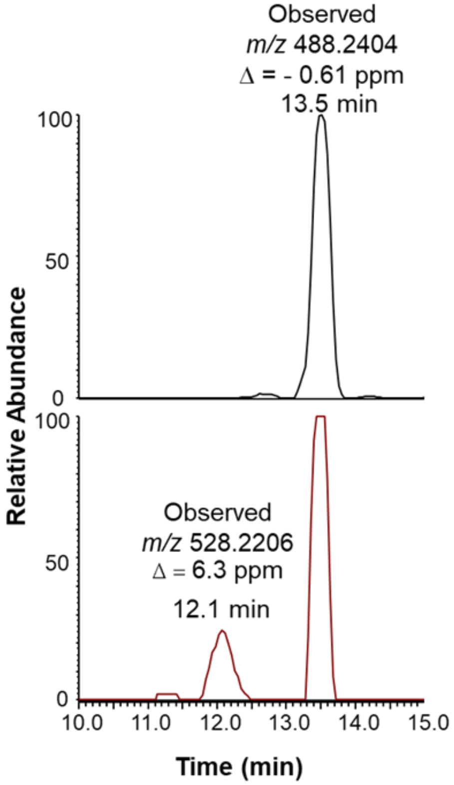
a


Observed
m/z 488.2404
Δ = - 0.61 ppm
13.5 min
100
50
0
100
50
0
Observed
m/z 528.2206
Δ = 6.3 ppm
12.1 min
Relative Abundance
10.0
11.0
12.0
13.0
14.0
15.0
Time (min)

b

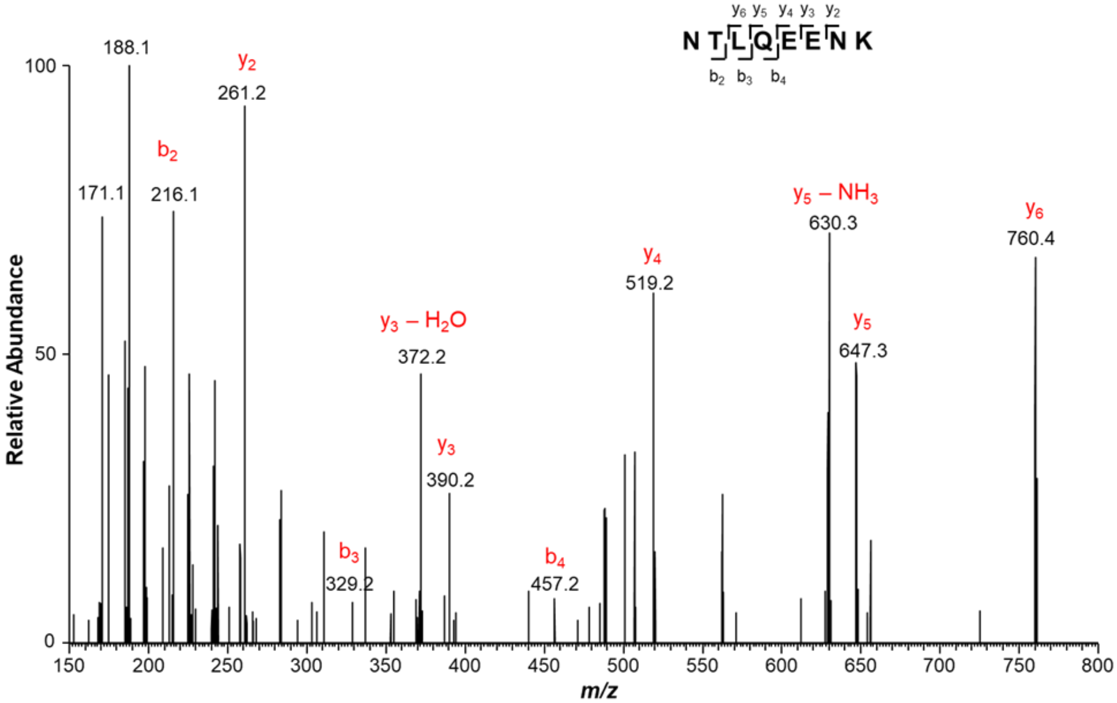

N T L Q E E N K
y6 y5 y4 y3 y2
b2 b3 b4
100
50
0
Relative Abundance
188.1
171.1
y2
261.2
b2
216.1
y3 – H2O
372.2
y3
390.2
b3
329.2
b4
457.2
y4
519.2
y5 – NH3
630.3
y5
647.3
y6
760.4
150
200
250
300
350
400
450
500
550
600
650
700
750
800
m/z

Figure S3. LC-MS and MS/MS for the identification of the unmodified CtIP peptide, NTLQEENK and the same peptide with Thr^{126} being phosphorylated from the irradiated sample. **a** Selected-ion chromatogram for the $[M + 2H]^{2+}$ ions of the unphosphorylated (top, calculated *m/z* 488.2407) and phosphorylated (bottom, calculated *m/z* 528.2239) peptide NTLQEENK. **b** Tandem mass spectrum (MS/MS) of the ESI-produced $[M+2H]^{2+}$ ion of the unphosphorylated peptide NTLQEENK. The spectrum was acquired by LC-MS/MS in the data-dependent acquisition mode on a QE Plus quadrupole-Orbitrap mass spectrometer.