

Supplementary Information:

Figure S1: Calculated Isotope distributions for the naturally acetylated (S1A) and *in vitro* d3-acetylated (S1B) tryptic peptide (residues 54-63) containing K56 of histone H3. S1C shows an overlaid plot of the both isotopic distributions. Note the overlap of the 4th isotope peaks of the naturally acetylated peptide with the monoisotopic peak of the d3-acetylated peptide. This overlap accounts for 8.60% of the area of the monoisotopic peak of the naturally acetylated peptide.

Figure S2: Calculated Isotope distributions for various isoforms of the d3-acetylated Histone H4 tail tryptic peptide (residues 4-17) containing (S2A) 0, (S2B) 1, (S2C) 2, (S2D) 3, and (S2E) 4 naturally acetylated lysines. S2F shows an overlaid plot of the isotopic distributions of all isoforms. Note the overlap of the 4 isotope peaks with monoisotopic peak of the isoform 3 Da heavier. This overlap is *ca.* 10.75% of the area of the monoisotopic peak.

FQK_{ac} STELLIR

Elemental Composition: C₅₈H₉₈N₁₅O₁₇

Resolution: 5500

Isotope Number	m/z	Percent Total	Percent Maximum
0	1276.72651	46.93	100.00
1	1277.72945	34.05	72.55
2	1278.73219	13.80	29.41
3	1279.73484	4.04	8.61
4	1280.73743	0.95	2.01
5	1281.73997	0.19	0.40
6	1282.74249	0.03	0.07
7	1283.74501	0.00	0.01
8	1284.74772	0.00	0.00
9	1285.75172	0.00	0.00

S1A

FQK_{d3-ac} STELLIR

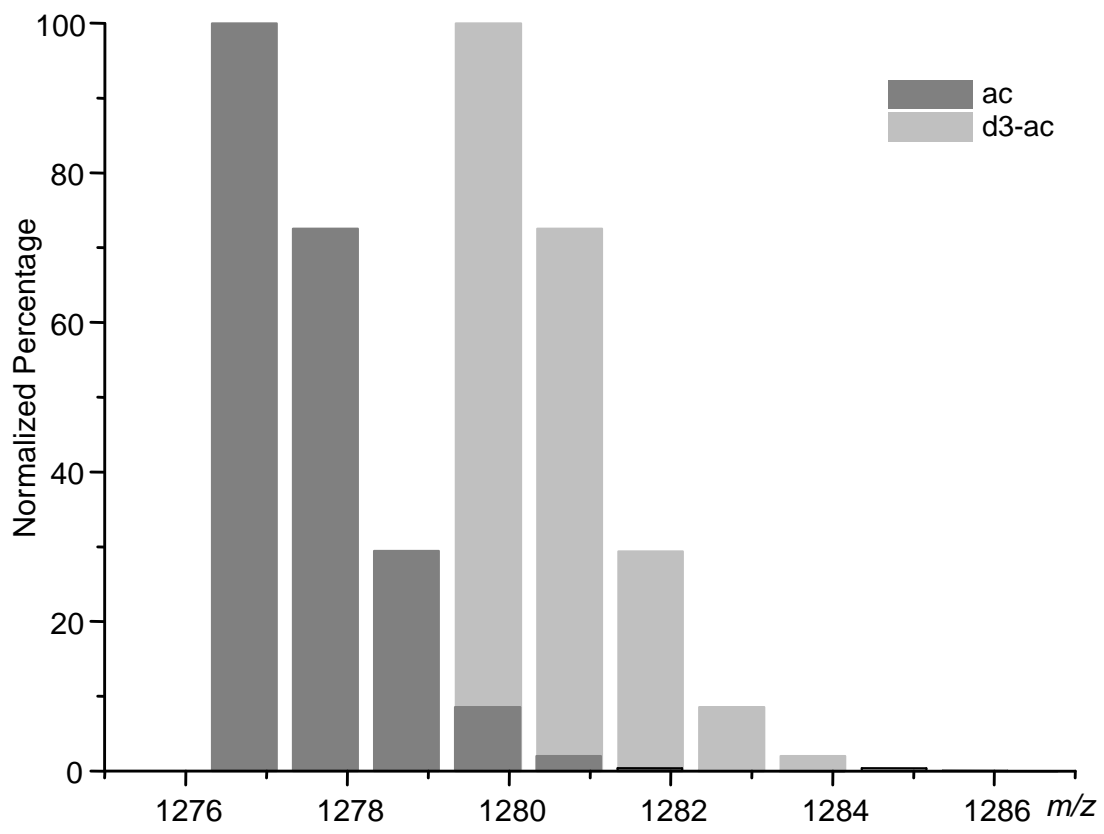
Elemental Composition: C₅₈H₉₅D₃N₁₅O₁₇

Resolution: 5500

Isotope Number	m/z	Percent Total	Percent Maximum
0	1279.74534	46.96	100.00
1	1280.74828	34.04	72.50
2	1281.75102	13.80	29.38
3	1282.75367	4.04	8.60
4	1283.75625	0.94	2.01
5	1284.75879	0.19	0.40
6	1285.76131	0.03	0.07
7	1286.76.83	0.00	0.01
8	1287.76654	0.00	0.00
9	1288.77055	0.00	0.00

S1B

S1C



GK_{ac}GGK_{ac}GLGK_{ac}GGAK_{ac}R
 Elemental Composition: C₆₁H₁₀₈N₂₁O₁₉
 Resolution: 5500

Isotope Number	m/z	Percent Total	Percent Maximum
0	1438.81304	44.12	100.00
1	1439.81584	34.57	78.34
2	1440.81847	15.07	34.16
3	1441.82103	4.74	10.74
4	1442.82354	1.19	2.69
5	1443.82601	0.25	0.57
6	1444.82846	0.05	0.10
7	1445.83088	0.01	0.02
8	1446.83340	0.00	0.00
9	1447.83648	0.00	0.00

S2A

GK_{d3-ac}GGK_{ac}GLGK_{ac}GGAK_{ac}R
 GK_{ac}GGK_{d3-ac}GLGK_{ac}GGAK_{ac}R
 GK_{ac}GGK_{ac}GLGK_{d3-ac}GGAK_{ac}R
 GK_{ac}GGK_{ac}GLGK_{ac}GGAK_{d3-ac}R
 Elemental Composition: C₆₁H₁₀₅D₃N₂₁O₁₉
 Resolution: 5500

Isotope Number	m/z	Percent Total	Percent Maximum
0	1441.83651	44.11	100.00
1	1442.83931	34.57	78.38
2	1443.84195	15.08	34.20
3	1444.84451	4.74	10.76
4	1445.84702	1.19	2.70
5	1446.84950	0.25	0.57
6	1447.85194	0.05	0.10
7	1448.85437	0.01	0.02
8	1449.85688	0.00	0.00
9	1450.85995	0.00	0.00

S2B

$GK_{d3-ac}GGK_{d3-ac}GLGK_{ac}GGAK_{ac}R$, $GK_{d3-ac}GGK_{ac}GLGK_{d3-ac}GGAK_{ac}R$,
 $GK_{d3-ac}GGK_{ac}GLGK_{ac}GGAK_{d3-ac}R$, $GK_{ac}GGK_{d3-ac}GLGK_{d3-ac}GGAK_{ac}R$,
 $GK_{ac}GGK_{d3-ac}GLGK_{ac}GGAK_{d3-ac}R$, $GK_{ac}GGK_{ac}GLGK_{d3-ac}GGAK_{d3-ac}R$
 Elemental Composition: $C_{61}H_{102}D_6N_{21}O_{19}$
 Resolution: 5500

S2C

Isotope Number	m/z	Percent Total	Percent Maximum
0	1444.85999	44.09	100.00
1	1445.86279	34.57	78.43
2	1446.86543	15.09	34.23
3	1447.86800	4.75	10.77
4	1448.87051	1.19	2.70
5	1449.87298	0.25	0.57
6	1450.87543	0.05	0.11
7	1451.87785	0.01	0.02
8	1452.88036	0.00	0.00
9	1453.88343	0.00	0.00

$GK_{d3-ac}GGK_{d3-ac}GLGK_{d3-ac}GGAK_{ac}R$
 $GK_{d3-ac}GGK_{d3-ac}GLGK_{ac}GGAK_{d3-ac}R$
 $GK_{d3-ac}GGK_{ac}GLGK_{d3-ac}GGAK_{d3-ac}R$
 $GK_{ac}GGK_{d3-ac}GLGK_{d3-ac}GGAK_{d3-ac}R$
 Elemental Composition: $C_{61}H_{99}D_9N_{21}O_{19}$
 Resolution: 5500

S2D

Isotope Number	m/z	Percent Total	Percent Maximum
0	1447.88346	44.07	100.00
1	1448.88627	34.58	78.47
2	1449.88891	15.10	34.27
3	1450.89148	4.75	10.79
4	1451.89399	1.19	2.71
5	1452.89646	0.25	0.57
6	1453.89891	0.05	0.11
7	1454.90135	0.01	0.02
8	1455.90385	0.00	0.00
9	1456.90690	0.00	0.00

GK_{d3-ac}GGK_{d3-ac}GLGK_{d3-ac}GGAK_{d3-ac}R
 Elemental Composition: C₆₁H₉₆D₁₂N₂₁O₁₉
 Resolution: 5500

Isotope Number	m/z	Percent Total	Percent Maximum
0	1450.90694	44.05	100.00
1	1451.90974	34.58	78.52
2	1452.91239	15.11	34.30
3	1453.91496	4.76	10.80
4	1454.91747	1.20	2.71
5	1455.91995	0.25	0.57
6	1456.92240	0.05	0.11
7	1457.92483	0.01	0.02
8	1458.92733	0.00	0.00
9	1459.93038	0.00	0.00

S2E

S2F

