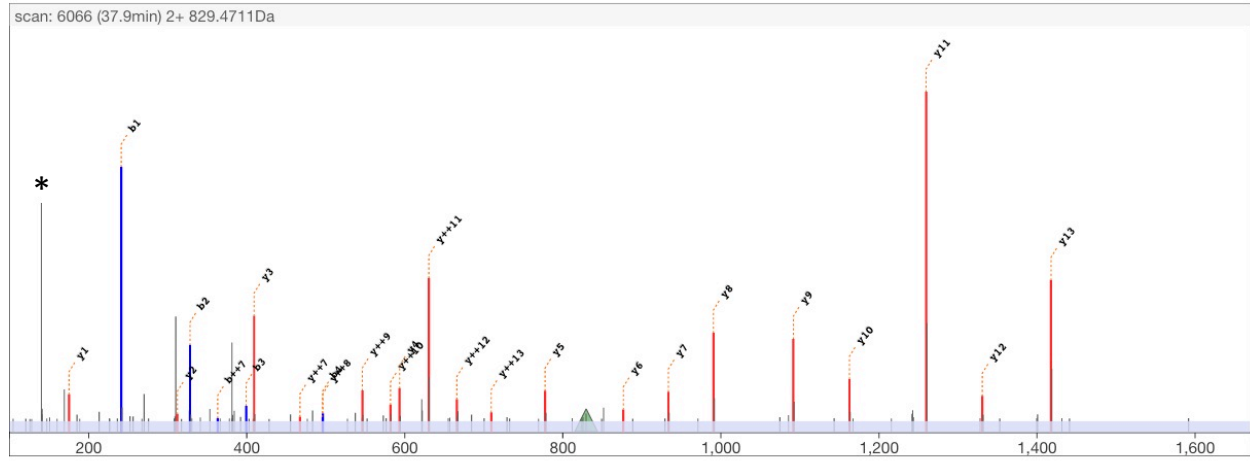
scan 6066
 retention time 37.9min
 precursor m/z 829.4711
 precursor charge 2+

Theoretical

M H²⁺ 829.4728
 MH Δ_{mass} Da -0.0036
 MH Δ_{mass} ppm -2.1

edit peptide

{Propionyl}K{Propionyl}SAPATGGV{Propionyl}K{Propionyl}PHR align



| | b++ | b | | y | y++ |
|----|--------|---------|-----------|---------|--------|
| | | | Propionyl | 1601.91 | 801.46 |
| 1 | 121.08 | 241.15 | K | 1417.79 | 709.40 |
| 2 | 164.60 | 328.19 | S | 1330.76 | 665.88 |
| 3 | 200.12 | 399.22 | A | 1259.72 | 630.36 |
| 4 | 248.64 | 496.28 | P | 1162.67 | 581.84 |
| 5 | 284.16 | 567.31 | A | 1091.63 | 546.32 |
| 6 | 334.68 | 668.36 | T | 990.58 | 495.80 |
| 7 | 363.20 | 725.38 | G | 933.56 | 467.29 |
| 8 | 391.71 | 782.40 | V | 876.54 | 438.77 |
| 9 | 441.24 | 881.47 | K | 777.47 | 389.24 |
| 10 | 533.30 | 1065.59 | Propionyl | 593.35 | 297.18 |
| 11 | 625.36 | 1249.72 | K | 409.23 | 205.12 |
| 12 | 673.89 | 1346.77 | P | 312.18 | 156.59 |
| 13 | 742.42 | 1483.83 | H | 175.12 | 88.06 |
| 14 | 820.47 | 1639.93 | R | | |

* = 140Da diagnostic ion

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

Experimental spectrum

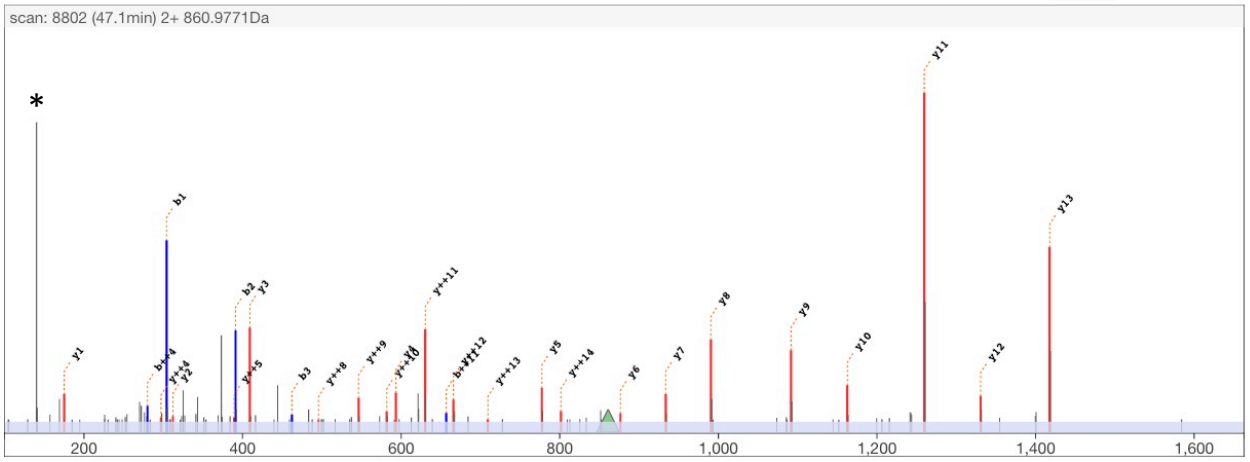
scan 8802
 retention time 47.1min
 precursor m/z 860.9771
 precursor charge 2+

Theoretical

M H²⁺ 860.9783
 MH Δ_{mass} Da -0.0025
 MH Δ_{mass} ppm -1.4

edit peptide

{PIC}K{Propionyl}SAPATGGV{Propionyl}K{Propionyl}PHR align



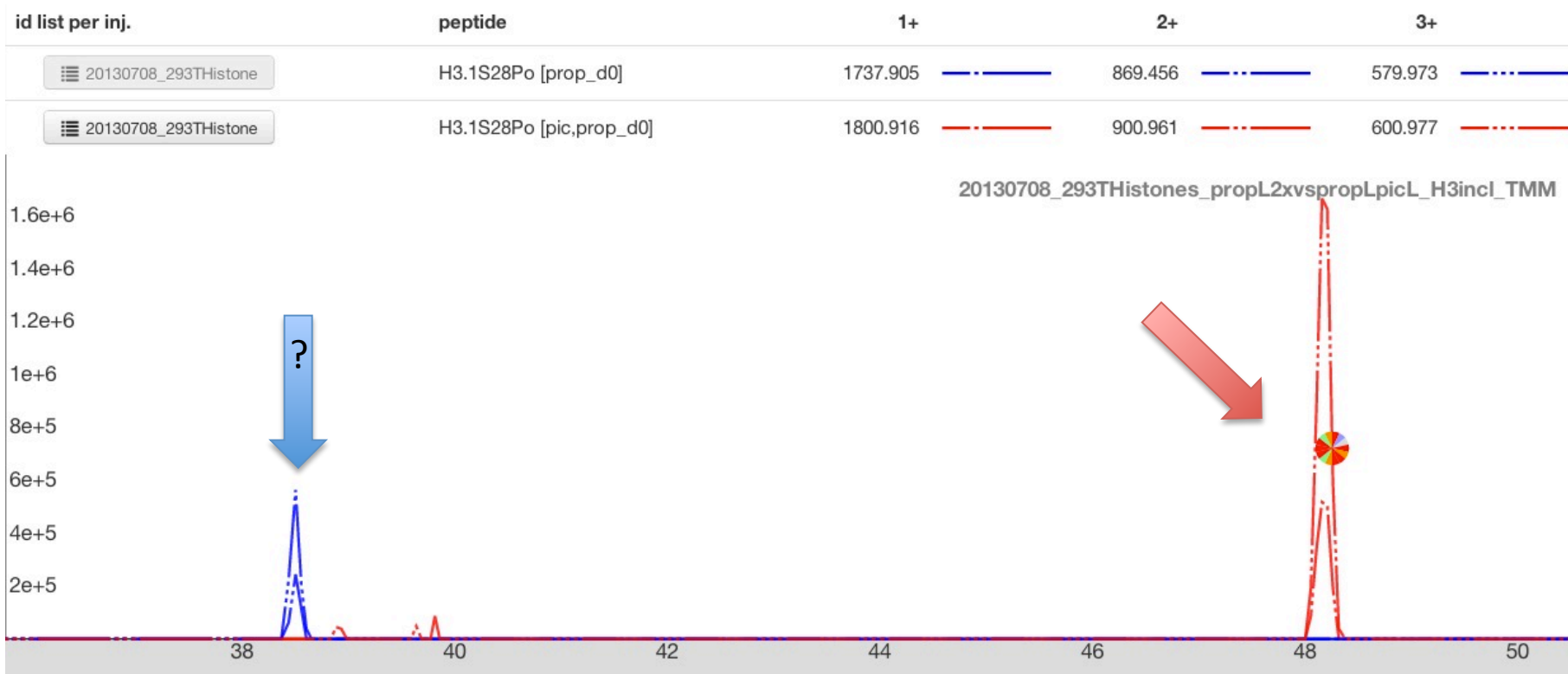
| | b++ | b | | y | y++ | |
|----|--------|---------|-----------|---------|--------|----|
| | 60.53 | 120.04 | PIC | 1601.91 | 801.46 | 14 |
| 1 | 152.59 | 304.17 | K | 1417.79 | 709.40 | 13 |
| 2 | 196.10 | 391.20 | S | 1330.76 | 665.88 | 12 |
| 3 | 231.62 | 462.23 | A | 1259.72 | 630.36 | 11 |
| 4 | 280.15 | 559.29 | P | 1162.67 | 581.84 | 10 |
| 5 | 315.67 | 630.32 | A | 1091.63 | 546.32 | 9 |
| 6 | 366.19 | 731.37 | T | 990.58 | 495.80 | 8 |
| 7 | 394.70 | 788.39 | G | 933.56 | 467.29 | 7 |
| 8 | 423.21 | 845.42 | V | 876.54 | 438.77 | 6 |
| 9 | 472.75 | 944.48 | K | 777.47 | 389.24 | 5 |
| 10 | 564.81 | 1128.60 | Propionyl | 593.35 | 297.18 | 4 |
| 11 | 656.87 | 1312.73 | K | 409.23 | 205.12 | 3 |
| 12 | 705.39 | 1409.78 | Propionyl | 312.18 | 156.59 | 2 |
| 13 | 773.92 | 1546.84 | P | 175.12 | 88.06 | 1 |
| 14 | 851.97 | 1702.94 | H | | | |
| | | | R | | | |

* = 140Da diagnostic ion

H3.1_K27-R40:

KSPoAPATGGVKKPHR

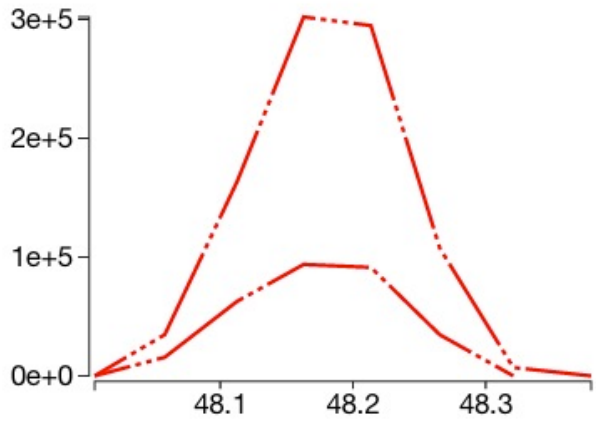
Putative peak for Prop-labeled peptide but no MS2 detected.



Quanti event: 47.5-49.0min



| injection | peptide | charge | m/z | auc |
|-----------------------------------------------------|-------------------------|--------|-----------|--------|
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1S28Po [prop_d0] | 1 | 1737.9047 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1S28Po [pic,prop_d0] | 1 | 1800.9156 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1S28Po [prop_d0] | 2 | 869.4560 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1S28Po [pic,prop_d0] | 2 | 900.9615 | 9.2e+5 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1S28Po [prop_d0] | 3 | 579.9731 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1S28Po [pic,prop_d0] | 3 | 600.9767 | 2.8e+6 |



No MS2 for Prop-labeling detected.

H3.1_K27-R40: PIC-KS^oAPATGGVKKPHR MS/MS

y13⁺⁺ - H3PO4

Experimental spectrum

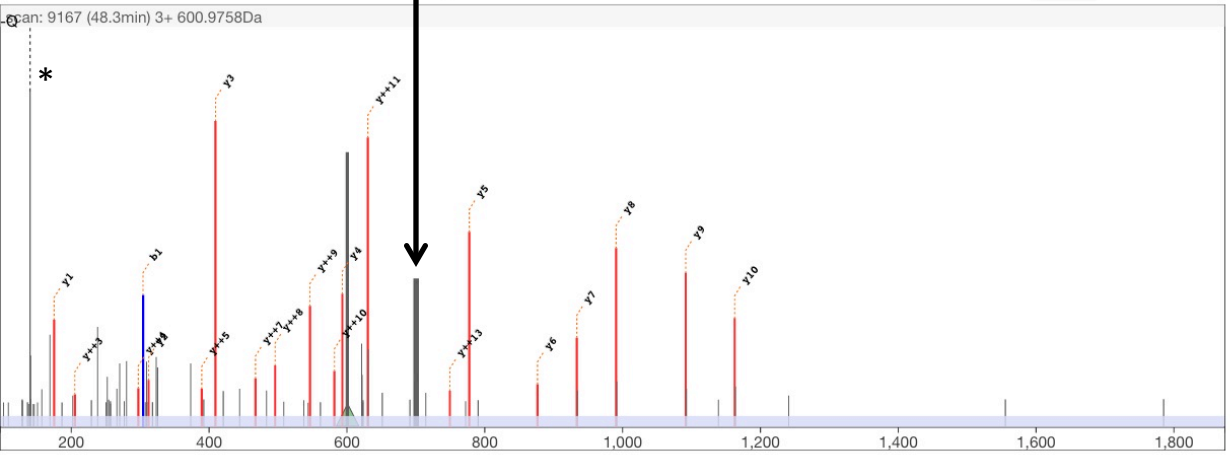
scan 9167
 retention time 48.3min
 precursor m/z 600.9758
 precursor charge 3+

Theoretical

M H³⁺ 600.9767
 MH Δ_{mass} Da -0.0027
 MH Δ_{mass} ppm -1.5

edit peptide

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



Anchor
 click on peak
 m/z 749.4084
 intensity 588
 int. rank 43

Current
 mouse over peak
 m/z 700.3926
 intensity 3208
 int. rank 7

Explanation?
 delta mass could be...
 Δ_{m/z} -49.01581

Tune the seq
 Align anchor peak

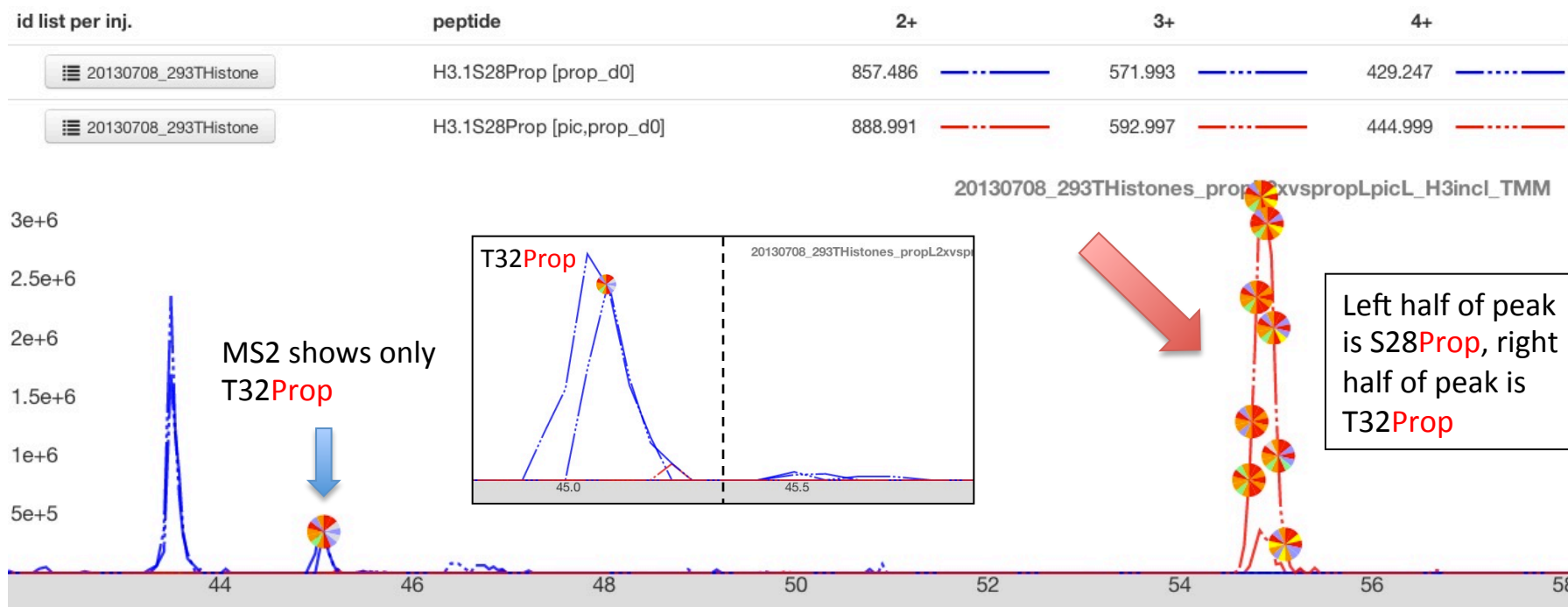
| | b ⁺⁺ | b | | y | y ⁺⁺ | |
|----|-----------------|---------|-----------|---------|-----------------|----|
| | 60.53 | 120.04 | PIC | 1681.88 | 841.44 | 14 |
| 1 | 152.59 | 304.17 | K | 1497.76 | 749.38 | 13 |
| 2 | 236.09 | 471.16 | S | 1330.76 | 665.88 | 12 |
| 3 | 271.60 | 542.20 | Phospho | 1259.72 | 630.36 | 11 |
| 4 | 320.13 | 639.25 | A | 1162.67 | 581.84 | 10 |
| 5 | 355.65 | 710.29 | P | 1091.63 | 546.32 | 9 |
| 6 | 406.17 | 811.34 | A | 990.58 | 495.80 | 8 |
| 7 | 434.68 | 868.36 | T | 933.56 | 467.29 | 7 |
| 8 | 463.19 | 925.38 | G | 876.54 | 438.77 | 6 |
| 9 | 512.73 | 1024.45 | V | 819.52 | 410.25 | 5 |
| 10 | 604.79 | 1208.57 | K | 777.47 | 389.24 | 5 |
| 11 | 696.85 | 1392.69 | Propionyl | 593.35 | 297.18 | 4 |
| 12 | 745.38 | 1489.75 | Propionyl | 409.23 | 205.12 | 3 |
| 13 | 813.91 | 1626.80 | P | 312.18 | 156.59 | 2 |
| 14 | 891.96 | 1782.91 | H | 175.12 | 88.06 | 1 |

* = 140Da diagnostic ion

H3.1_K27-R40:

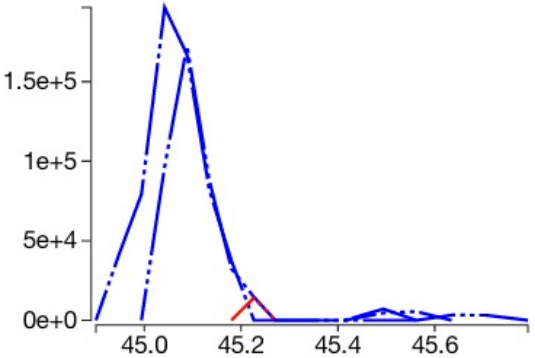
KSProp? APATProp? GGVKKPHR

Calculated AUCs for both variations. Only T32-prop MS2 shown.



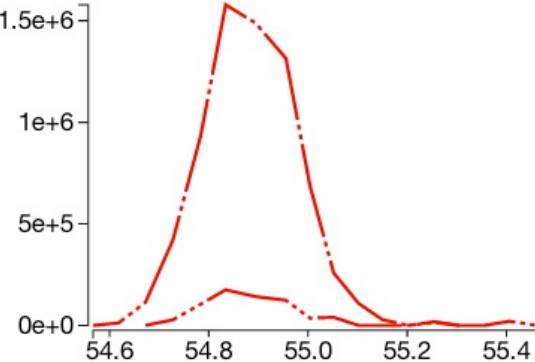
Quanti event: 44.8-45.9min

| injection | peptide | charge | m/z | auc |
|-----------------------------------------------------|---------------------------|--------|----------|--------|
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1S28Prop [prop_d0] | 2 | 857.4860 | 1.7e+6 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1S28Prop [pic,prop_d0] | 2 | 888.9914 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1S28Prop [prop_d0] | 3 | 571.9931 | 1.2e+6 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1S28Prop [pic,prop_d0] | 3 | 592.9967 | 3.8e+4 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1S28Prop [prop_d0] | 4 | 429.2466 | 4.4e+4 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1S28Prop [pic,prop_d0] | 4 | 444.9993 | 0.0e+0 |



Quanti event: 54.4-55.7min

| injection | peptide | charge | m/z | auc |
|-----------------------------------------------------|---------------------------|--------|----------|--------|
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1S28Prop [prop_d0] | 2 | 857.4860 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1S28Prop [pic,prop_d0] | 2 | 888.9914 | 2.3e+7 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1S28Prop [prop_d0] | 3 | 571.9931 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1S28Prop [pic,prop_d0] | 3 | 592.9967 | 2.2e+6 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1S28Prop [prop_d0] | 4 | 429.2466 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1S28Prop [pic,prop_d0] | 4 | 444.9993 | 0.0e+0 |



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

Experimental spectrum

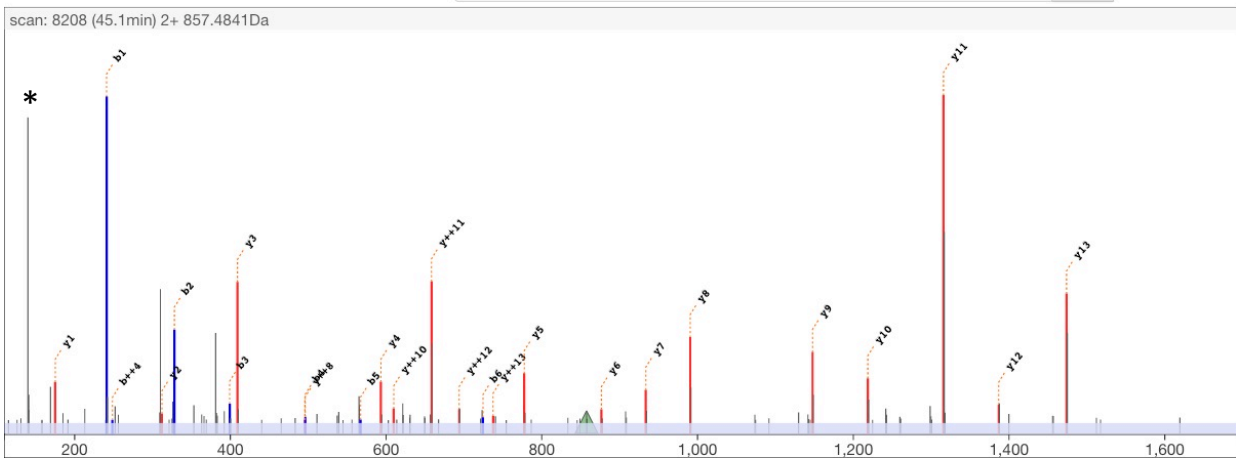
scan 8208
retention time 45.1min
precursor m/z 857.4841
precursor charge 2+

Theoretical

M H²⁺ 857.4860
MH Δ_{mass} Da -0.0036
MH Δ_{mass} ppm -2.1

edit peptide

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



| | b++ | b | | y | y++ | |
|----|--------|---------|-----------|---------|--------|----|
| | | | Propionyl | 1657.94 | 829.47 | 14 |
| 1 | 121.08 | 241.15 | K | 1473.82 | 737.41 | 13 |
| | | | Propionyl | | | |
| 2 | 164.60 | 328.19 | S | 1386.79 | 693.90 | 12 |
| | | | A | | | |
| 3 | 200.12 | 399.22 | P | 1315.75 | 658.38 | 11 |
| | | | A | | | |
| 4 | 248.64 | 496.28 | T | 1218.70 | 609.85 | 10 |
| | | | A | | | |
| 5 | 284.16 | 567.31 | G | 1147.66 | 574.33 | 9 |
| | | | T | | | |
| 6 | 362.70 | 724.39 | Propionyl | 990.58 | 495.80 | 8 |
| | | | G | | | |
| 7 | 391.21 | 781.41 | V | 933.56 | 467.29 | 7 |
| | | | G | | | |
| 8 | 419.72 | 838.43 | V | 876.54 | 438.77 | 6 |
| | | | K | | | |
| 9 | 469.25 | 937.50 | V | 777.47 | 389.24 | 5 |
| | | | Propionyl | | | |
| 10 | 561.31 | 1121.62 | K | 593.35 | 297.18 | 4 |
| | | | Propionyl | | | |
| 11 | 653.37 | 1305.74 | K | 409.23 | 205.12 | 3 |
| | | | P | | | |
| 12 | 701.90 | 1402.79 | H | 312.18 | 156.59 | 2 |
| | | | R | | | |
| 13 | 770.43 | 1539.85 | | 175.12 | 88.06 | 1 |
| 14 | 848.48 | 1695.95 | | | | |

* = 140Da diagnostic ion

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

Experimental spectrum

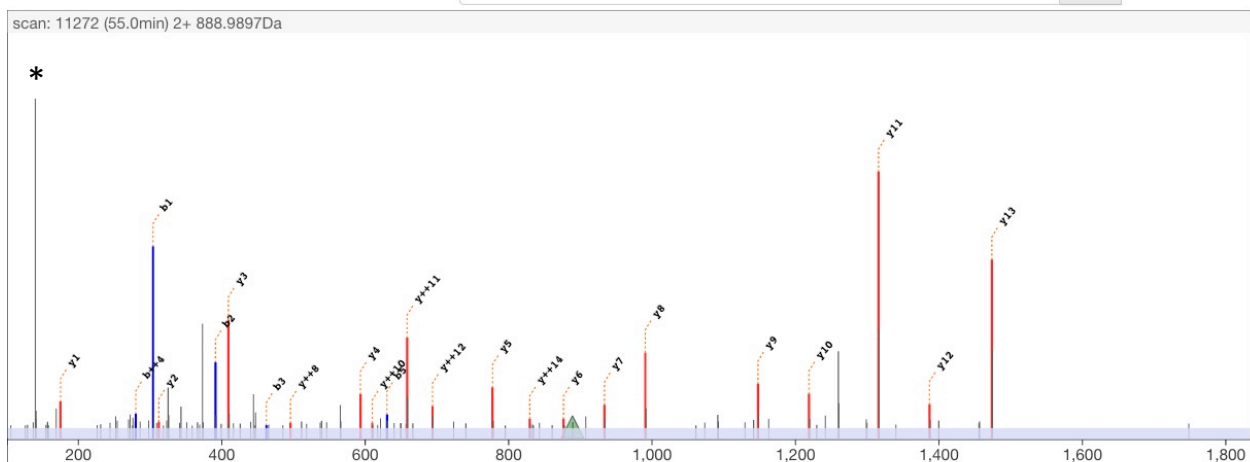
scan 11272
 retention time 55.0min
 precursor m/z 888.9897
 precursor charge 2+

Theoretical

M H²⁺ 888.9914
 MH Δ_{mass} Da -0.0034
 MH Δ_{mass} ppm -1.9

edit peptide

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

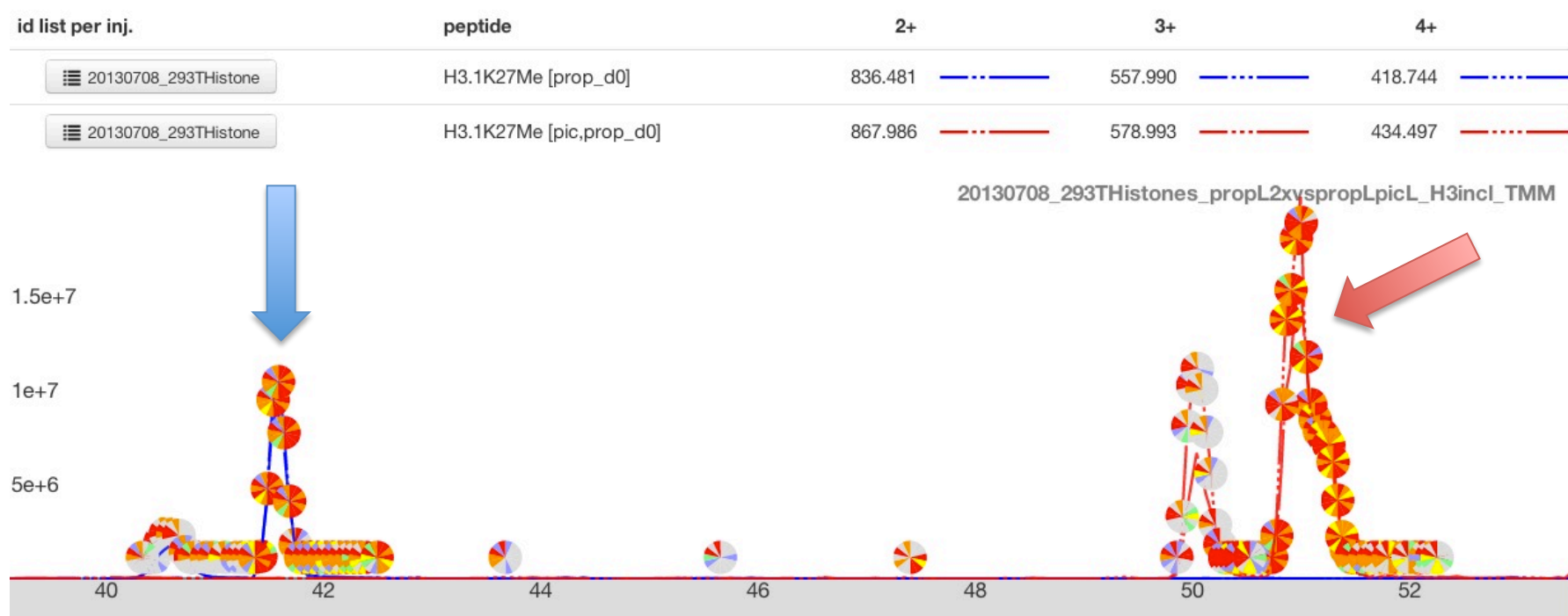


| | b++ | b | | y | y++ | |
|----|--------|---------|----------------|---------|--------|----|
| | 60.53 | 120.04 | PIC | 1657.94 | 829.47 | 14 |
| 1 | 152.59 | 304.17 | K Propionyl | 1473.82 | 737.41 | 13 |
| 2 | 196.10 | 391.20 | S | 1386.79 | 693.90 | 12 |
| 3 | 231.62 | 462.23 | A | 1315.75 | 658.38 | 11 |
| 4 | 280.15 | 559.29 | P | 1218.70 | 609.85 | 10 |
| 5 | 315.67 | 630.32 | A | 1147.66 | 574.33 | 9 |
| 6 | 394.20 | 787.40 | T Propionyl | 990.58 | 495.80 | 8 |
| 7 | 422.71 | 844.42 | G | 933.56 | 467.29 | 7 |
| 8 | 451.22 | 901.44 | V | 876.54 | 438.77 | 6 |
| 9 | 500.76 | 1000.51 | K | 777.47 | 389.24 | 5 |
| 10 | 592.82 | 1184.63 | K Propionyl | 593.35 | 297.18 | 4 |
| 11 | 684.88 | 1368.75 | K | 409.23 | 205.12 | 3 |
| 12 | 733.41 | 1465.80 | P | 312.18 | 156.59 | 2 |
| 13 | 801.94 | 1602.86 | H | 175.12 | 88.06 | 1 |
| 14 | 879.99 | 1758.96 | R | | | |

* = 140Da diagnostic ion

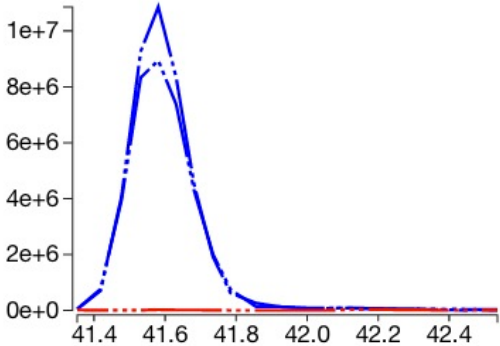
H3.1_K27-R40:

KMe1SAPATGGVKKPHR



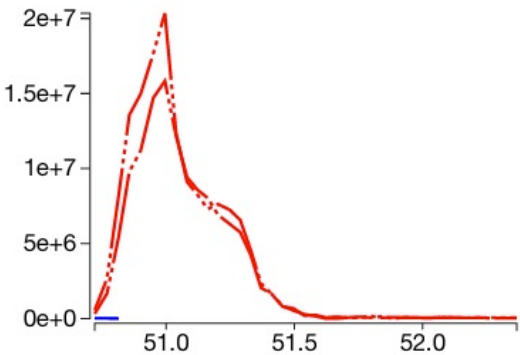
Quanti event: 41.3-42.5min

| injection | peptide | charge | m/z | auc |
|-----------------------------------------------------|-------------------------|--------|----------|--------|
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me [prop_d0] | 2 | 836.4807 | 1.3e+8 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me [pic,prop_d0] | 2 | 867.9861 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me [prop_d0] | 3 | 557.9895 | 1.2e+8 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me [pic,prop_d0] | 3 | 578.9932 | 6.8e+5 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me [prop_d0] | 4 | 418.7440 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me [pic,prop_d0] | 4 | 434.4967 | 0.0e+0 |



Quanti event: 50.7-52.4min

| injection | peptide | charge | m/z | auc |
|-----------------------------------------------------|-------------------------|--------|----------|--------|
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me [prop_d0] | 2 | 836.4807 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me [pic,prop_d0] | 2 | 867.9861 | 3.3e+8 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me [prop_d0] | 3 | 557.9895 | 1.0e+5 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me [pic,prop_d0] | 3 | 578.9932 | 3.9e+8 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me [prop_d0] | 4 | 418.7440 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me [pic,prop_d0] | 4 | 434.4967 | 0.0e+0 |



H3.1_K27-R40: Prop-KMe1SAPATGGVKKPHR MS/MS

Experimental spectrum

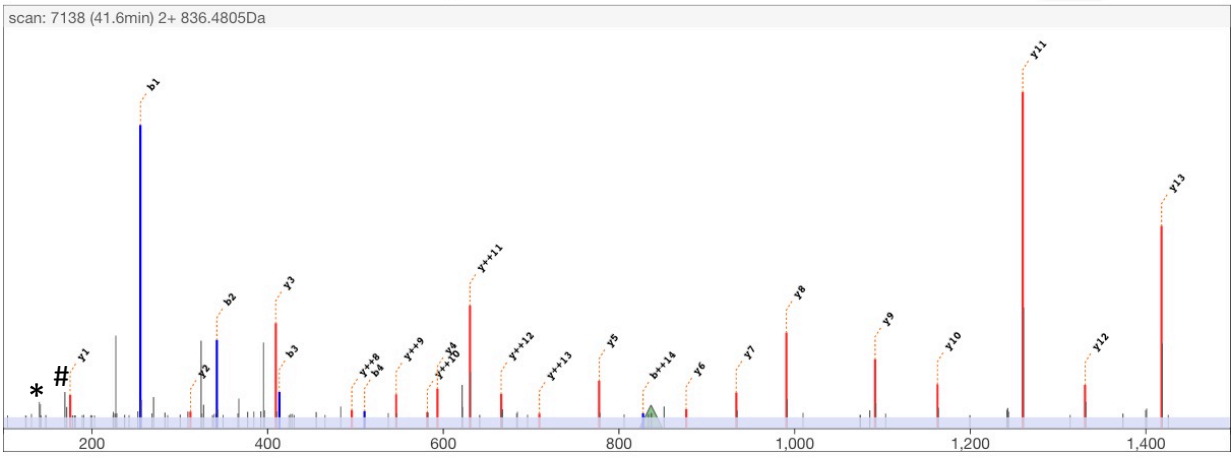
scan 7138
 retention time 41.6min
 precursor m/z 836.4805
 precursor charge 2+

Theoretical

M H²⁺ 836.4807
 MH Δ_{mass} Da -0.0003
 MH Δ_{mass} Ppm -0.2

edit peptide

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



| | b++ | b | | y | y++ | |
|----|--------|---------|-------------------|---------|--------|----|
| | | | Propionyl | 1615.93 | 808.47 | 14 |
| 1 | 128.09 | 255.17 | K | 1417.79 | 709.40 | 13 |
| | | | Methyl(Propionyl) | | | |
| 2 | 171.60 | 342.20 | S | 1330.76 | 665.88 | 12 |
| 3 | 207.12 | 413.24 | A | 1259.72 | 630.36 | 11 |
| 4 | 255.65 | 510.29 | P | 1162.67 | 581.84 | 10 |
| 5 | 291.17 | 581.33 | A | 1091.63 | 546.32 | 9 |
| 6 | 341.69 | 682.38 | T | 990.58 | 495.80 | 8 |
| 7 | 370.20 | 739.40 | G | 933.56 | 467.29 | 7 |
| 8 | 398.71 | 796.42 | V | 876.54 | 438.77 | 6 |
| 9 | 448.25 | 895.49 | K | 777.47 | 389.24 | 5 |
| 10 | 540.31 | 1079.61 | Propionyl | 593.35 | 297.18 | 4 |
| 11 | 632.37 | 1263.73 | K | 409.23 | 205.12 | 3 |
| 12 | 680.90 | 1360.78 | P | 312.18 | 156.59 | 2 |
| 13 | 749.42 | 1497.84 | H | 175.12 | 88.06 | 1 |
| 14 | 827.48 | 1653.94 | R | | | |

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

H3.1_K27-R40: PIC-KMe1SAPATGGVKKPHR MS/MS

Experimental spectrum

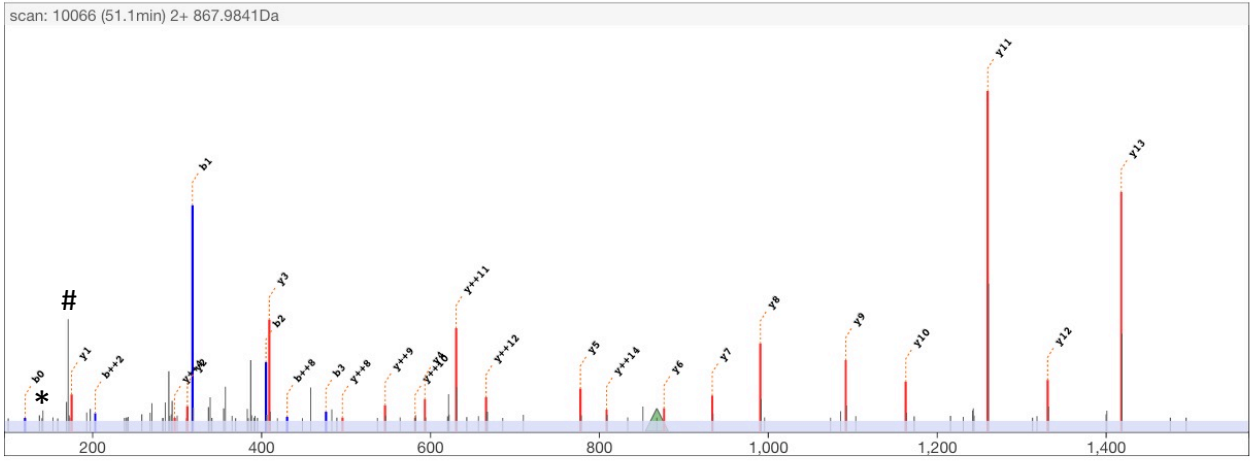
scan 10066
 retention time 51.1min
 precursor m/z 867.9841
 precursor charge 2+

Theoretical

M H²⁺ 867.9861
 MH Δ_{mass} Da -0.0041
 MH Δ_{mass} ppm -2.4

edit peptide

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



| | b++ | b | | y | y++ | |
|----|--------|---------|--------------------|---------|--------|----|
| | 60.53 | 120.04 | PIC | 1615.93 | 808.47 | 14 |
| 1 | 159.59 | 318.18 | Methyl/Propionyl K | 1417.79 | 709.40 | 13 |
| 2 | 203.11 | 405.21 | S | 1330.76 | 665.88 | 12 |
| 3 | 238.63 | 476.25 | A | 1259.72 | 630.36 | 11 |
| 4 | 287.16 | 573.30 | P | 1162.67 | 581.84 | 10 |
| 5 | 322.67 | 644.34 | A | 1091.63 | 546.32 | 9 |
| 6 | 373.20 | 745.39 | T | 990.58 | 495.80 | 8 |
| 7 | 401.71 | 802.41 | G | 933.56 | 467.29 | 7 |
| 8 | 430.22 | 859.43 | V | 876.54 | 438.77 | 6 |
| 9 | 479.75 | 958.50 | K | 777.47 | 389.24 | 5 |
| 10 | 571.81 | 1142.62 | Propionyl K | 593.35 | 297.18 | 4 |
| 11 | 663.87 | 1326.74 | Propionyl K | 409.23 | 205.12 | 3 |
| 12 | 712.40 | 1423.79 | P | 312.18 | 156.59 | 2 |
| 13 | 780.93 | 1560.85 | H | 175.12 | 88.06 | 1 |
| 14 | 858.98 | 1716.95 | R | | | |

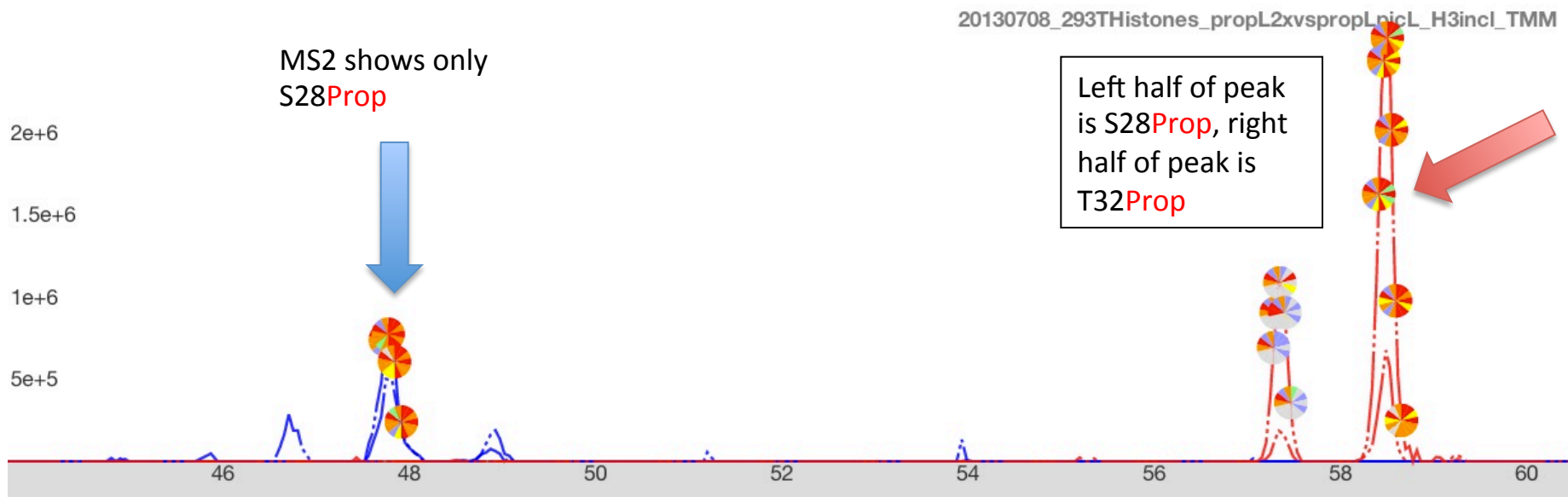
* = 140Da diagnostic ion
 # = 171Da diagnostic ion

H3.1_K27-R40:

KMe1SProp?APATProp?GGVKKPHR

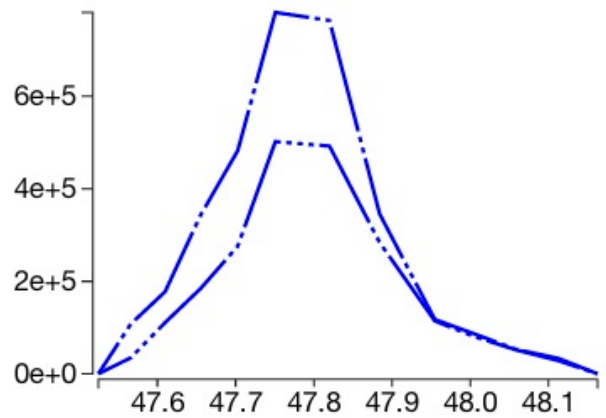
Calculated AUCs for both variations, MS2 for S28-Prop shown.

| id list per inj. | peptide | 2+ | 3+ | 4+ |
|----------------------|--------------------------------|---------|---------|---------|
| 20130708_293THistone | H3.1K27MeS28Prop [prop_d0] | 864.494 | 576.665 | 432.751 |
| 20130708_293THistone | H3.1K27MeS28Prop [pic,prop_d0] | 895.999 | 597.669 | 448.503 |



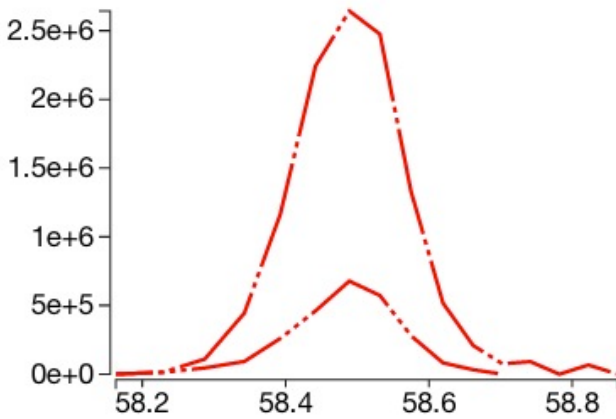
Quanti event: 47.5-48.2min

| injection | peptide | charge | m/z | auc |
|-----------------------------------------------------|--------------------------------|--------|----------|--------|
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27MeS28Prop [prop_d0] | 2 | 864.4938 | 1.1e+7 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27MeS28Prop [pic,prop_d0] | 2 | 895.9992 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27MeS28Prop [prop_d0] | 3 | 576.6649 | 7.5e+6 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27MeS28Prop [pic,prop_d0] | 3 | 597.6686 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27MeS28Prop [prop_d0] | 4 | 432.7505 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27MeS28Prop [pic,prop_d0] | 4 | 448.5033 | 0.0e+0 |



Quanti event: 58.1-58.9min

| injection | peptide | charge | m/z | auc |
|-----------------------------------------------------|--------------------------------|--------|----------|--------|
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27MeS28Prop [prop_d0] | 2 | 864.4938 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27MeS28Prop [pic,prop_d0] | 2 | 895.9992 | 3.1e+7 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27MeS28Prop [prop_d0] | 3 | 576.6649 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27MeS28Prop [pic,prop_d0] | 3 | 597.6686 | 6.9e+6 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27MeS28Prop [prop_d0] | 4 | 432.7505 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27MeS28Prop [pic,prop_d0] | 4 | 448.5033 | 0.0e+0 |



H3.1_K27-R40: Prop-KMe1SPropAPATGGVKKPHR MS/MS

Experimental spectrum

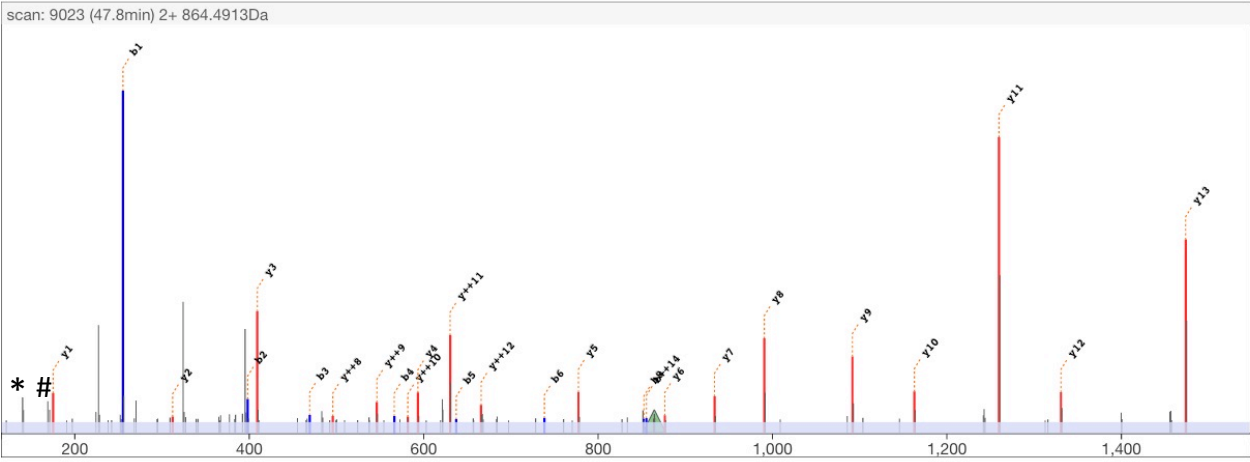
scan 9023
 retention time 47.7min
 precursor m/z 864.4913
 precursor charge 2+

Theoretical

M H²⁺ 864.4938
 MH Δ_{mass} Da -0.0049
 MH Δ_{mass} ppm -2.8

edit peptide

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



| | b++ | b | | y | y++ | |
|----|--------|---------|------------------|---------|--------|----|
| | | | Propionyl | 1671.95 | 836.48 | 14 |
| 1 | 128.09 | 255.17 | K | 1473.82 | 737.41 | 13 |
| | | | Methyl,Propionyl | | | |
| 2 | 199.62 | 398.23 | S | 1330.76 | 665.88 | 12 |
| 3 | 235.14 | 469.27 | A | 1259.72 | 630.36 | 11 |
| 4 | 283.66 | 566.32 | P | 1162.67 | 581.84 | 10 |
| 5 | 319.18 | 637.36 | A | 1091.63 | 546.32 | 9 |
| 6 | 369.71 | 738.40 | T | 990.58 | 495.80 | 8 |
| 7 | 398.22 | 795.42 | G | 933.56 | 467.29 | 7 |
| 8 | 426.73 | 852.45 | V | 876.54 | 438.77 | 6 |
| 9 | 476.26 | 951.51 | K | 777.47 | 389.24 | 5 |
| 10 | 568.32 | 1135.64 | Propionyl | 593.35 | 297.18 | 4 |
| 11 | 660.38 | 1319.76 | K | 409.23 | 205.12 | 3 |
| 12 | 708.91 | 1416.81 | P | 312.18 | 156.59 | 2 |
| 13 | 777.44 | 1553.87 | H | 175.12 | 88.06 | 1 |
| 14 | 855.49 | 1709.97 | R | | | |

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

Experimental spectrum

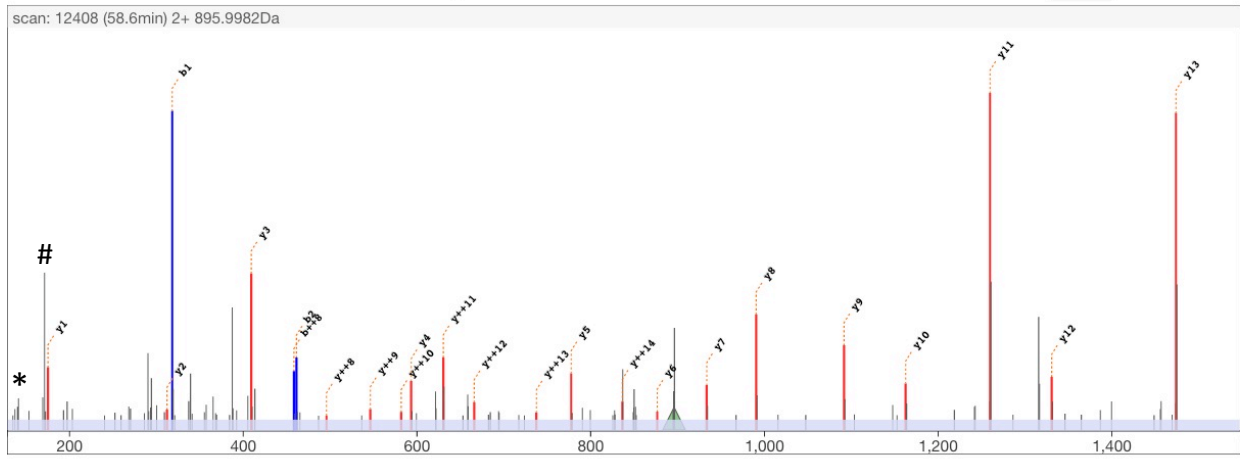
scan 12408
 retention time 58.6min
 precursor m/z 895.9982
 precursor charge 2+

Theoretical

M H²⁺ 895.9992
 MH Δ_{mass} Da -0.0020
 MH Δ_{mass} ppm -1.1

edit peptide

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

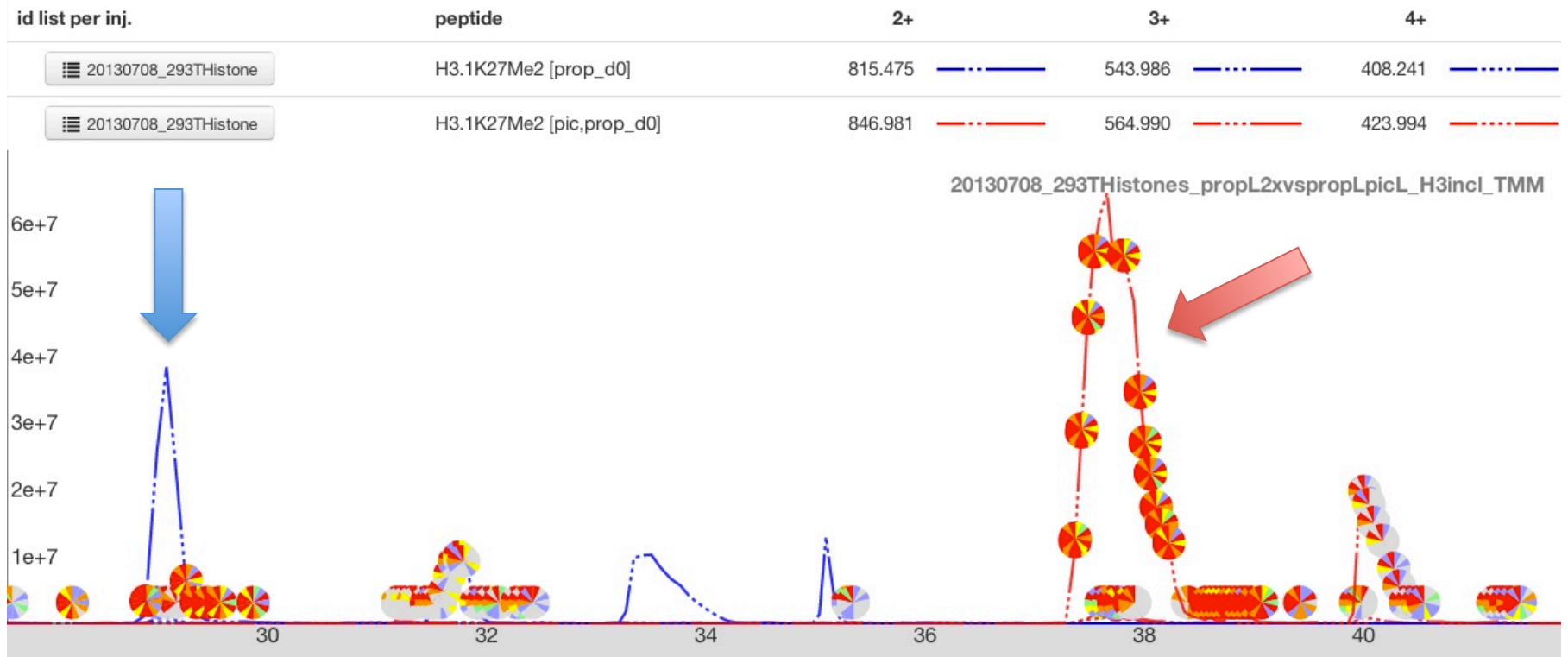


| | b++ | b | | y | y++ | |
|----|--------|---------|------------------|---------|--------|----|
| | 60.53 | 120.04 | PIC | 1671.95 | 836.48 | 14 |
| 1 | 159.59 | 318.18 | K | 1473.82 | 737.41 | 13 |
| 2 | 231.12 | 461.24 | Methyl,Propionyl | 1330.76 | 665.88 | 12 |
| 3 | 266.64 | 532.28 | S | 1259.72 | 630.36 | 11 |
| 4 | 315.17 | 629.33 | A | 1162.67 | 581.84 | 10 |
| 5 | 350.69 | 700.37 | P | 1091.63 | 546.32 | 9 |
| 6 | 401.21 | 801.41 | A | 990.58 | 495.80 | 8 |
| 7 | 429.72 | 858.44 | T | 933.56 | 467.29 | 7 |
| 8 | 458.23 | 915.46 | G | 876.54 | 438.77 | 6 |
| 9 | 507.77 | 1014.53 | V | 777.47 | 389.24 | 5 |
| 10 | 599.83 | 1198.65 | K | 593.35 | 297.18 | 4 |
| 11 | 691.89 | 1382.77 | Propionyl | 409.23 | 205.12 | 3 |
| 12 | 740.41 | 1479.82 | K | 312.18 | 156.59 | 2 |
| 13 | 808.94 | 1616.88 | P | 175.12 | 88.06 | 1 |
| 14 | 886.99 | 1772.98 | H | | | |
| | | | R | | | |

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

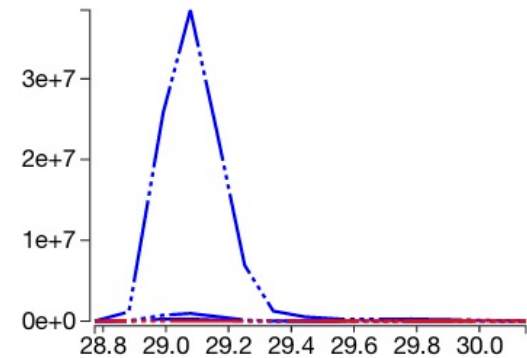
H3.1_K27-R40:

KMe2SAPATGGVKKPHR



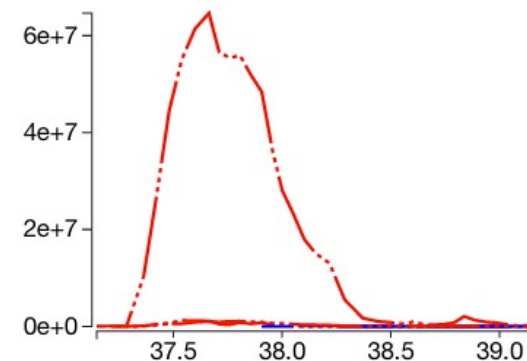
Quanti event: 28.7-30.2min

| injection | peptide | charge | m/z | auc |
|-----------------------------------------------------|--------------------------|--------|----------|--------|
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2 [prop_d0] | 2 | 815.4754 | 4.0e+6 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2 [pic,prop_d0] | 2 | 846.9808 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2 [prop_d0] | 3 | 543.9860 | 5.3e+8 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2 [pic,prop_d0] | 3 | 564.9897 | 5.8e+4 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2 [prop_d0] | 4 | 408.2413 | 1.4e+7 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2 [pic,prop_d0] | 4 | 423.9941 | 4.2e+5 |



Quanti event: 37.1-39.2min

| injection | peptide | charge | m/z | auc |
|-----------------------------------------------------|--------------------------|--------|----------|--------|
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2 [prop_d0] | 2 | 815.4754 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2 [pic,prop_d0] | 2 | 846.9808 | 3.0e+7 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2 [prop_d0] | 3 | 543.9860 | 7.8e+4 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2 [pic,prop_d0] | 3 | 564.9897 | 2.2e+9 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2 [prop_d0] | 4 | 408.2413 | 9.8e+4 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2 [pic,prop_d0] | 4 | 423.9941 | 3.6e+7 |



H3.1_K27-R40: Prop-KMe2SAPATGGVKKPHR MS/MS

Experimental spectrum

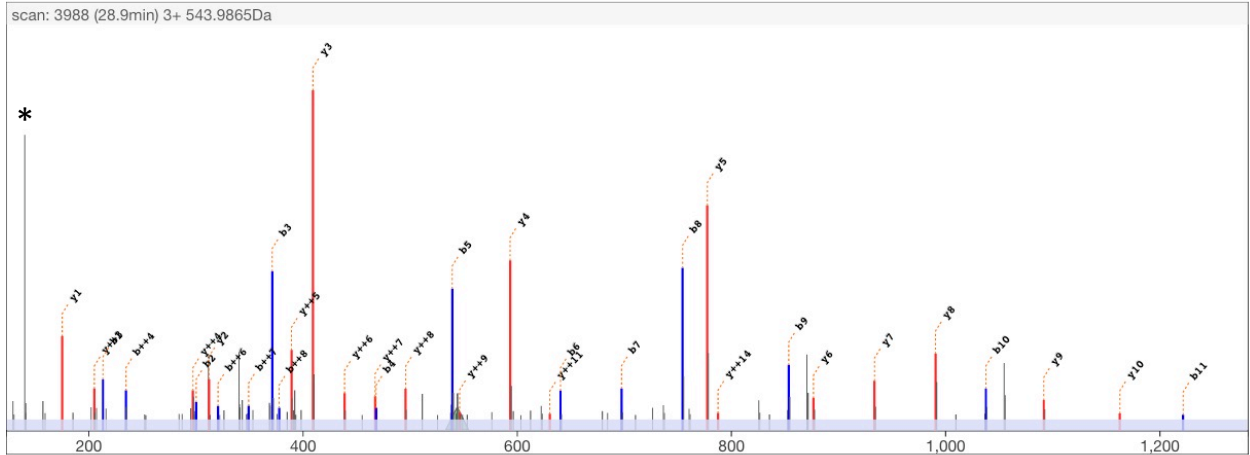
scan 3988
 retention time 28.9min
 precursor m/z 543.9865
 precursor charge 3+

Theoretical

M H³⁺ 543.9860
 MH Δ_{mass} Da 0.0015
 MH Δ_{mass} ppm 0.9

edit peptide

{Propionyl}K{Dimethyl}SAPATGGV{K{Propionyl}K{Propionyl}PHR align



| | b++ | b | y | y++ | |
|----|--------|---------|---------|--------|----|
| | | | 1573.92 | 787.46 | 14 |
| 1 | 107.08 | 213.16 | 1417.79 | 709.40 | 13 |
| 2 | 150.60 | 300.19 | 1330.76 | 665.88 | 12 |
| 3 | 186.12 | 371.23 | 1259.72 | 630.36 | 11 |
| 4 | 234.64 | 468.28 | 1162.67 | 581.84 | 10 |
| 5 | 270.16 | 539.32 | 1091.63 | 546.32 | 9 |
| 6 | 320.69 | 640.37 | 990.58 | 495.80 | 8 |
| 7 | 349.20 | 697.39 | 933.56 | 467.29 | 7 |
| 8 | 377.71 | 754.41 | 876.54 | 438.77 | 6 |
| 9 | 427.24 | 853.48 | 777.47 | 389.24 | 5 |
| 10 | 519.30 | 1037.60 | 593.35 | 297.18 | 4 |
| 11 | 611.36 | 1221.72 | 409.23 | 205.12 | 3 |
| 12 | 659.89 | 1318.77 | 312.18 | 156.59 | 2 |
| 13 | 728.42 | 1455.83 | 175.12 | 88.06 | 1 |
| 14 | 806.47 | 1611.93 | | | |

* = 140Da diagnostic ion

H3.1_K27-R40: PIC-KMe2SAPATGGVKKPHR MS/MS

Experimental spectrum

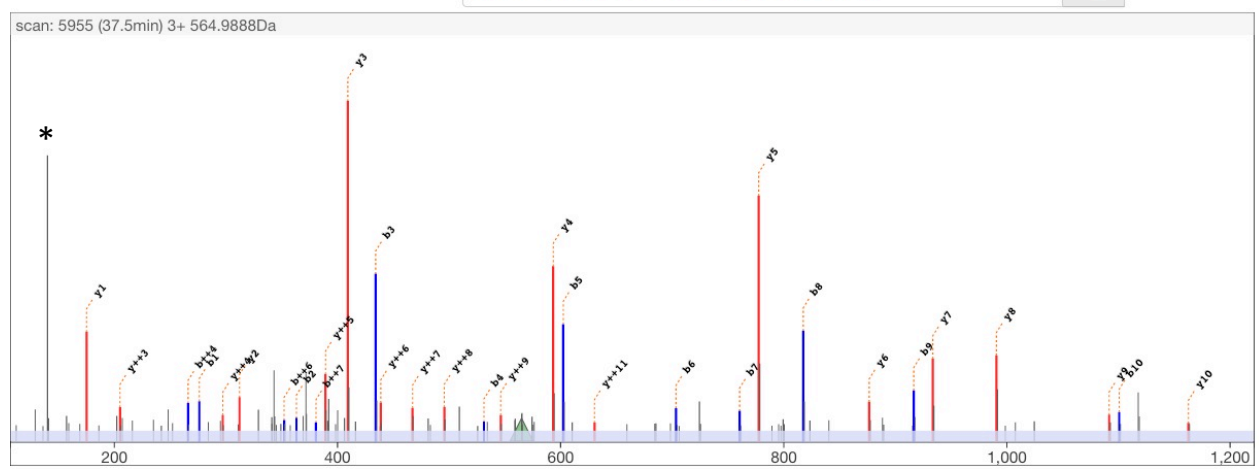
scan 5955
 retention time 37.5min
 precursor m/z 564.9888
 precursor charge 3+

Theoretical

M H³⁺ 564.9897
 MH Δ_{mass} Da -0.0025
 MH Δ_{mass} ppm -1.5

edit peptide

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

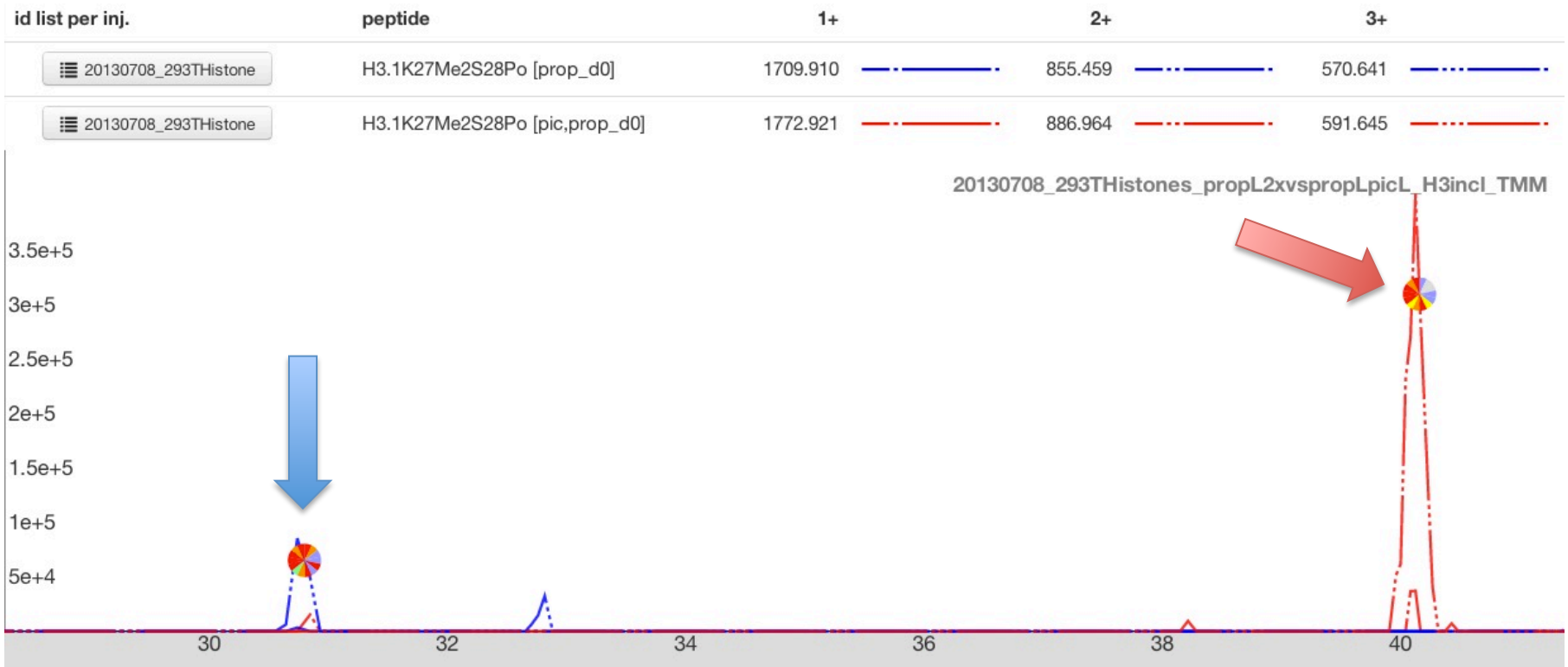


| | b++ | b | | y | y++ | |
|----|--------|---------|-----|---------|--------|----|
| | 60.53 | 120.04 | PIC | 1573.92 | 787.46 | 14 |
| 1 | 138.59 | 276.17 | K | 1417.79 | 709.40 | 13 |
| 2 | 182.10 | 363.20 | S | 1330.76 | 665.88 | 12 |
| 3 | 217.62 | 434.24 | A | 1259.72 | 630.36 | 11 |
| 4 | 266.15 | 531.29 | P | 1162.67 | 581.84 | 10 |
| 5 | 301.67 | 602.33 | A | 1091.63 | 546.32 | 9 |
| 6 | 352.19 | 703.38 | T | 990.58 | 495.80 | 8 |
| 7 | 380.70 | 760.40 | G | 933.56 | 467.29 | 7 |
| 8 | 409.21 | 817.42 | V | 876.54 | 438.77 | 6 |
| 9 | 458.75 | 916.49 | K | 777.47 | 389.24 | 5 |
| 10 | 550.81 | 1100.61 | K | 593.35 | 297.18 | 4 |
| 11 | 642.87 | 1284.73 | P | 409.23 | 205.12 | 3 |
| 12 | 691.40 | 1381.78 | H | 312.18 | 156.59 | 2 |
| 13 | 759.93 | 1518.84 | R | 175.12 | 88.06 | 1 |
| 14 | 837.98 | 1674.94 | | | | |

* = 140Da diagnostic ion

H3.1_K27-R40:

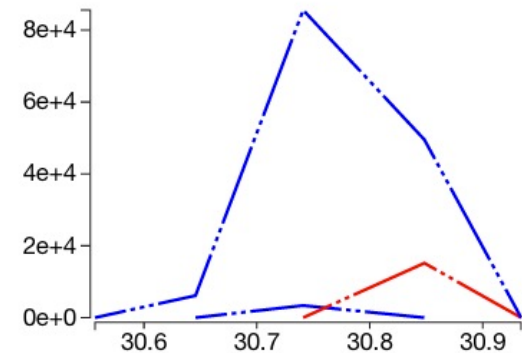
KMe2SPoAPATGGVKKPHR



Quanti event: 29.7-31.4min

x

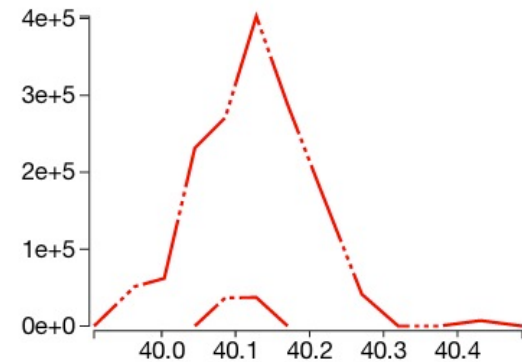
| injection | peptide | charge | m/z | auc |
|-----------------------------------------------------|-------------------------------|--------|-----------|--------|
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Po [prop_d0] | 1 | 1709.9098 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Po [pic,prop_d0] | 1 | 1772.9207 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Po [prop_d0] | 2 | 855.4586 | 2.1e+4 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Po [pic,prop_d0] | 2 | 886.9640 | 8.8e+4 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Po [prop_d0] | 3 | 570.6415 | 8.4e+5 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Po [pic,prop_d0] | 3 | 591.6451 | 0.0e+0 |



Quanti event: 39.4-41.0min

x

| injection | peptide | charge | m/z | auc |
|-----------------------------------------------------|-------------------------------|--------|-----------|--------|
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Po [prop_d0] | 1 | 1709.9098 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Po [pic,prop_d0] | 1 | 1772.9207 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Po [prop_d0] | 2 | 855.4586 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Po [pic,prop_d0] | 2 | 886.9640 | 1.9e+5 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Po [prop_d0] | 3 | 570.6415 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Po [pic,prop_d0] | 3 | 591.6451 | 4.0e+6 |



Experimental spectrum

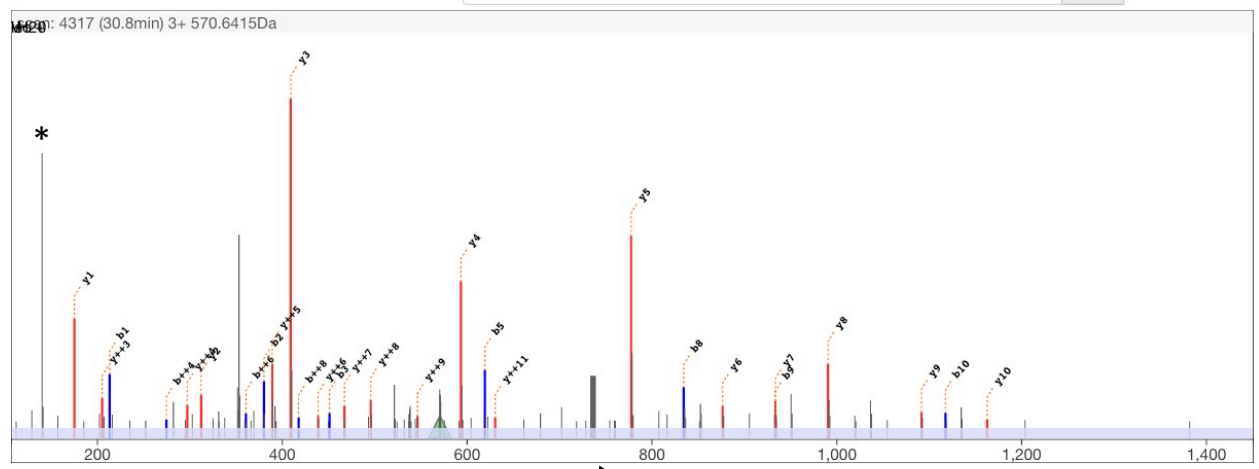
scan 4317
 retention time 30.8min
 precursor m/z 570.6415
 precursor charge 3+

Theoretical

M H³⁺ 570.6415
 MH Δ_{mass} Da 0.0002
 MH Δ_{mass} ppm 0.1

edit peptide

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



Anchor
 click on peak
 m/z 834.3704
 intensity 1323
 int. rank 13

Current
 mouse over peak
 m/z 736.3955
 intensity 1695
 int. rank 9

Explanation?
 delta mass could be...
 $\Delta_{m/z}$ -97.97491

Tune the seq
 Align anchor peak

b8 - H3PO4

* = 140Da diagnostic ion

| | b++ | b | y | y++ | |
|----|--------|---------|---------|--------|----|
| | | | 1653.88 | 827.45 | 14 |
| 1 | 107.08 | 213.16 | 1497.76 | 749.38 | 13 |
| 2 | 190.58 | 380.16 | 1330.76 | 665.88 | 12 |
| 3 | 226.10 | 451.20 | 1259.72 | 630.36 | 11 |
| 4 | 274.63 | 548.25 | 1162.67 | 581.84 | 10 |
| 5 | 310.15 | 619.29 | 1091.63 | 546.32 | 9 |
| 6 | 360.67 | 720.33 | 990.58 | 495.80 | 8 |
| 7 | 389.18 | 777.35 | 933.56 | 467.29 | 7 |
| 8 | 417.69 | 834.38 | 876.54 | 438.77 | 6 |
| 9 | 467.23 | 933.44 | 777.47 | 389.24 | 5 |
| 10 | 559.29 | 1117.57 | 593.35 | 297.18 | 4 |
| 11 | 651.35 | 1301.69 | 409.23 | 205.12 | 3 |
| 12 | 699.87 | 1398.74 | 312.18 | 156.59 | 2 |
| 13 | 768.40 | 1535.80 | 175.12 | 88.06 | 1 |
| 14 | 846.45 | 1691.90 | | | |

Phospho-loss also on b2 and b5 ions.

H3.1_K27-R40: PIC-KMe2SPoAPATGGVKKPHR MS/MS

Experimental spectrum

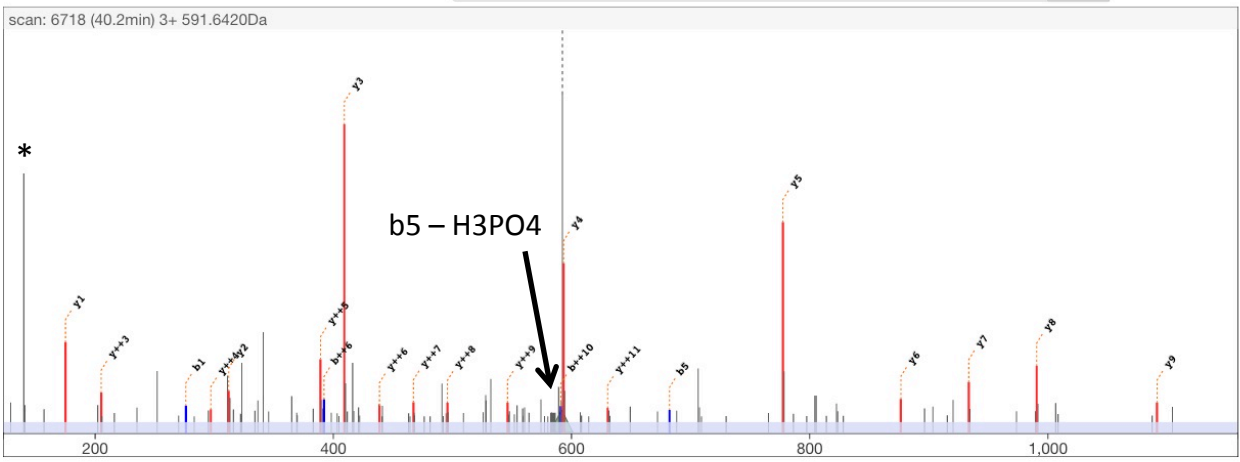
scan 6718
 retention time 40.2min
 precursor m/z 591.6420
 precursor charge 3+

Theoretical

M H³⁺ 591.6451
 MH Δ_{mass} Da -0.0092
 MH Δ_{mass} ppm -5.2

edit peptide

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



| Anchor | Current |
|----------------------|------------------------|
| <i>click on peak</i> | <i>mouse over peak</i> |
| m/z 682.3036 | m/z 584.3321 |
| intensity 1258 | intensity 976 |
| int. rank 63 | int. rank 82 |

Explanation?
 delta mass could be...
 $\Delta_{m/z}$ -97.97156

Tune the seq
 Align anchor peak

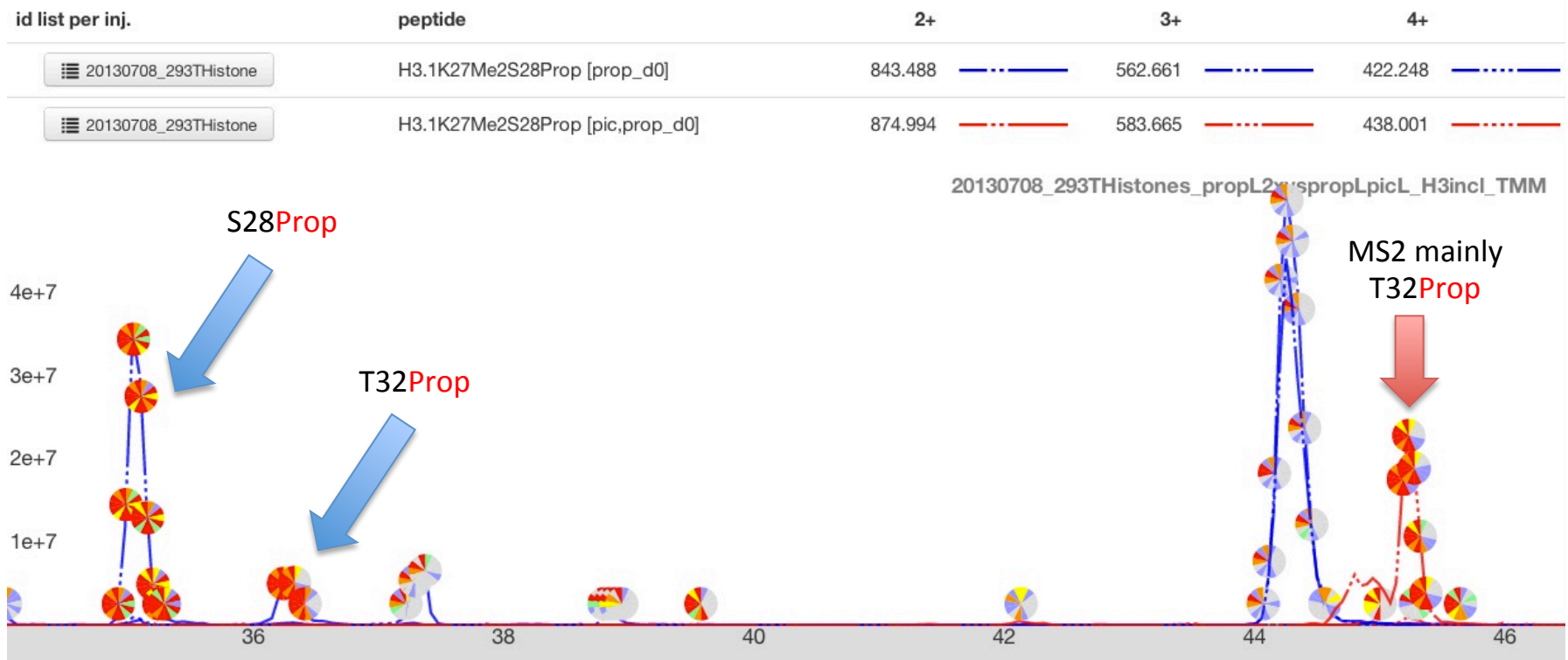
| | b++ | b | | y | y++ | |
|----|--------|---------|-----|---------|--------|----|
| | 60.53 | 120.04 | PIC | 1653.88 | 827.45 | 14 |
| 1 | 138.59 | 276.17 | K | 1497.76 | 749.38 | 13 |
| 2 | 222.09 | 443.17 | S | 1330.76 | 665.88 | 12 |
| 3 | 257.61 | 514.21 | A | 1259.72 | 630.36 | 11 |
| 4 | 306.13 | 611.26 | P | 1162.67 | 581.84 | 10 |
| 5 | 341.65 | 682.30 | A | 1091.63 | 546.32 | 9 |
| 6 | 392.18 | 783.34 | T | 990.58 | 495.80 | 8 |
| 7 | 420.69 | 840.37 | G | 933.56 | 467.29 | 7 |
| 8 | 449.20 | 897.39 | V | 876.54 | 438.77 | 6 |
| 9 | 498.73 | 996.46 | K | 777.47 | 389.24 | 5 |
| 10 | 590.79 | 1180.58 | K | 593.35 | 297.18 | 4 |
| 11 | 682.85 | 1364.70 | P | 409.23 | 205.12 | 3 |
| 12 | 731.38 | 1461.75 | H | 312.18 | 156.59 | 2 |
| 13 | 799.91 | 1598.81 | R | 175.12 | 88.06 | 1 |
| 14 | 877.96 | 1754.91 | | | | |

* = 140Da diagnostic ion

H3.1_K27-R40:

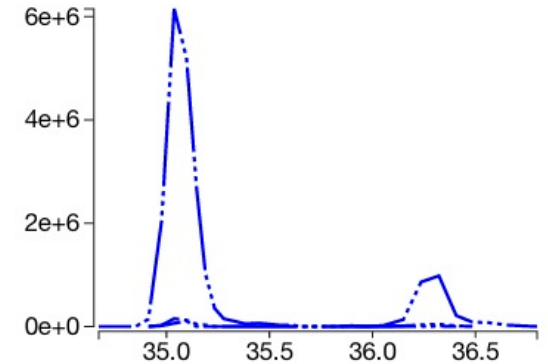
KMe2SProp?APATProp?GGVKKPHR

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



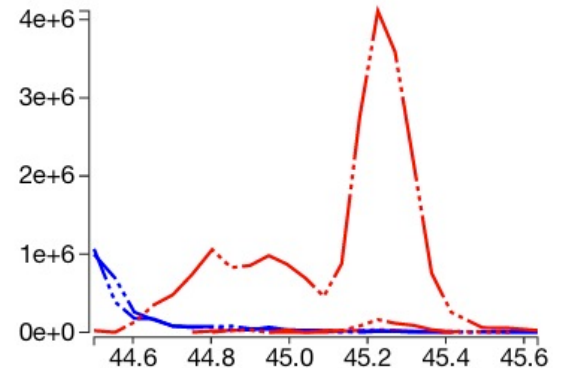
Quanti event: 34.6-36.9min

| injection | peptide | charge | m/z | auc |
|-----------------------------------------------------|---------------------------------|--------|----------|--------|
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Prop [prop_d0] | 2 | 843.4885 | 6.6e+5 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Prop [pic,prop_d0] | 2 | 874.9939 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Prop [prop_d0] | 3 | 562.6614 | 7.2e+7 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Prop [pic,prop_d0] | 3 | 583.6651 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Prop [prop_d0] | 4 | 422.2479 | 1.8e+6 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Prop [pic,prop_d0] | 4 | 438.0006 | 0.0e+0 |



Quanti event: 44.5-45.7min

| injection | peptide | charge | m/z | auc |
|-----------------------------------------------------|---------------------------------|--------|----------|--------|
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Prop [prop_d0] | 2 | 843.4885 | 6.5e+6 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Prop [pic,prop_d0] | 2 | 874.9939 | 4.7e+5 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Prop [prop_d0] | 3 | 562.6614 | 5.5e+6 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Prop [pic,prop_d0] | 3 | 583.6651 | 6.2e+7 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Prop [prop_d0] | 4 | 422.2479 | 0.0e+0 |
| 20130708_293THistones_propL2xvspropLpicL_H3incl_TMM | H3.1K27Me2S28Prop [pic,prop_d0] | 4 | 438.0006 | 1.8e+6 |



H3.1_K27-R40: Prop-KMe2SAPATPropGGVKKPHR MS/MS

Experimental spectrum

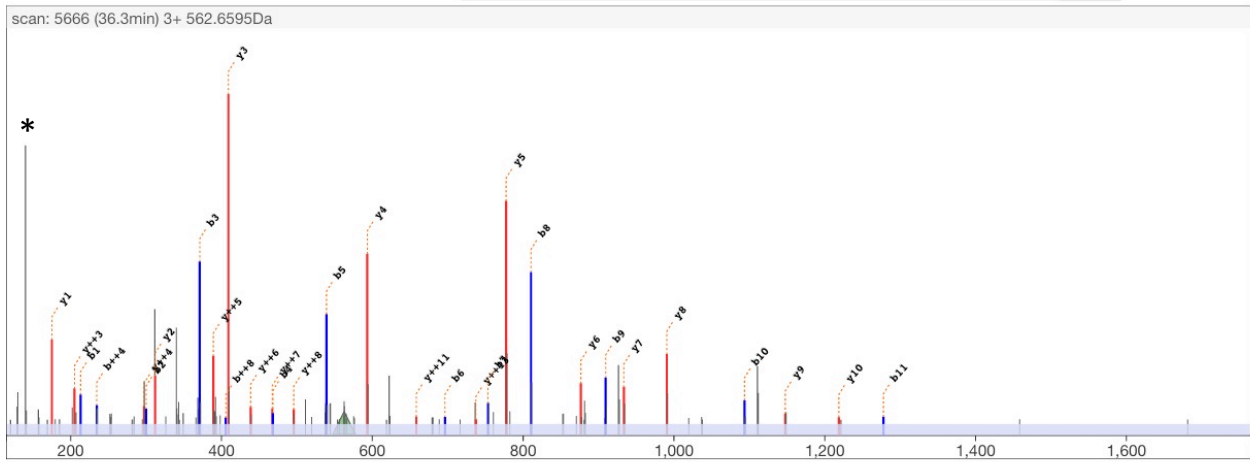
scan 5666
 retention time 36.2min
 precursor m/z 562.6595
 precursor charge 3+

Theoretical

M H³⁺ 562.6614
 MH Δ_{mass} Da -0.0056
 MH Δ_{mass} ppm -3.3

edit peptide

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



| | b++ | b | | y | y++ |
|----|--------|---------|-----------|---------|--------|
| | | | Propionyl | 1629.94 | 815.48 |
| 1 | 107.08 | 213.16 | K | 1473.82 | 737.41 |
| | | | Dimethyl | | |
| 2 | 150.60 | 300.19 | S | 1386.79 | 693.90 |
| 3 | 186.12 | 371.23 | A | 1315.75 | 658.38 |
| 4 | 234.64 | 468.28 | P | 1218.70 | 609.85 |
| 5 | 270.16 | 539.32 | A | 1147.66 | 574.33 |
| 6 | 348.70 | 696.39 | T | 990.58 | 495.80 |
| 7 | 377.21 | 753.41 | G | 933.56 | 467.29 |
| 8 | 405.72 | 810.44 | V | 876.54 | 438.77 |
| 9 | 455.26 | 909.50 | K | 777.47 | 389.24 |
| 10 | 547.32 | 1093.63 | Propionyl | 593.35 | 297.18 |
| 11 | 639.38 | 1277.75 | K | 409.23 | 205.12 |
| 12 | 687.90 | 1374.80 | Propionyl | 312.18 | 156.59 |
| 13 | 756.43 | 1511.86 | P | 175.12 | 88.06 |
| 14 | 834.48 | 1667.96 | H | | |
| | | | R | | |

* = 140Da diagnostic ion

H3.1_K27-R40: PIC-KMe2SAPATPropGGVKKPHR MS/MS

Experimental spectrum

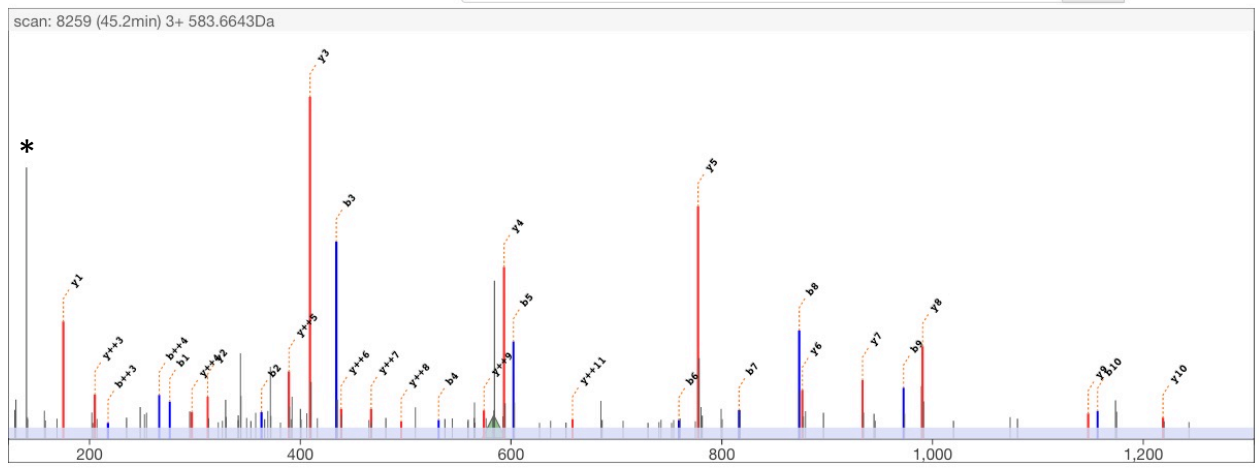
scan 8259
 retention time 45.2min
 precursor m/z 583.6643
 precursor charge 3+

Theoretical

M H³⁺ 583.6651
 MH Δ_{mass} Da -0.0023
 MH Δ_{mass} ppm -1.3

edit peptide

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



| | b++ | b | | y | y++ | |
|----|--------|---------|-----|---------|--------|----|
| | 60.53 | 120.04 | PIC | 1629.94 | 815.48 | 14 |
| 1 | 138.59 | 276.17 | K | 1473.82 | 737.41 | 13 |
| 2 | 182.10 | 363.20 | S | 1386.79 | 693.90 | 12 |
| 3 | 217.62 | 434.24 | A | 1315.75 | 658.38 | 11 |
| 4 | 266.15 | 531.29 | P | 1218.70 | 609.85 | 10 |
| 5 | 301.67 | 602.33 | A | 1147.66 | 574.33 | 9 |
| 6 | 380.21 | 759.40 | T | 990.58 | 495.80 | 8 |
| 7 | 408.72 | 816.43 | G | 933.56 | 467.29 | 7 |
| 8 | 437.23 | 873.45 | V | 876.54 | 438.77 | 6 |
| 9 | 486.76 | 972.51 | K | 777.47 | 389.24 | 5 |
| 10 | 578.82 | 1156.64 | K | 593.35 | 297.18 | 4 |
| 11 | 670.88 | 1340.76 | K | 409.23 | 205.12 | 3 |
| 12 | 719.41 | 1437.81 | P | 312.18 | 156.59 | 2 |
| 13 | 787.94 | 1574.87 | H | 175.12 | 88.06 | 1 |
| 14 | 865.99 | 1730.97 | R | | | |

* = 140Da diagnostic ion