Supplementary Information

Table S1. Percentage of oxidized product ions observed in the CID spectrum of the doubly charged ion of the oxidized OVA peptide $(M+O+2H)^{2+}$.

Product Ion	$m/z_{unoxidized}$[a]	$m/z_{oxidized}$[a]	Percentage oxidized[b,c]
y_3	303	319	0
y_4	432	448	0
y_5	546	562	0
y_6	659	675	0
y_7	788	804	0
y_8	859	875	0
y_9	996	1012	22 ± 7
y_{10}	1067	1083	63 ± 0.4
y_{11}	1138	1154	69 ± 1
y_{12}	1275	1291	100
y_{13}	1374	1390	100
y_{14}	1445	1461	100
b_5	499	515	0
b_6	636	652	17 ± 1
b_7	707	723	25 ± 2
b_8	778	794	38 ± 2
b_9	915	931	100
b_{10}	986	1002	100
b_{11}	1115	1131	100
b_{12}	1228	1244	100
b_{13}	1342	1358	100
b_{14}	1471	1487	100
b_{15}	1542	1558	100
b_{16}	1599	1615	100

[a] These m/z ratios correspond to the nominal m/z ratio of the observed product ions.
[b] The percentage oxidized is obtained by dividing the ion abundance of the oxidized product ion by the sum of the oxidized and unoxidized product ions.
[c] The error associated with oxidized percentage value corresponds to the standard deviation from at least three separate measurements

Table S2. Percentage of oxidized product ions observed in the CID spectrum of the doubly charged ion of the oxidized β-amyloid peptide $(M+O+2H)^{2+}$.

Product Ion	$m/z_{unoxidized}$[a]	$m/z_{oxidized}$[a]	Percentage oxidized[b,c]
y_2	313	329	10 ± 2
y_3	412	428	0
y_5	653	669	0
y_6	781	797	0
y_7	918	934	55.0 ± 0.7
y_8	1055	1071	100
y_9	1154	1170	100
y_9^{2+}	578	586	100
b_2	293	309	14 ± 1
b_3	392	408	28 ± 1
b_4	529	545	45 ± 3
b_5	666	682	83.0 ± 0.4
b_6	794	810	78 ± 1
b_7	922	938	73 ± 1
b_8	1035	1051	54 ± 2
b_9	1134	1150	85 ± 1
b_9^{2+}	567	575	88 ± 3
b_{10}^{2+}	641	649	83 ± 1

[a] These m/z ratios correspond to the nominal m/z ratio of the observed product ions.
[b] The percentage oxidized is obtained by dividing the ion abundance of the oxidized product ion by the sum of the oxidized and unoxidized product ions.
[c] The error associated with oxidized percentage value corresponds to the standard deviation from at least three separate measurements.

Table S3. Percentage of oxidized product ions observed in the CID spectrum of the triply charged ion of the oxidized MPP peptide $(M+O+3H)^{3+}$.

Product Ion	$m/z_{unoxidized}$[a]	$m/z_{oxidized}$[a]	Percentage oxidized[b,c]
y_2	294	310	0
y_5^{2+}	322	330	20±0.5
y_6	700	716	40±0.8
y_7	813	829	41±1.1
y_{11}^{2+}	649	657	63±0.9
b_2	225	241	11±0.2
b_5	523	539	47±0.4
b_8	879	895	61±1.5
b_9	1016	1032	100
b_{11}^{2+}	615	623	100
b_{12}^{2+}	679	687	100
b_{12}^{3+}	453	458	100

[a] These m/z ratios correspond to the nominal m/z ratio of the observed product ions.
[b] The percentage oxidized is obtained by dividing the ion abundance of the oxidized product ion by the sum of the oxidized and unoxidized product ions.
[c] The error associated with oxidized percentage value corresponds to the standard deviation from at least three separate measurements

Figure S1. MS^3 of the y_4+O product ion of oxidized angiotensin I $(M+O+2H)^{2+}$, which helps confirm that oxidation only occurs at His9 and not Pro7 or Phe8. The asterisks indicate the product ions that are oxidized.

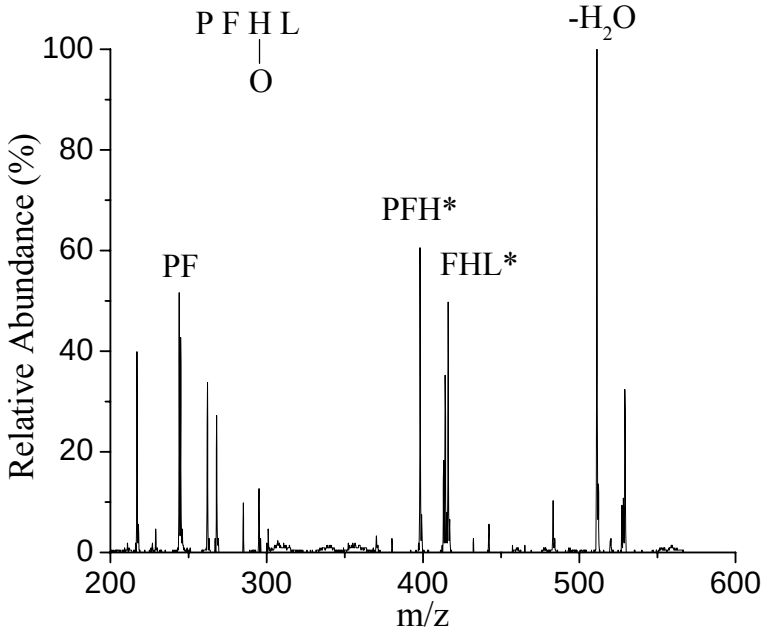


Figure S2. MS^3 of the $(b_9+O)^{2+}$ product ion of oxidized angiotensin I $(M+O+2H)^{2+}$, which helps confirm that oxidation only occurs at His6 and His9 and not Pro7 or Phe8. The asterisks indicate the product ions that are oxidized.

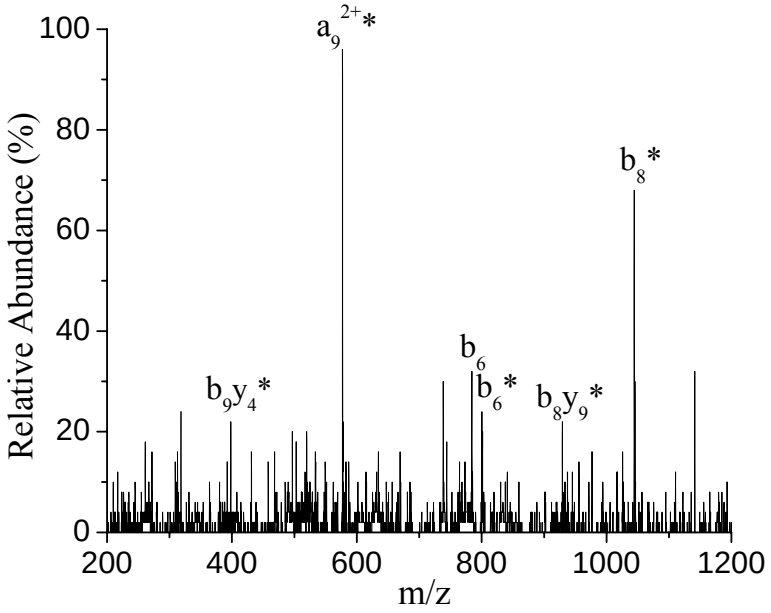


Figure S3. MS^3 of the b_8+O product ion of oxidized angiotensin I $(M+O+2H)^{2+}$, which helps confirm that oxidation only occurs at His6 and His9 and not Pro7 or Phe8. The asterisks indicate the product ions that are oxidized.

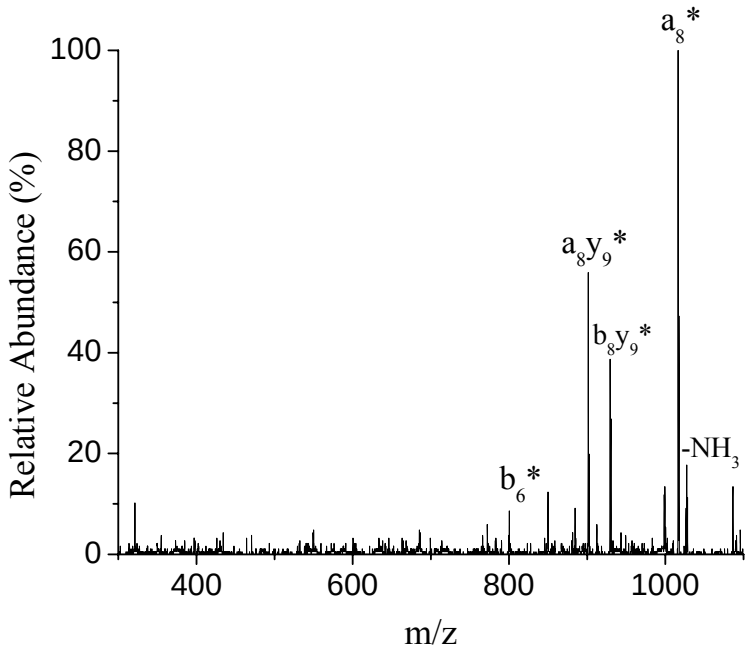
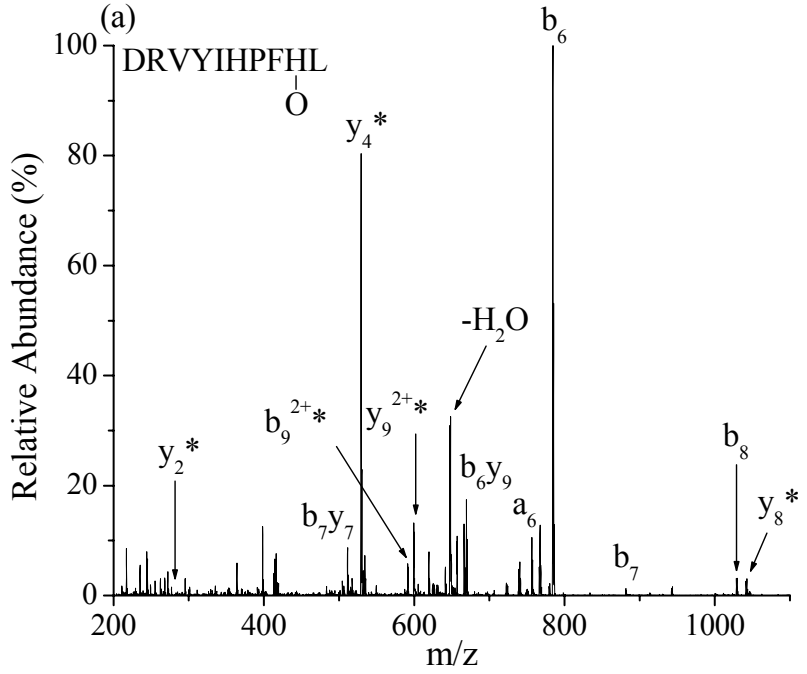


Figure S4. (a) CID of His9-oxidized angiotensin I $(M+O+2H)^{2+}$. (b) CID of His6-oxidized angiotensin I $(M+O+2H)^{2+}$. The individual oxidized His6 and oxidized His9 isomers were obtained by separating them by HPLC. The asterisks indicate the product ions that are oxidized.



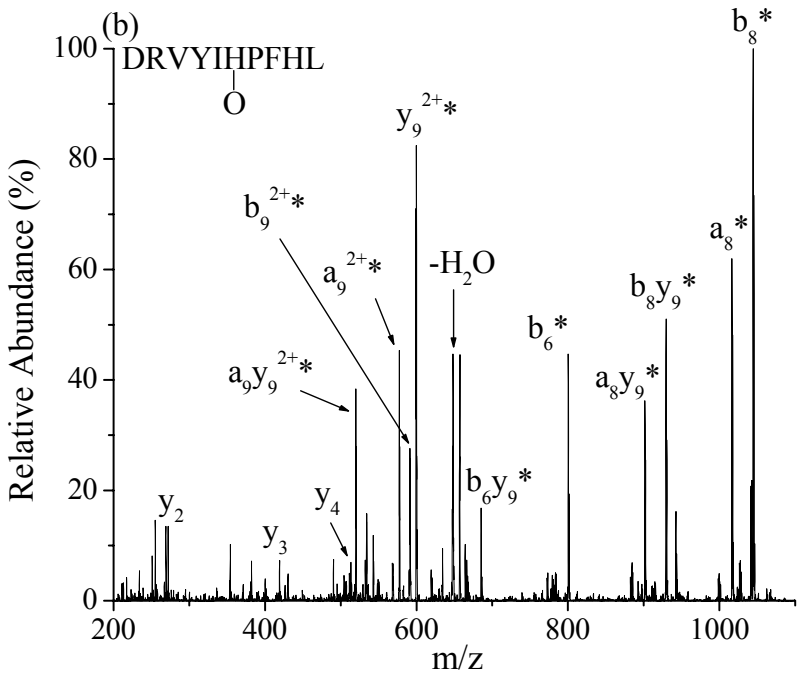
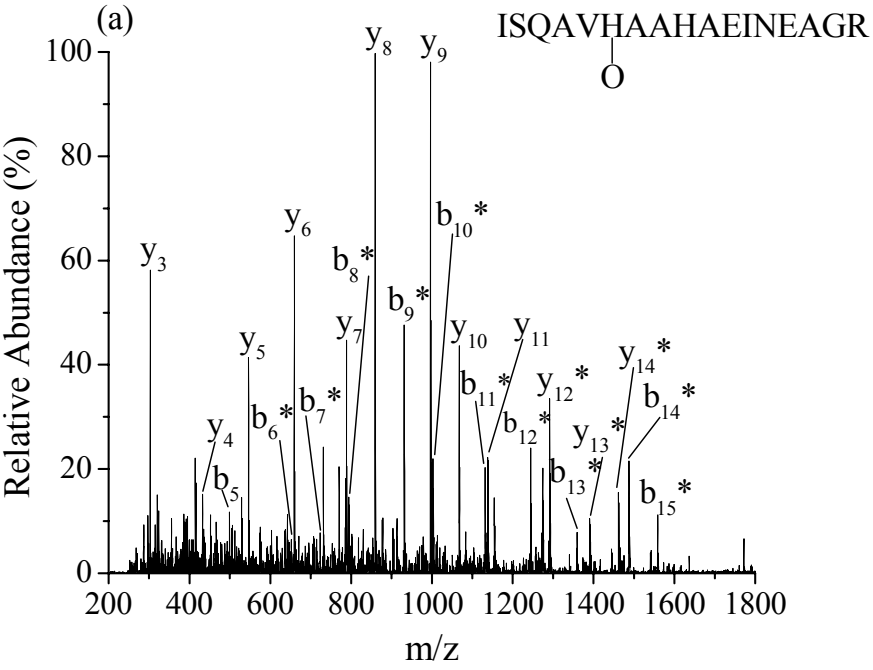


Figure S5. (a) CID of His6-oxidized OVA peptide $(M+O+2H)^{2+}$ (b) CID of His9-oxidized OVA peptide $(M+O+2H)^{2+}$. The individual oxidized His6 and oxidized His9 isomers were obtained by separating them by HPLC. The asterisks indicate the product ions that are oxidized.



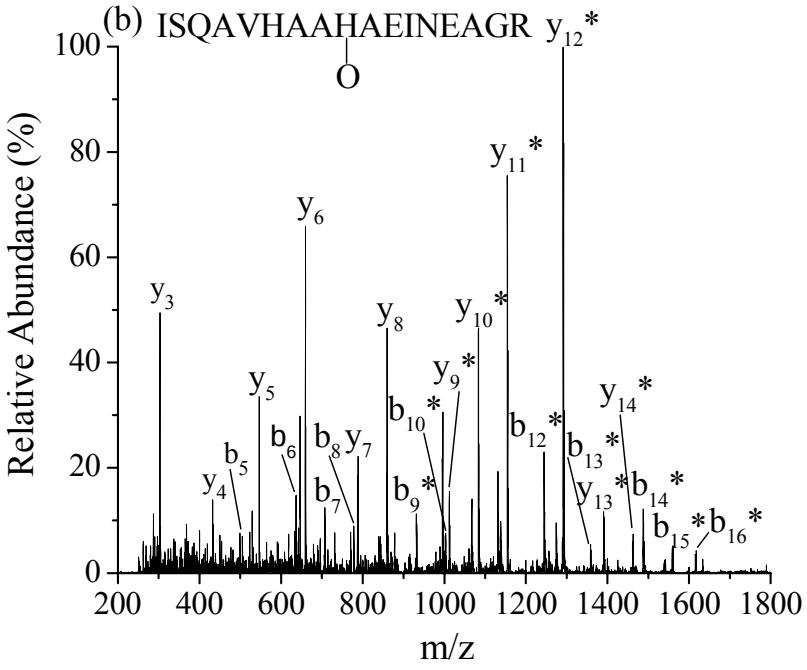


Figure S6. ETD of the triply-charged ion of oxidized OVA peptide $(M+O+3H)^{3+}$ without prior LC separation. The asterisks indicate the product ions that are oxidized.

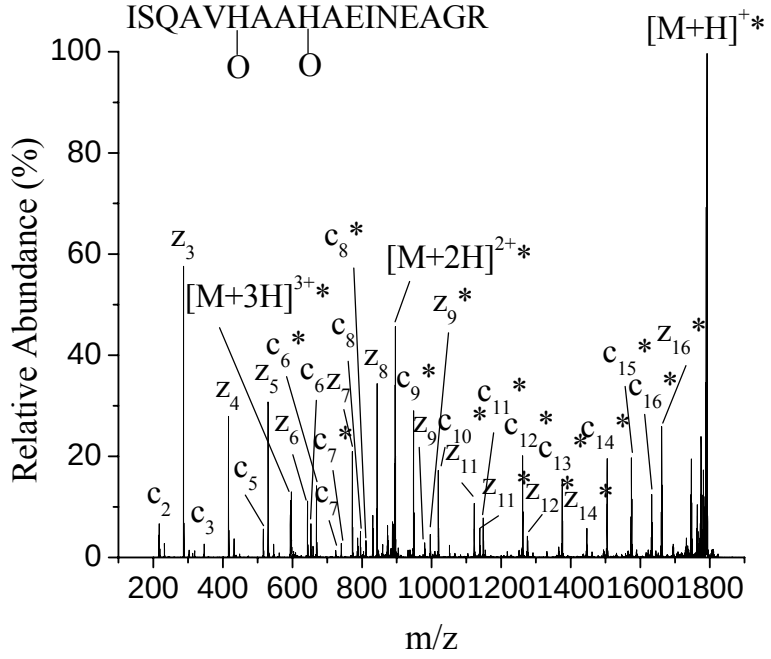
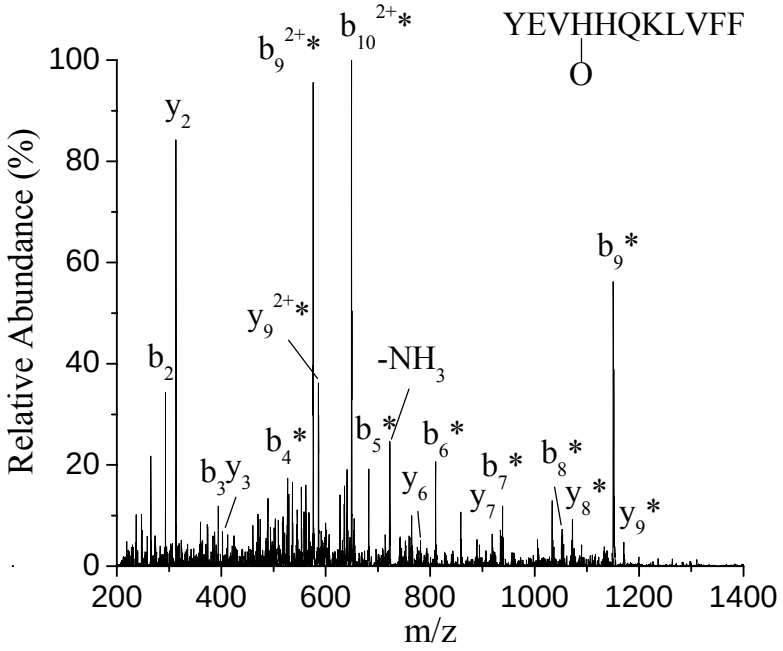
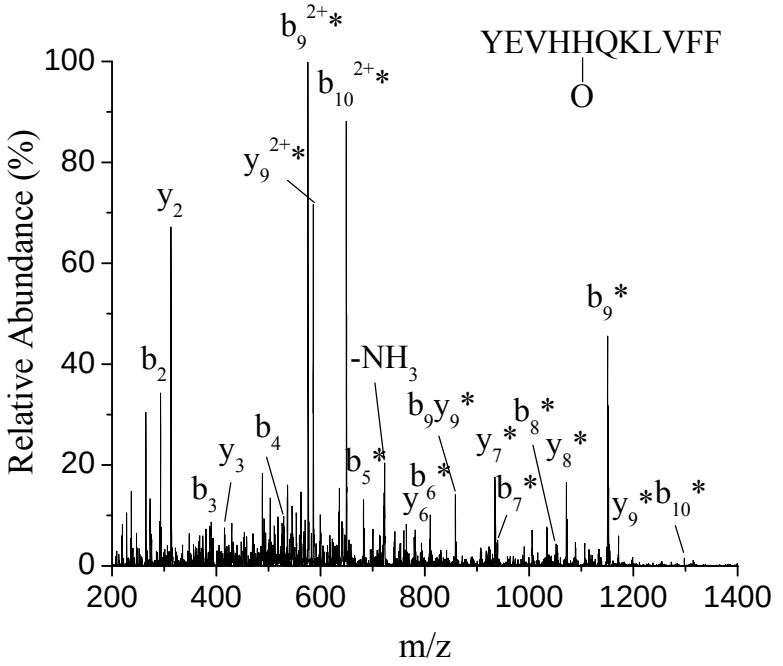


Figure S7. (a) CID of His4-oxidized β-amyloid peptide $(M+O+2H)^{2+}$. (b) CID of His5-oxidized β-amyloid peptide $(M+O+2H)^{2+}$. (c) CID of Phe10-oxidized β-amyloid peptide $(M+O+2H)^{2+}$. (d) CID of Phe11-oxidized β-amyloid peptide $(M+O+2H)^{2+}$. The individual oxidized isomers were obtained by separating them by HPLC. The asterisks indicate the product ions that are oxidized.

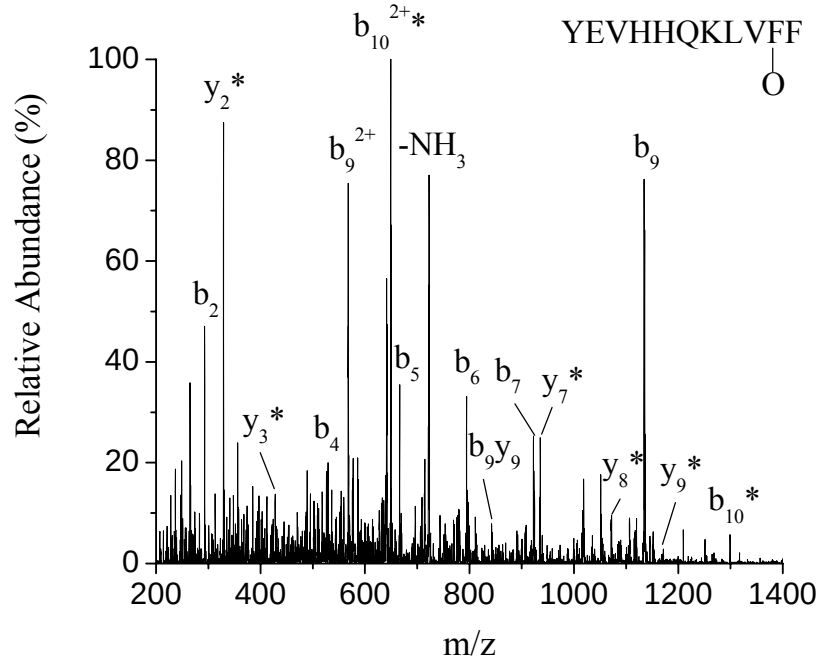
(a)



(b)



(c)


YEVHHQKLVFF
O
Relative Abundance (%)
m/z
b10 2+*
y2*
b9 2+
-NH3
b9
b2
b5
b6
b7
y7*
y3*
b4
b9y9
y8*
y9*
b10*

(d)

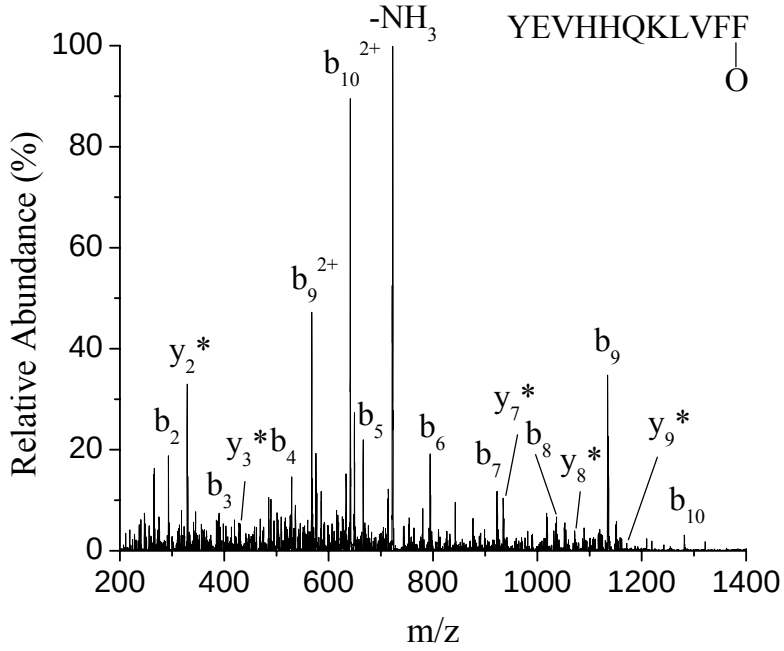

-NH3
YEVHHQKLVFF
O
Relative Abundance (%)
m/z
b10 2+
b9 2+
y2*
b9
y7*
b2
b5
b6
y3*b4
b8
y9*
b7
y8*
b3
b10

Figure S8. ETD of the triply-charged ion of oxidized β-amyloid peptide $(M+O+3H)^{3+}$ without prior LC separation. The asterisks indicate the product ions that are oxidized.