

Supplemental Materials

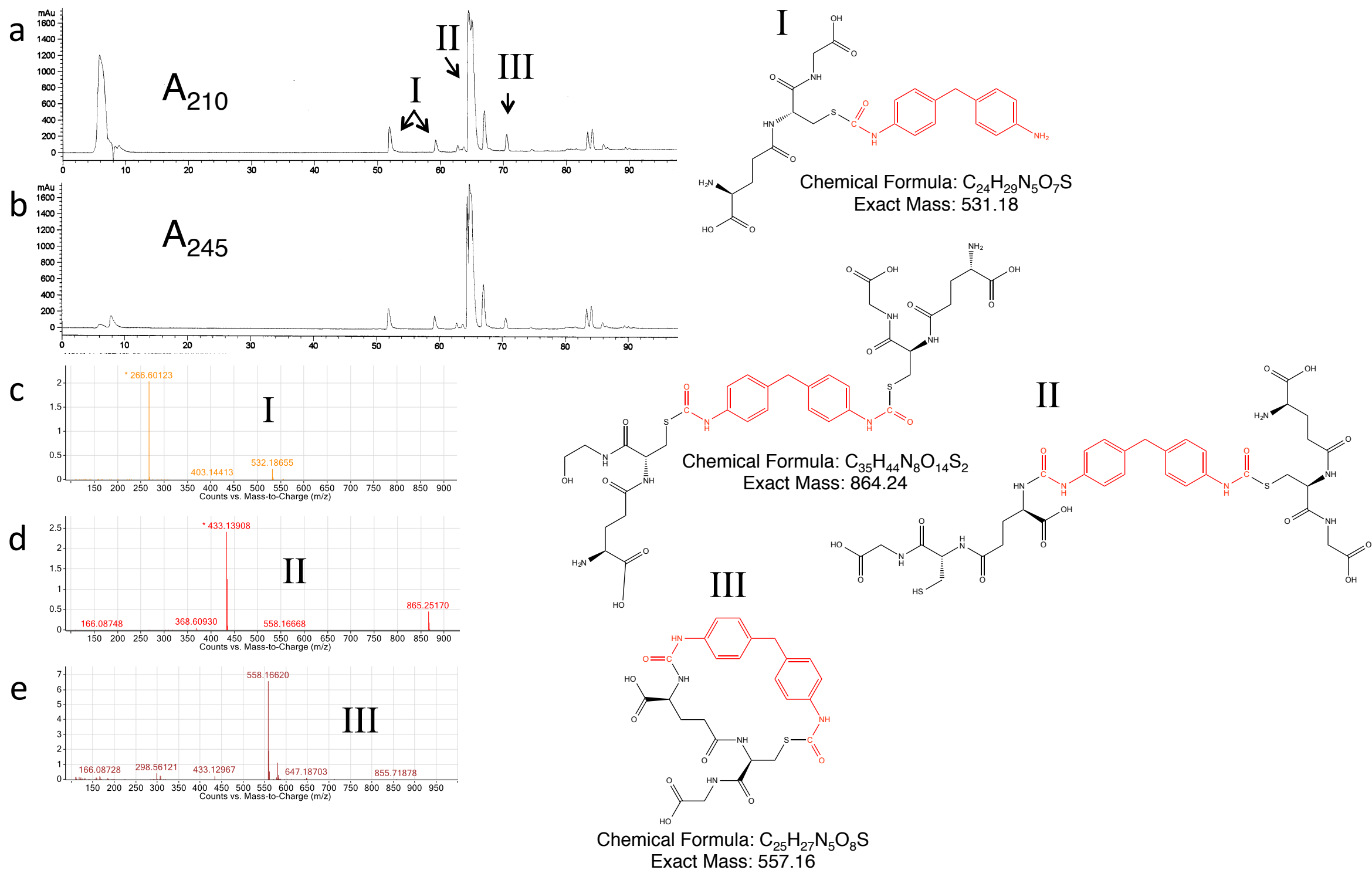
**Glutathione Reaction Products with the Chemical Allergen,
Methylene-Diphenyl Diisocyanate, Stimulate Alternative Macrophage
Activation and Eosinophilic Airway Inflammation**

*Adam V Wisnewski*¹, Jian Liu¹, Christopher M Colangelo²*

Departments of Internal Medicine¹ and Molecular Biophysics & Biochemistry²; Yale University

School of Medicine, New Haven, CT

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Supplemental Figure S1. Data characterizing the GSH-MDI reaction products generated in vitro. Panels a & b show A_{210} and A_{245} of different fractions of GSH-MDI reaction products separated by reverse phase HPLC as described. Panels c, d, and e show LC-MS data for different purified fractions (labeled I, II, III), which correspond to the structures shown on the right, as previously described,¹⁻³ or an asymmetric (*S,N'*-linked) bis(GSH)-MDI also shown, which could theoretically form via direct reactivity between GSH and MDI, or via inter- or intra-molecular rearrangement of (*S,S'*-linked) bis(GSH)-MDI.

Supplemental Figure S2. MS/MS data defining unique modification of murine albumin K⁴¹⁴. Data from iTRAQ experiments were queried for the expected 614 atomic mass unit modification due to GSH-MDI addition and carbamidomethylation (during sample workup). Raw data from the MASCOT search engine showing b- and y-ions confirming amino acid sequence, and modification on the K residue.

MATRIX SCIENCE Mascot Search Results

Peptide View

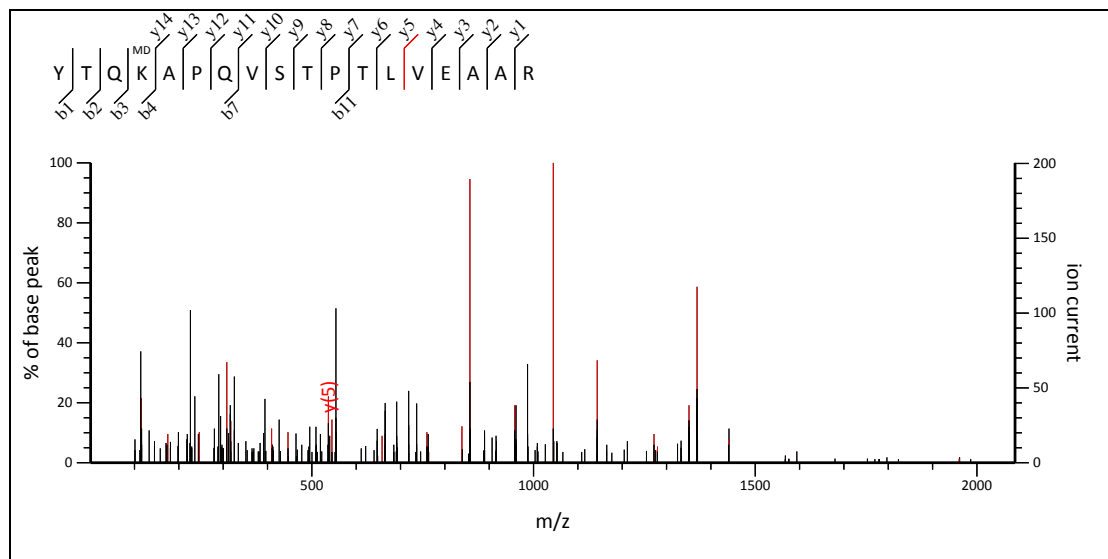
MS/MS Fragmentation of **YTQKAPQVSTPTLVEAAR**

Found in **ALBU_MOUSE** in **SwissProt**, Serum albumin OS=Mus musculus GN=Alb PE=1 SV=3

Match to Query 94630: 2717.352432 from(906.791420,3+) rtinseconds(5898) index(28730)

Title: Locus:1.1.1.9243.3 File:"5600TT14-1047.wiff"

Data file C:\Program Files (x86)\Matrix Science\Mascot Daemon\mgf\835 Copy of Wisnewski 4-PLEX MDI mod 10 fractions\mascot_daemon_merge.mgf



Label all possible matches Label matches used for scoring

Monoisotopic mass of neutral peptide Mr(calc): 2717.3241

Fixed modifications: Carbamidomethyl (C), iTRAQ4plex (N-term), iTRAQ4plex (K) (apply to specified residues or termini only)

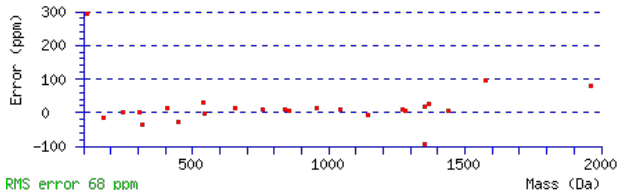
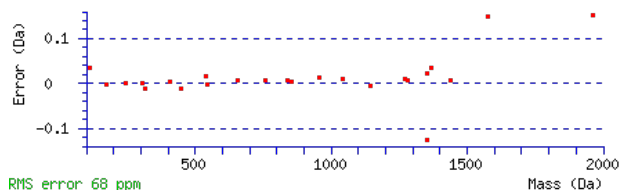
Variable modifications:

K4 : MDI_614_KNH (HKN)

Ions Score: 54 **Expect:** 8e-06

Matches : 24/192 fragment ions using 97 most intense peaks ([help](#))

#	b	b ⁺⁺	b [*]	b ⁺⁺⁺	b ⁰	b ⁰⁺⁺	Seq.	y	y ⁺⁺	y [*]	y ⁺⁺⁺	y ⁰	y ⁰⁺⁺	#
1	308.1727	154.5900					Y							18
2	409.2203	205.1138			391.2098	196.1085	T	2411.1660	1206.0866	2394.1394	1197.5734	2393.1554	1197.0813	17
3	537.2789	269.1431	520.2524	260.6298	519.2684	260.1378	Q	2310.1183	1155.5628	2293.0918	1147.0495	2292.1077	1146.5575	16
4	1279.5534	640.2803	1262.5268	631.7671	1261.5428	631.2750	K	2182.0597	1091.5335	2165.0332	1083.0202	2164.0492	1082.5282	15
5	1350.5905	675.7989	1333.5639	667.2856	1332.5799	666.7936	A	1439.7853	720.3963	1422.7587	711.8830	1421.7747	711.3910	14
6	1447.6433	724.3253	1430.6167	715.8120	1429.6327	715.3200	P	1368.7482	684.8777	1351.7216	676.3644	1350.7376	675.8724	13
7	1575.7018	788.3546	1558.6753	779.8413	1557.6913	779.3493	Q	1271.6954	636.3513	1254.6688	627.8381	1253.6848	627.3461	12
8	1674.7703	837.8888	1657.7437	829.3755	1656.7597	828.8835	V	1143.6368	572.3220	1126.6103	563.8088	1125.6263	563.3168	11
9	1761.8023	881.4048	1744.7757	872.8915	1743.7917	872.3995	S	1044.5684	522.7878	1027.5419	514.2746	1026.5578	513.7826	10
10	1862.8500	931.9286	1845.8234	923.4153	1844.8394	922.9233	T	957.5364	479.2718	940.5098	470.7586	939.5258	470.2665	9
11	1959.9027	980.4550	1942.8762	971.9417	1941.8922	971.4497	P	856.4887	428.7480	839.4621	420.2347	838.4781	419.7427	8
12	2060.9504	1030.9788	2043.9239	1022.4656	2042.9398	1021.9736	T	759.4359	380.2216	742.4094	371.7083	741.4254	371.2163	7
13	2174.0345	1087.5209	2157.0079	1079.0076	2156.0239	1078.5156	L	658.3883	329.6978	641.3617	321.1845	640.3777	320.6925	6
14	2273.1029	1137.0551	2256.0763	1128.5418	2255.0923	1128.0498	V	545.3042	273.1557	528.2776	264.6425	527.2936	264.1504	5
15	2402.1455	1201.5764	2385.1189	1193.0631	2384.1349	1192.5711	E	446.2358	223.6215	429.2092	215.1083	428.2252	214.6162	4
16	2473.1826	1237.0949	2456.1560	1228.5817	2455.1720	1228.0897	A	317.1932	159.1002	300.1666	150.5870			3
17	2544.2197	1272.6135	2527.1932	1264.1002	2526.2091	1263.6082	A	246.1561	123.5817	229.1295	115.0684			2
18							R	175.1190	88.0631	158.0924	79.5498			1



NCBI BLAST search of **YTQKAPQVSTPTLVEAAR**

(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)

Other BLAST [web gateways](#)

All matches to this query

Score	Mr(calc)	Delta	Sequence
54.4	2717.3241	0.0283	YTQKAPQVSTPTLVEAAR

Mascot: <http://www.matrixscience.com/>

Supplemental Table S1. Peptides from BAL Fluid Positively Matched to Mouse Albumin or Mouse Albumin + MDI-GSH. List of the ion masses that match peptides of mouse albumin, or MDI modified mouse albumin, from samples of airway fluid of GSH-MDI exposed mice. Data from the MASCOT search engine includes the MASCOT Score, Expectation, Deduced Peptide Sequence, Start/End position in the mature albumin protein, m/z, Measured Ion Mass, Calculated Ion Mass, the difference from the expected value, the relative difference in ppm, and the ion charge. The ion mass corresponding to the GSH-MDI modified murine albumin peptide of interest is highlighted.

Score	Expectation	Peptide Sequence	Start	End	M/Z	Ion Mass	Ion Mass(calc)	Delta	ppm	Charge
164.24	6.20E-14	K.AHCLSEVEHDTMPADLPAIAADFVEDQEVECK.N	287	317	947.2069	3784.7986	3784.7626	0.0359	9.5	4
131.96	1.10E-10	K.AHCLSEVEHDTMPADLPAIAADFVEDQEVECK.N	287	317	757.9645	3784.7862	3784.7626	0.0236	6.2	5
123.07	8.90E-10	K.AHCLSEVEHDTMPADLPAIAADFVEDQEVECK.N + Oxidation (M)	287	317	951.2038	3800.7863	3800.7576	0.0287	7.6	4
122.94	2.50E-10	K.TVMDDFAQFLDTCKK.A + Oxidation (M)	546	560	1077.996	2153.9774	2153.9676	0.0099	4.6	2
122.46	2.70E-10	K.TVMDDFAQFLDTCKK.A	546	560	1070.0015	2137.9885	2137.9727	0.0158	7.4	2
120.78	1.60E-10	R.LSQTFFPNADFAEITK.L	219	233	985.5344	1969.0542	1969.04	0.0142	7.2	2
119.53	5.50E-10	K.TVMDDFAQFLDTCKK.A + Oxidation (M)	546	560	718.998	2153.9722	2153.9676	0.0047	2.2	3
112.97	2.30E-09	K.ENPTTFMGHLYHEVAR.R + Oxidation (M)	129	144	516.2534	2060.9844	2060.986	-0.0016	-0.8	4
111.21	1.20E-08	R.RHPYFYAPPELLYAAEQYNEILTQCCAEADK.E	145	174	1011.7459	4042.9547	4042.9113	0.0434	10.7	4
110.85	1.30E-08	R.RHPYFYAPPELLYAAEQYNEILTQCCAEADK.E	145	174	809.5971	4042.9492	4042.9113	0.0379	9.4	5
110.8	1.40E-08	R.HPYFYAPPELLYAAEQYNEILTQCCAEADK.E	146	174	972.7193	3886.8483	3886.8102	0.0381	9.8	4
109.86	1.10E-08	K.CCAEANPPACYGTVLAEFQPLVEEPK.N	360	385	1080.1943	3237.561	3237.5388	0.0222	6.9	3
108.57	6.50E-09	K.TVMDDFAQFLDTCKK.A + Oxidation (M)	546	560	539.4965	2153.9571	2153.9676	-0.0105	-4.9	4
108.22	3.70E-10	K.GLVLIASFQYLQK.A	21	33	590.0268	1767.0585	1767.0538	0.0047	2.7	3
108.16	2.60E-08	R.HPYFYAPPELLYAAEQYNEILTQCCAEADK.E	146	174	778.3763	3886.8453	3886.8102	0.0351	9	5
105.42	1.40E-08	K.TVMDDFAQFLDTCKK.A	546	560	535.4996	2137.9693	2137.9727	-0.0034	-1.6	4
104.25	5.00E-09	K.LGEYGFQNAIVLR.Y	398	410	541.9699	1622.8878	1622.8902	-0.0025	-1.5	3
100.37	1.80E-08	R.LSQTFFPNADFAEITK.L	219	233	657.3571	1969.0494	1969.04	0.0094	4.8	3
96.83	5.30E-08	K.DVFLGTFLYEYSR.R	324	336	585.3025	1752.8856	1752.8845	0.0011	0.6	3
96.44	5.50E-08	K.TCVADESAANCDK.S	52	64	576.9322	1727.7748	1727.7698	0.005	2.9	3
95.96	5.00E-08	R.LPCVEDYLSAILNR.V	446	459	602.9908	1805.9506	1805.9467	0.0038	2.1	3
93.48	5.00E-08	K.APQVSTPTLVEAAR.N	415	428	528.6339	1582.8799	1582.8801	-0.0002	-0.1	3
92.07	6.90E-08	K.ECCHGDLLCADDR.A	244	257	631.9308	1892.7707	1892.7573	0.0133	7	3
90.99	2.30E-07	K.DTCFSTEGPNLVTR.C	565	578	580.951	1739.8313	1739.8271	0.0042	2.4	3
89.73	1.00E-07	K.LVQEVTFDAK.T	42	51	479.9442	1436.8108	1436.8119	-0.0011	-0.8	3
88.41	6.20E-07	K.ENPTTFMGHLYHEVAR.R	129	144	512.2547	2044.9897	2044.9911	-0.0014	-0.7	4
87.89	7.20E-07	K.AETTFHSDICTLPEK.E	504	519	546.7771	2183.0794	2183.0813	-0.0019	-0.9	4
87.88	2.60E-07	R.LPCVEDYLSAILNR.V + iTRAQ4plex (Y)	446	459	651.0242	1950.0508	1950.0488	0.002	1	3
87.87	1.80E-07	R.HPDYSVSLLLR.L	338	348	481.9402	1442.7989	1442.8003	-0.0014	-1	3
87.55	3.40E-07	R.LPCVEDYLSAILNR.V	446	459	903.9837	1805.9528	1805.9467	0.0061	3.4	2
86.94	0.0000034	K.AHCLSEVEHDTMPADLPAIAADFVEDQEVECK.N	287	317	631.8064	3784.7949	3784.7626	0.0322	8.5	6
84.52	0.0000038	K.CCAEANPPACYGTVLAEFQPLVEEPK.N	360	385	810.3964	3237.5565	3237.5388	0.0176	5.4	4
84.46	3.30E-07	R.RHPDYSVSLLLR.L	337	348	533.975	1598.9031	1598.9014	0.0016	1	3
82.94	0.0000022	K.ENPTTFMGHLYHEVAR.R	129	144	682.6732	2044.9977	2044.9911	0.0066	3.2	3
82.52	5.20E-07	K.APQVSTPTLVEAAR.N	415	428	792.4525	1582.8904	1582.8801	0.0104	6.6	2
81.26	0.0000014	R.YNDLGEQHF.K.G	11	20	513.5988	1537.7746	1537.7769	-0.0023	-1.5	3
80.91	0.0000023	K.DTCFSTEGPNLVTR.C	565	578	870.9261	1739.8377	1739.8271	0.0107	6.1	2
79.86	0.0000024	R.ENYGELADCTK.Q	82	93	583.2672	1746.7797	1746.7796	0.0001	0.1	3
79.44	0.000016	R.RHPYFYAPPELLYAAEQYNEILTQCCAEADK.E + iTRAQ4plex (Y)	145	174	838.4158	4187.0425	4187.0134	0.0292	7	5
78.56	0.0000017	K.ECCHGDLLCADDR.A	244	257	947.3946	1892.7747	1892.7573	0.0174	9.2	2
77.96	0.0000014	K.LVQEVTFDAK.T	42	51	719.4154	1436.8162	1436.8119	0.0043	3	2
76.97	0.0000089	K.AETTFHSDICTLPEK.E	504	519	728.7003	2183.0791	2183.0813	-0.0022	-1	3
76.24	0.000043	R.RHPYFYAPPELLYAAEQYNEILTQCCAEADK.E	145	174	674.8287	4042.9285	4042.9113	0.0172	4.3	6
75.54	9.10E-07	K.QTALAELVK.H	526	534	420.929	1259.7652	1259.7693	-0.004	-3.2	3
74.54	0.000016	K.AADKDTCFSTEGPNLVTR.C	561	578	757.3831	2269.1275	2269.1252	0.0023	1	3
73.98	0.000011	K.YMCENQATISSK.L + Oxidation (M)	263	274	579.2796	1734.8169	1734.816	0.0009	0.5	3
73.52	0.000012	K.YMCENQATISSK.L	263	274	573.9484	1718.8233	1718.8211	0.0022	1.3	3
70.94	0.00001	K.LGEYGFQNAIVLR.Y	398	410	812.4528	1622.891	1622.8902	0.0008	0.5	2
70.25	0.0000015	K.GLVLIASFQYLQK.C + iTRAQ4plex (Y)	21	33	478.7948	1911.1501	1911.1559	-0.0058	-3	4
70.16	0.000026	R.RPCFSALTVDETVVPK.E	485	500	724.3834	2170.1283	2170.1336	-0.0053	-2.4	3
69.32	0.000011	R.RHPDYSVSLLLR.L	337	348	400.7323	1598.9	1598.9014	-0.0014	-0.9	4
68.86	0.0000042	K.QTALAELVK.H	526	534	630.8913	1259.7681	1259.7693	-0.0011	-0.9	2
67.5	0.000074	K.ENPTTFMGHLYHEVAR.R + iTRAQ4plex (Y)	129	144	438.8252	2189.0899	2189.0931	-0.0033	-1.5	5
66.71	0.00002	R.YTQKAPQVSTPTLVEAAR.N	411	428	750.0915	2247.2528	2247.2467	0.0062	2.8	3
65.78	0.000023	K.SLHTLFGDK.L	65	73	435.9182	1304.7326	1304.7332	-0.0006	-0.5	3
65.67	0.0000048	K.GLVLIASFQYLQK.C + iTRAQ4plex (Y)	21	33	638.0565	1911.1476	1911.1559	-0.0083	-4.3	3
64.93	0.000074	R.LSQTFFPNADFAEITK.L	219	233	493.2666	1969.0371	1969.04	-0.0029	-1.5	4
64.69	0.000084	K.DVFLGTFLYEYSR.R	324	336	877.4534	1752.8922	1752.8845	0.0078	4.4	2
64.26	0.000003	K.QTALAELVK.H	525	534	511.6644	1531.9712	1531.9663	0.0049	3.2	3
63.45	0.000098	R.ENYGELADCTK.Q	82	93	437.7003	1746.7719	1746.7796	-0.0077	-4.4	4
62.75	0.000064	K.TNCDLYEK.L	390	397	665.8298	1329.645	1329.6478	-0.0029	-2.2	2
60.53	0.000091	R.YTQKAPQVSTPTLVEAAR.N	411	428	562.819	2247.2471	2247.2467	0.0004	0.2	4
59.88	0.000099	K.TPVEHVTK.C	467	475	429.2495	1284.7266	1284.7281	-0.0016	-1.2	3
57.89	0.00018	K.LGEYGFQNAIVLR.Y + iTRAQ4plex (Y)	398	410	442.7531	1766.9833	1766.9923	-0.009	-5.1	4
57.81	0.000055	K.CCSGSLVER.R	476	484	606.2842	1210.5538	1210.5556	-0.0018	-1.5	2
57.59	0.00016	K.TPVEHVTK.C	467	475	643.373	1284.7314	1284.7281	0.0033	2.6	2

57.14	0.00044	K.DVFLGTFLYEYSR.R + iTRAQ4plex (Y)	324	336	633.3375	1896.9907	1896.9865	0.0042	2.2	3
56.71	0.0002	K.LGEYGFQNAILVR.Y + iTRAQ4plex (Y)	398	410	590.0044	1766.9914	1766.9923	-0.0008	-0.5	3
55.4	0.0028	K.DDNPSLPPFERPEAEAMCTSFK.E + Oxidation (M)	107	128	711.3392	2841.3278	2841.3193	0.0085	3	4
54.35	0.0022	R.YTQKAPQVSTPTLVEAAR.N + MDI_614_KNH (HKN)	411	428	906.7914	2717.3524	2717.3481	0.0043	1.5	3
54.07	0.00012	K.LATDLTK.V	234	240	525.3246	1048.6347	1048.6372	-0.0025	-2.4	2
53.92	0.00032	K.ECCHGDLLECADDR.A	244	257	474.1965	1892.7571	1892.7573	-0.0003	-0.2	4
53.35	0.0043	K.DDNPSLPPFERPEAEAMCTSFK.E	107	128	707.3398	2825.3301	2825.3244	0.0057	2	4
53.24	0.0005	K.LGEYGFQNAILVRYTQK.A	398	414	572.8237	2287.2658	2287.2568	0.009	3.9	4
52.51	0.00025	K.ATAEQLK.T	539	545	524.8152	1047.6157	1047.6168	-0.001	-1	2
51.82	0.0051	K.ECCHGDLLECADDR.AELAK.Y	244	262	638.2968	2549.158	2549.1552	0.0028	1.1	4
51.75	0.0031	K.DTCFSTEGPNLVTRCK.D	565	580	544.0215	2172.0569	2172.0547	0.0022	1	4
50.82	0.00078	K.YEATLEK.C	353	359	571.3211	1140.6277	1140.627	0.0007	0.6	2
50.03	0.00068	R.VCLLHEK.T	460	466	593.845	1185.6753	1185.6783	-0.003	-2.5	2
50.03	0.014	R.RHPYFYAPPELLYAEQYNEILTQCCAEADK.E + iTRAQ4plex (Y)	145	174	698.8474	4187.0407	4187.0134	0.0273	6.5	6
49.57	0.0006	K.CCTLPEDQR.L	437	445	661.8012	1321.5878	1321.5877	0.0001	0.1	2
49.51	0.01	K.DDNPSLPPFERPEAEAMCTSFK.E	107	128	942.7874	2825.3404	2825.3244	0.016	5.7	3
49.18	0.0017	R.NECFLQHK.D	99	106	455.2388	1362.6946	1362.6958	-0.0012	-0.9	3
49.1	0.00027	K.ALVSVR.Q	189	195	438.2742	874.5339	874.5358	-0.0019	-2.2	2
49.1	0.0035	K.DTCFSTEGPNLVTR.C	565	578	435.9644	1739.8287	1739.8271	0.0016	0.9	4
48.75	0.0018	R.NECFLQHK.D	99	106	682.3575	1362.7004	1362.6958	0.0046	3.4	2
48.51	0.0056	K.ENPTTFMGHYLHEVAR.R + iTRAQ4plex (Y)	129	144	730.7072	2189.0998	2189.0931	0.0066	3	3
47.2	0.0039	R.RPCFSALTVDETYVPK.E + iTRAQ4plex (Y)	485	500	579.5665	2314.237	2314.2357	0.0013	0.6	4
45.82	0.0019	K.NYAEAK.D	318	323	492.273	982.5314	982.5327	-0.0013	-1.3	2
44.82	0.0062	R.RPCFSALTVDETYVPK.E + iTRAQ4plex (Y)	485	500	463.8556	2314.2415	2314.2357	0.0058	2.5	5
43.98	0.015	R.LSQTFPNADF AIEITK.L + MDI_224_KNH (HKN)	219	233	684.0144	2049.0213	2049.0329	-0.0116	-5.7	3
43.29	0.017	R.ENYGELADCCTK.Q + iTRAQ4plex (Y)	82	93	473.7279	1890.8825	1890.8817	0.0008	0.4	4
43.25	0.016	R.ENYGELADCCTK.Q + iTRAQ4plex (Y)	82	93	631.3046	1890.8921	1890.8817	0.0103	5.4	3
42.27	0.046	K.LCAIPNLRENYGELADCCTK.Q	74	93	672.0804	2684.2925	2684.2964	-0.0039	-1.5	4
40.73	0.0048	K.CSYDEHAK.L	34	41	433.2058	1296.5957	1296.6012	-0.0055	-4.2	3
40.47	0.0012	K.SEIAHR.Y	5	10	428.7398	855.4649	855.4684	-0.0035	-4.1	2
39.37	0.0094	K.ESCLTPK.L	175	181	561.8084	1121.6023	1121.5994	0.0029	2.6	2
38.4	0.031	K.DVFLGTFLYEYSR.R + iTRAQ4plex (Y)	324	336	475.2572	1896.9997	1896.9865	0.0132	7	4
36.71	0.04	K.TNCDLYEK.L + iTRAQ4plex (Y)	390	397	492.2542	1473.7408	1473.7499	-0.0091	-6.2	3
36.31	0.016	R.RHPDYSVSLLLR.L + iTRAQ4plex (Y)	337	348	436.7577	1743.0016	1743.0035	-0.0019	-1.1	4
35.01	0.021	K.LCAIPNL.R.E	74	81	550.8215	1099.6284	1099.6294	-0.001	-0.9	2
34.99	0.019	K.KYEATLEK.C	352	359	471.9488	1412.8244	1412.824	0.0004	0.3	3
34.04	0.0066	R.AELAK.Y	258	262	410.262	818.5094	818.5105	-0.0011	-1.3	2
31.32	0.015	K.AWAVAR.L	213	218	409.2423	816.4701	816.4728	-0.0027	-3.3	2
29.81	0.016	K.LDGVK.E	182	186	410.2625	818.5104	818.5105	-0.0001	-0.1	2

Supplemental Table S2. Identification of GSH-MDI modified albumin peptide in samples from GSH-MDI exposed mice (114, 115) not control mice exposed to MDI-m (116, 117). Differences in amount of different ions with masses that match peptides of mouse albumin, or MDI modified mouse albumin from GSH-MDI exposed mice (e.g. 114 and 115) vs. controls (116 and 117). Shown are the Score, Expectation, Sequence and Charge data (same as Table S1), paired with quantitation of the respective amounts of ion with 114, 115, 116, or 117 labels, and their relative ratios as labeled. The ion mass corresponding to the GSH-MDI modified murine albumin peptide of interested is highlighted.

Score	Expectation	Peptide Sequence	Charge	115/114	116/114	117/114	114	115	116	117
164.24	6.20E-14	K.AHCLSEVEHDTMPADLPAIAADFVEDQEVCK.N	4	1.13	1.092	0.988	1000.544	1524.748	1258.692	864.539
131.96	1.10E-10	K.AHCLSEVEHDTMPADLPAIAADFVEDQEVCK.N	5	1.059	1.023	0.956	336.277	479.944	396.33	281.045
123.07	8.90E-10	K.AHCLSEVEHDTMPADLPAIAADFVEDQEVCK.N + Oxidation (M)	4	0.874	0.701	1.06	186.863	220.235	150.83	173.152
122.94	2.50E-10	K.TVMDDFAQFLDTCKC.A + Oxidation (M)	2	1.082	0.682	0.727	137.761	201.017	108.186	87.587
122.46	2.70E-10	K.TVMDDFAQFLDTCKC.A	2	1.35	1.259	0.818	122.228	222.517	177.269	87.446
120.78	1.60E-10	R.LSQTFPNADFAEITK.L	2	1.311	1.372	1.335	1649.839	2914.993	2606.508	1926.182
119.53	5.50E-10	K.TVMDDFAQFLDTCKC.A + Oxidation (M)	3	1.038	0.987	0.898	6087.801	8521.661	6918.267	4778.308
112.97	2.30E-09	K.ENPTTFMGHYLHEVAR.R + Oxidation (M)	4	1.09	1.136	1.095	56.345	82.785	73.693	53.973
111.21	1.20E-08	R.RHPYFYAPPELLYAEQYNEILTQCCAEADK.E	4	0.827	1.051	0.886	506.678	564.806	613.258	392.682
110.85	1.30E-08	R.RHPYFYAPPELLYAEQYNEILTQCCAEADK.E	5	0.758	1.027	0.792	571.914	584.572	676.707	396.065
110.8	1.40E-08	R.RHPYFYAPPELLYAEQYNEILTQCCAEADK.E	4	0.905	0.864	0.91	324.103	395.393	322.391	258.005
109.86	1.10E-08	K.CCAEANPPACYGTVLAEFQPLVEEPK.N	3	1.234	0.487	0.368	86.254	143.481	48.356	27.793
108.57	6.50E-09	K.TVMDDFAQFLDTCKC.A + Oxidation (M)	4	1.065	0.9	0.81	380.075	545.494	393.858	269.189
108.22	3.70E-10	K.GLVLIAFSQYLQK.C	3	0.994	1.442	0.813	143.335	192.094	237.968	101.839
108.16	2.60E-08	R.HPYFYAPPELLYAEQYNEILTQCCAEADK.E	5	0.867	0.877	0.752	281.399	329.021	284.215	184.936
105.42	1.40E-08	K.TVMDDFAQFLDTCKC.A	4	0.928	0.836	0.764	459.105	574.581	442.242	306.845
104.25	5.00E-09	K.LGEYGFQNALV.R.Y	3	0.82	0.759	0.584	316.474	349.802	276.644	161.473
100.37	1.80E-08	R.LSQTFPNADFAEITK.L	3	1.061	0.901	1.02	4902.894	7010.584	5086.214	4373.495
96.83	5.30E-08	K.DVFLGTFLYEYSR.R	3	1.168	1.359	0.992	276.943	435.991	433.352	240.328
96.44	5.50E-08	K.TCVADESAANCDK.S	3	1.364	1.115	1.036	735.166	1351.518	943.954	665.769
95.96	5.00E-08	R.LPCVEDYLSAILNR.V	3	1.283	1.128	0.942	189.913	328.533	246.758	156.458
93.48	5.00E-08	K.APQVSTPTLVEAAR.N	3	0.906	0.417	0.869	80.762	98.602	38.812	61.358
92.07	6.90E-08	K.ECCHGDLLCADDR.A	3	0.932	0.978	0.785	284.027	356.932	319.958	195.07
90.99	2.30E-07	K.DTCFSTEGPNLVTR.C	3	0.732	1.373	0.864	290.917	286.913	459.846	219.827
89.73	1.00E-07	K.LVQEVTFDAK.T	3	0.935	1.13	1.107	97.464	122.808	126.79	94.342
88.41	6.20E-07	K.ENPTTFMGHYLHEVAR.R	4	0.841	0.927	0.669	1333.428	1512.284	1423.651	779.787
87.89	7.20E-07	K.AETTFHSDICTLPEK.E	4	0.91	0.886	0.958	885.134	1085.517	903.437	741.623
87.88	2.60E-07	R.LPCVEDYLSAILNR.V + iTRAQ4plex (Y)	3	---	---	---	---	---	---	---
87.87	1.80E-07	R.HPDYSVSLLR.L	3	1.05	1.106	1.145	986.101	1395.621	1255.832	987.113
87.55	3.40E-07	R.LPCVEDYLSAILNR.V	2	1.202	0.981	0.97	1814.009	2939.292	2048.939	1538.808
86.94	0.0000034	K.AHCLSEVEHDTMPADLPAIAADFVEDQEVCK.N	6	1.956	1.335	0.75	41.334	109.022	63.559	27.09
85.1	0.0000056	K.AHCLSEVEHDTMPADLPAIAADFVEDQEVCK.N + Oxidation (M)	5	0.96	0.687	1.102	216.783	280.449	171.544	208.875
84.52	0.0000038	K.CCAEANPPACYGTVLAEFQPLVEEPK.N	4	1.178	1.086	0.706	883.677	1403.222	1104.804	545.325
84.46	3.30E-07	R.RHPDYSVSLLR.L	3	2.535	2.173	1.037	695.841	2378.196	1741.32	631.236
82.94	0.0000022	K.ENPTTFMGHYLHEVAR.R	3	1.037	0.559	0.873	99.274	138.734	63.856	75.744
82.52	5.20E-07	K.APQVSTPTLVEAAR.N	2	1.068	1.062	0.957	4519.768	6506.785	5526.288	3782.262
81.26	0.0000014	R.YNDLGEQHF.K.G	3	1.24	1.266	1.271	463.412	774.519	675.434	514.969
80.91	0.0000023	K.DTCFSTEGPNLVTR.C	2	1.028	0.916	1.032	3834.933	5317.357	4045.273	3460.655
79.86	0.0000024	R.ENYGELADCCTK.Q	3	1.056	0.9	1.223	1129.025	1606.791	1170.413	1207.494
79.44	0.000016	R.RHPYFYAPPELLYAEQYNEILTQCCAEADK.E + iTRAQ4plex (Y)	5	---	---	---	---	---	---	---
78.56	0.0000017	K.ECCHGDLLCADDR.A	2	0.96	1.088	0.968	667.094	863.502	835.5	564.436
77.96	0.0000014	K.LVQEVTFDAK.T	2	1.112	1.082	1.245	4971.943	7453.262	6196.095	5412.037
76.97	0.0000089	K.AETTFHSDICTLPEK.E	3	0.884	0.899	0.869	1425.2	1699.445	1474.729	1083.266
76.24	0.000043	R.RHPYFYAPPELLYAEQYNEILTQCCAEADK.E	6	0.823	0.75	0.716	126.157	139.986	109.035	78.997
75.54	9.10E-07	K.QTALAELVK.H	3	1.338	1.146	1.124	3048.488	5497.75	4024.009	2996.128
74.54	0.000016	K.AADKDTCFSTEGPNLVTR.C	3	0.222	0.432	0.108	154.012	46.154	76.609	14.498
73.98	0.000011	K.YMCENQATISSK.L + Oxidation (M)	3	1.257	1.348	0.76	35.31	59.858	54.804	23.454
73.52	0.000012	K.YMCENQATISSK.L	3	0.969	0.884	0.67	2631.077	3436.489	2678.19	1541.174
70.94	0.00001	K.LGEYGFQNALV.R.Y	2	0.93	0.868	0.634	2479.885	3109.351	2479.402	1373.72
70.25	0.0000015	K.GLVLIAFSQYLQK.C + iTRAQ4plex (Y)	4	---	---	---	---	---	---	---
70.16	0.000026	R.RPCFSALTVEDETVVPK.E	3	1.379	1.283	1.239	222.527	413.616	328.731	241.118
69.32	0.000011	R.RHPDYSVSLLR.L	4	1.47	1.43	1.185	589.484	1168.459	970.723	610.984
68.86	0.0000042	K.QTALAELVK.H	2	1.042	0.971	0.911	1496.185	2102.222	1672.721	1192.235
67.5	0.000074	K.ENPTTFMGHYLHEVAR.R + iTRAQ4plex (Y)	5	---	---	---	---	---	---	---
66.71	0.00002	R.YTQKAPQVSTPTLVEAAR.N	3	0.237	0.329	0.368	117.598	37.582	44.531	37.834
65.78	0.000023	K.SLHTLFGDK.L	3	0.98	1.049	1.081	302.483	399.683	365.343	285.887
65.67	0.0000048	K.GLVLIAFSQYLQK.C + iTRAQ4plex (Y)	3	---	---	---	---	---	---	---
64.93	0.000074	R.LSQTFPNADFAEITK.L	4	0.941	0.74	0.925	311.199	394.828	265.363	251.801
64.69	0.000084	K.DVFLGTFLYEYSR.R	2	1.103	1.039	1.112	416.174	618.738	498.192	404.721
64.26	0.000003	K.KQTALAELVK.H	3	0.857	0.485	0.308	1288.727	1488.647	719.862	347.638
63.45	0.000098	R.ENYGELADCCTK.Q	4	0.994	0.784	0.949	527.307	706.576	476.061	437.414
62.75	0.000064	K.TNCDLYEK.L	2	1.567	0.61	0.713	22.651	47.857	15.92	14.119
60.53	0.000091	R.YTQKAPQVSTPTLVEAAR.N	4	0.778	0.576	0.544	112.634	118.158	74.691	53.594
59.88	0.000099	K.TPVSEHVTK.C	3	1.419	1.264	1.183	107.52	205.688	156.492	111.204
57.89	0.00018	K.LGEYGFQNALV.R.Y + iTRAQ4plex (Y)	4	---	---	---	---	---	---	---
57.81	0.000055	K.CCSGSLVER.R	2	1.424	1.418	1.37	18.607	35.719	30.38	22.291
57.59	0.00016	K.TPVSEHVTK.C	2	1.28	1.273	1.14	156.716	270.536	229.747	156.267
57.14	0.00044	K.DVFLGTFLYEYSR.R + iTRAQ4plex (Y)	3	---	---	---	---	---	---	---
56.71	0.0002	K.LGEYGFQNALV.R.Y + iTRAQ4plex (Y)	3	---	---	---	---	---	---	---
55.4	0.0028	K.DDNPSLPPFERPEAEAMCTSFK.E + Oxidation (M)	4	0.956	0.847	0.72	6861.314	8841.969	6690.812	4320.424
54.35	0.0022	R.YTQKAPQVSTPTLVEAAR.N + MDI_614_KNH (HKN)	3	0.612	0.098	-0.007	65.574	54.072	7.422	-0.42
54.07	0.00012	K.LATDLTK.V	2	2.29	1.592	1.956	136.262	420.62	249.839	233.048
53.92	0.00032	K.ECCHGDLLCADDR.A	4	1.403	1.547	1.283	40.338	76.293	71.879	45.27
53.35	0.0043	K.DDNPSLPPFERPEAEAMCTSFK.E	4	1.04	0.91	0.822	2226.642	3122.468	2332.973	1600.534

53.24	0.0005	K.LGEYGFQNAILVRYTQK.A	4	0.423	0.246	0.255	157.378	89.802	44.645	35.109
52.51	0.00025	K.ATAEQLK.T	2	1.062	0.97	1.125	3307.143	4733.199	3696.103	3253.184
51.82	0.0051	K.ECCHGDLLCADDRALAK.Y	4	2.71	1.672	0.516	82.829	302.59	159.518	37.358
51.75	0.0031	K.DTCFSTEGPNLVTRCK.D	4	1.06	0.62	0.688	67.88	96.966	48.486	40.824
50.82	0.00078	K.YEATLEK.C	2	1.091	0.736	0.666	4098.41	6028.849	3472.669	2386.04
50.03	0.014	R.RHPYFYAPELlyYAEQYNEILTQCCAEADK.E + iTRAQ4plex (Y)	6	---	---	---	---	---	---	---
50.03	0.00068	R.VCLLHEK.T	2	0.808	0.844	0.876	146.195	159.262	142.111	111.954
49.57	0.0006	K.CCTLPEDQR.L	2	1	1.286	0.735	40.797	54.989	60.399	26.22
49.51	0.01	K.DDNPSLPPFERPEAEAMCTSFK.E	3	0.67	1.548	1.033	31.677	28.611	56.483	28.604
49.18	0.0017	R.NECFLQHK.D	3	0.947	1.031	0.664	929.045	1185.869	1102.995	539.155
49.1	0.0035	K.DTCFSTEGPNLVTR.C	4	0.733	1.443	0.99	13.702	13.539	22.767	11.864
49.1	0.00027	K.ALVSVR.Q	2	1.286	1.302	1.177	6363.091	11034.403	9542.412	6551.469
48.75	0.0018	R.NECFLQHK.D	2	0.879	1.308	0.992	60.879	72.161	91.693	52.816
48.51	0.0056	K.ENPTTFMGHYLHEVAR.R + iTRAQ4plex (Y)	3	---	---	---	---	---	---	---
47.2	0.0039	R.RPCFSALTVDETYVPK.E + iTRAQ4plex (Y)	4	---	---	---	---	---	---	---
45.82	0.0019	K.NYAEAK.D	2	1.299	1.295	1.493	1689.788	2959.362	2520.208	2205.597
44.82	0.0062	R.RPCFSALTVDETYVPK.E + iTRAQ4plex (Y)	5	---	---	---	---	---	---	---
43.98	0.015	R.LSQTFPNADFAEITK.L + MDI_224_KNH (HKN)	3	0.685	1.034	0.871	42.218	38.97	50.268	32.142
43.29	0.017	R.ENYGELADCCTK.Q + iTRAQ4plex (Y)	4	---	---	---	---	---	---	---
43.25	0.016	R.ENYGELADCCTK.Q + iTRAQ4plex (Y)	3	---	---	---	---	---	---	---
42.27	0.046	K.LCAIPNLRENYGELADCCTK.Q	4	17.455	-0.922	0.7	22.163	521.543	-23.527	13.568
42.14	0.059	K.DDNPSLPPFERPEAEAMCTSFK.E + Oxidation (M)	3	0.939	0.854	0.745	1636.777	2071.693	1609.36	1066.566
40.73	0.0048	K.CSYDEHAK.L	3	1.215	0.797	0.574	76.943	126.006	70.611	38.633
40.47	0.0012	K.SEIAHR.Y	2	0.507	1.001	0.518	27.581	18.858	31.806	12.5
39.37	0.0094	K.ESCLTPK.L	2	2.736	1.487	1.243	26.736	98.613	45.792	29.048
38.4	0.031	K.DVFLGTFlyEYSR.R + iTRAQ4plex (Y)	4	---	---	---	---	---	---	---
36.71	0.04	K.TNCDLYEK.L + iTRAQ4plex (Y)	3	---	---	---	---	---	---	---
36.31	0.016	R.RHPDYSVSLLLR.L + iTRAQ4plex (Y)	4	---	---	---	---	---	---	---
35.01	0.021	K.LCAIPNLR.E	2	1.147	1.11	1.042	791.722	1224.496	1011.908	721.039
34.99	0.019	K.KYEATLEK.C	3	1.193	1.28	0.709	143.577	230.867	211.671	89.009
34.04	0.0066	R.AELAK.Y	2	1.081	0.937	1.112	2237.619	3262.597	2414.247	2176.381
31.32	0.015	K.AWAVAR.L	2	0.962	1.015	0.887	1825.25	2367.133	2134.352	1416.22
29.81	0.016	K.LDGVK.E	2	1.433	1.026	0.872	365.843	706.57	432.401	279.043

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