Supplemental Materials for:

Reaction Products of Hexamethylene Diisocyanate Vapors with "Self" Molecules in the Airways of Rabbits Exposed Via Tracheostomy

Adam V. Wisnewski, Jean Kanyo, Jennifer Asher, James A. Goodrich, Grace Barnett, Lyn Patrylak, Jian Liu, Carrie A. Redlich and Ala F. Nassar

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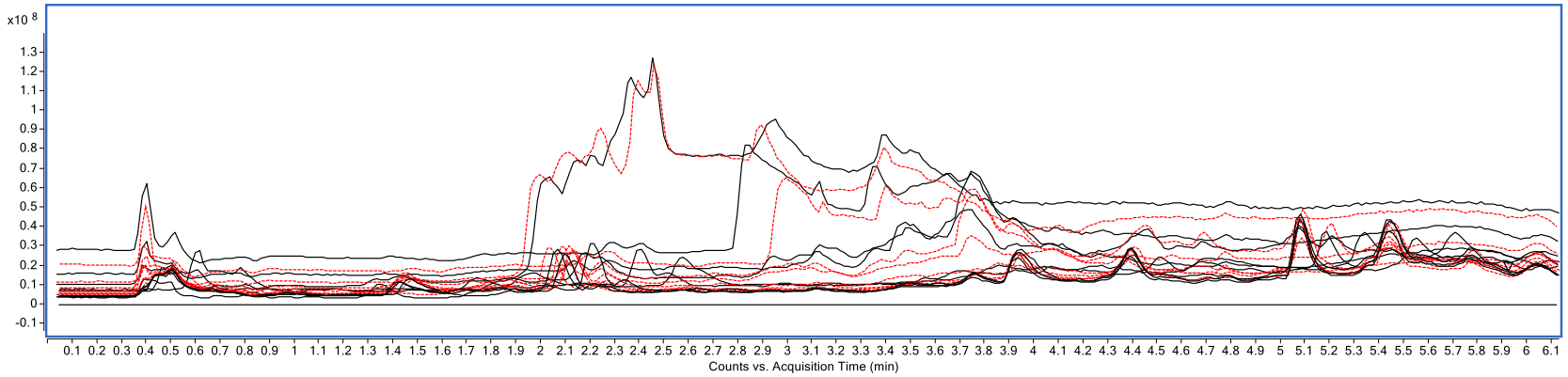


Figure S1. Qualitative similarity of airway lavage fluid from HDI vapor exposed and control rabbit. Total ion current (TIC) from LC-MS analysis of different fractions (N=9 each) of concentrated airway lavage fluid from HDI vapor exposed (black solid lines) and control (O_2) exposed rabbits (red dashed lines). Airway lavage was concentrated by solid phase absorption (C18 column) and eluted in N=3 fractions each at 20%, 60% and 100% acetonitrile.

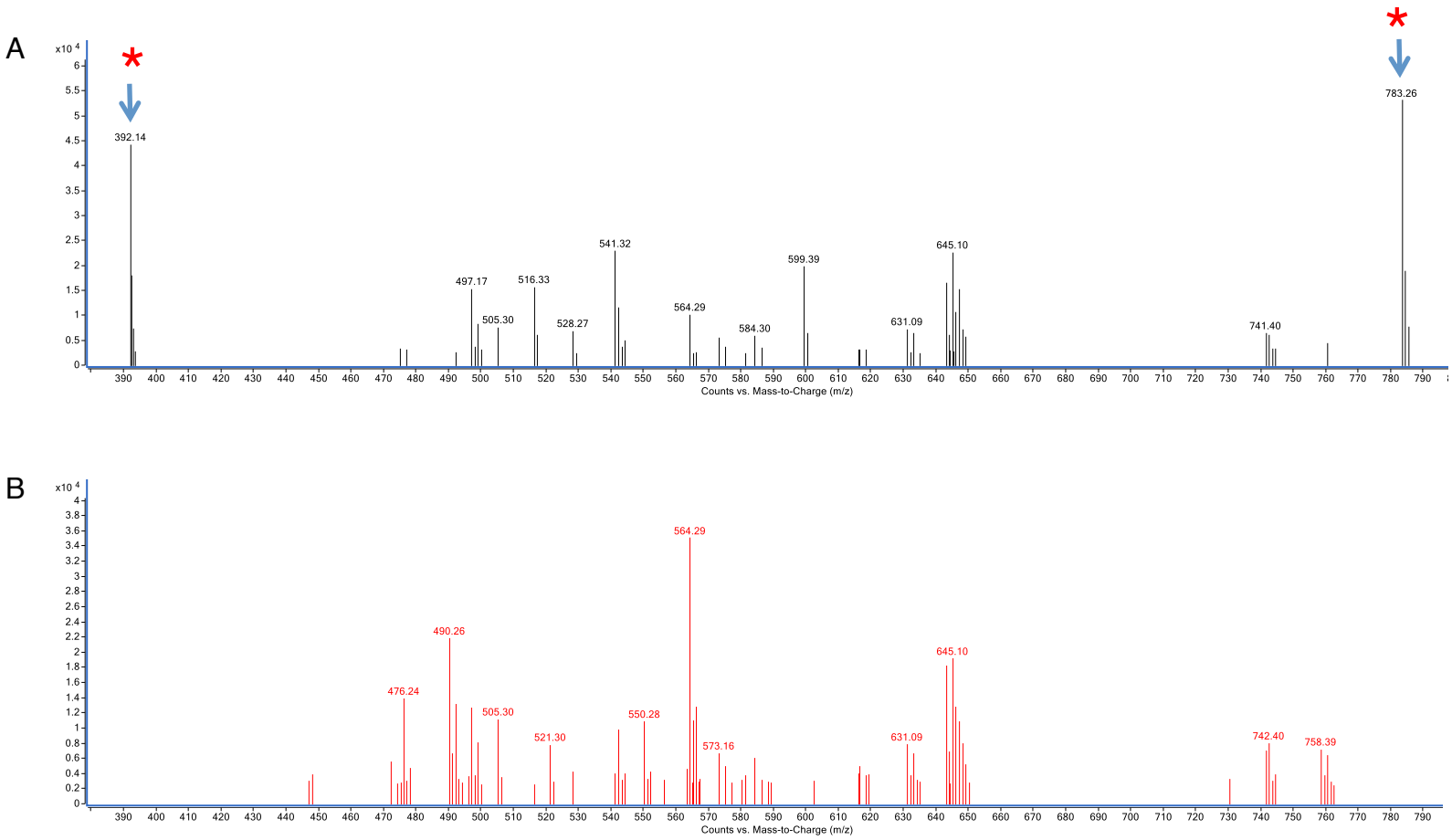


Figure S2. Identification of bis(GSH)-HDI by LC-MS. MS data on concentrated airway fluid from an HDI vapor exposed (A) and control rabbit (B), eluting from the LC column ~2.78 minutes in the Agilent system as described in the methods and Figure 2 of the main manuscript. Singly and doubly charged ions with *m/z*'s (783.26 and 392.14) corresponding to bis(GSH)-HDI are uniquely observed in the HDI vapor exposed rabbit as highlighted by arrows with *.

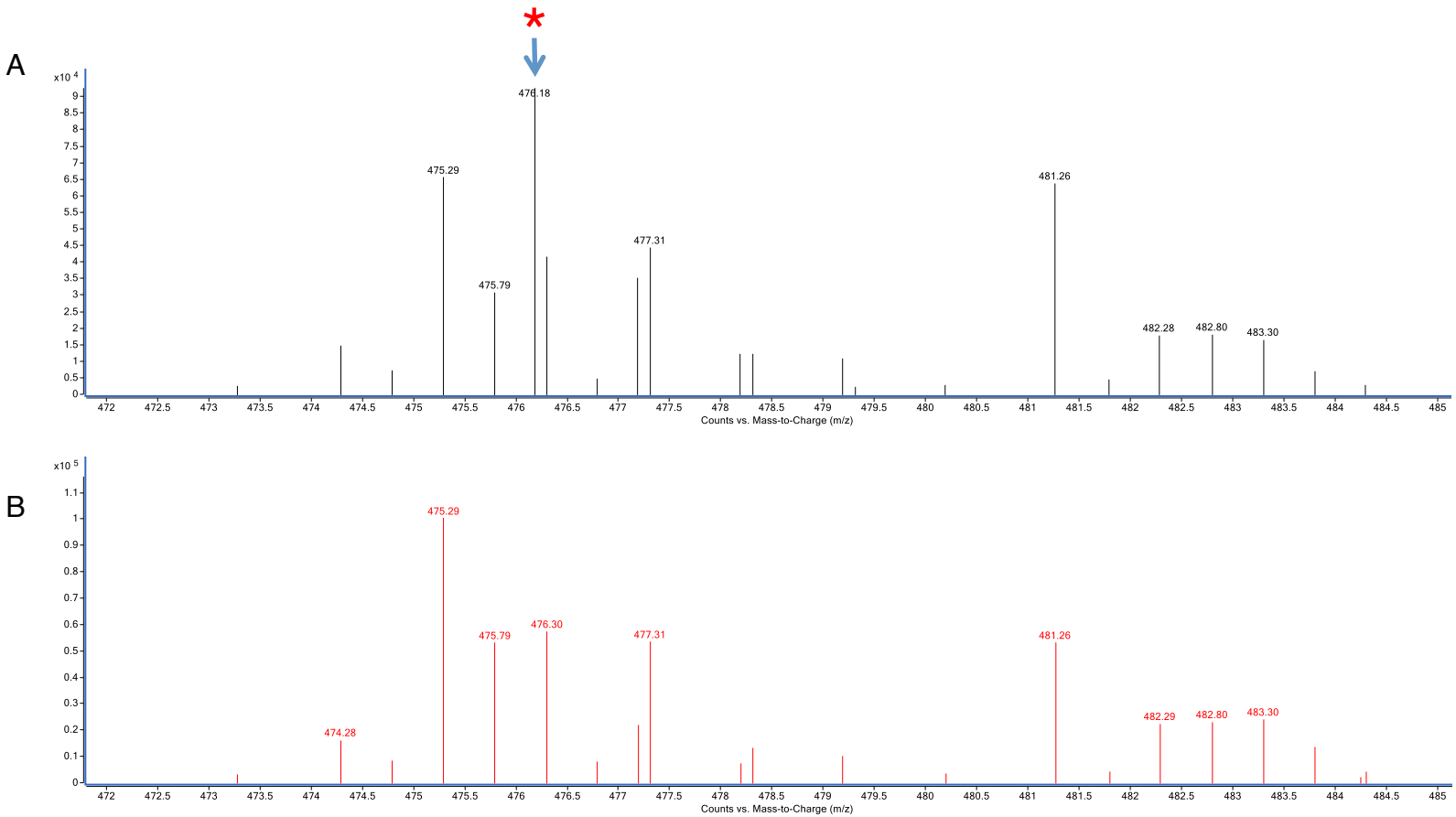


Figure S3. Identification of mono(GSH)-HDI by LC-MS. MS data on concentrated airway fluid from an HDI vapor exposed (A) and control rabbit (B), eluting from the LC column ~3.28 minutes in the Agilent system as described in the methods and Figure 2 of the main manuscript. The $[M+H]^+$ ion with an *m/z* (476.18) corresponding to mono(GSH)-HDI is uniquely present in the HDI vapor exposed rabbit as highlighted by arrow with *.

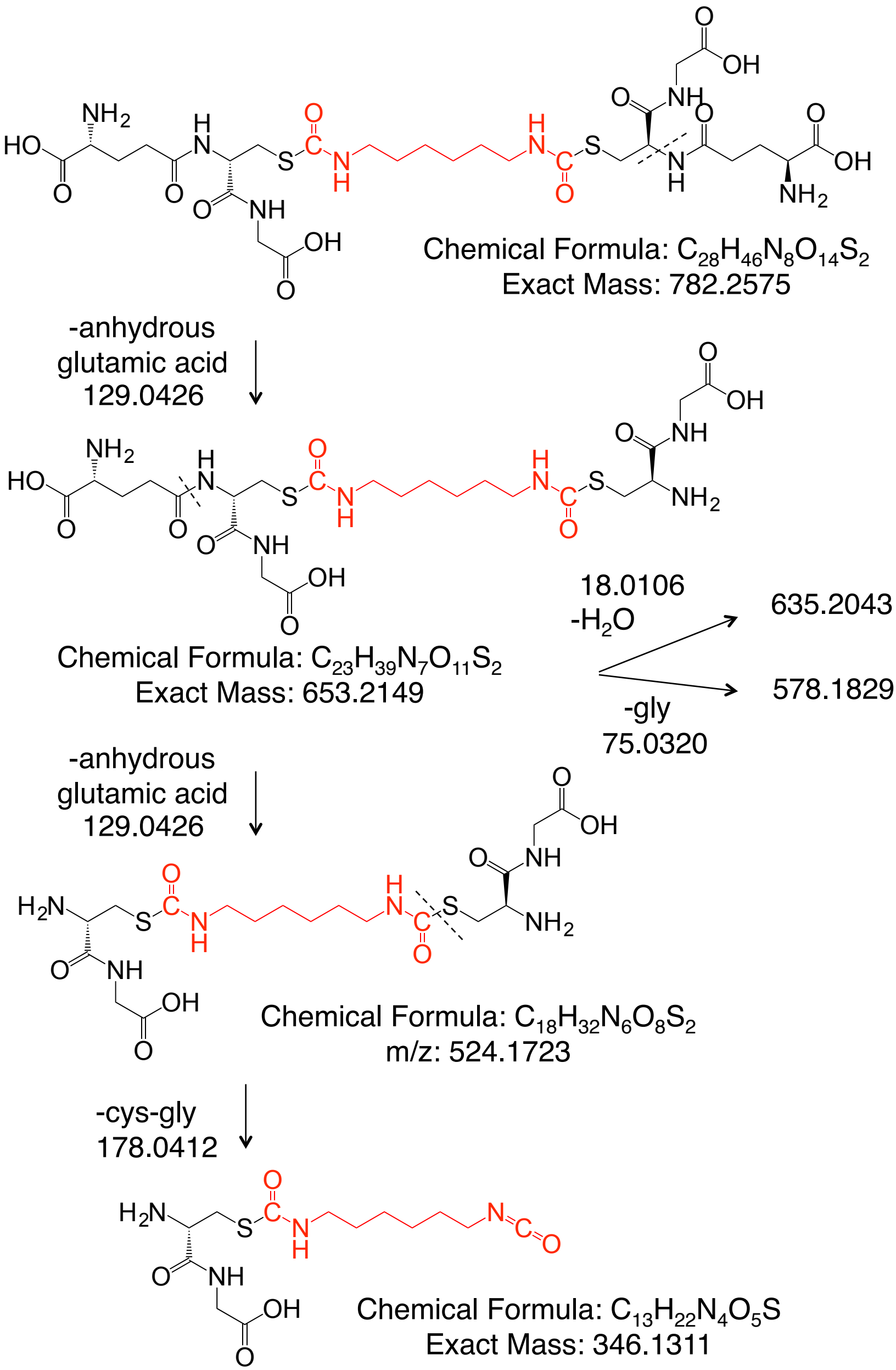
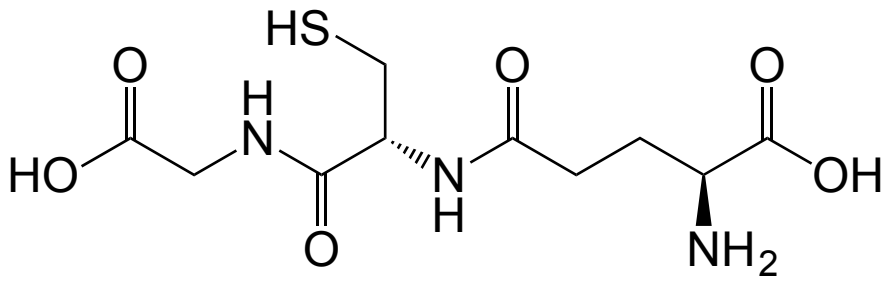
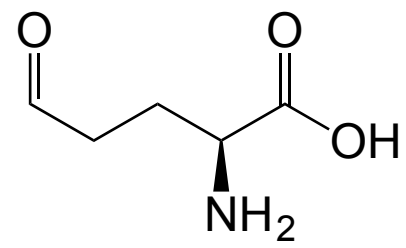


Figure S4. Predicted HCD Fragments of bis(GSH)-HDI

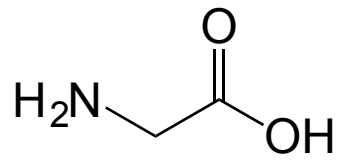


Chemical Formula: $C_{10}H_{17}N_3O_6S$
Exact Mass: 307.0838



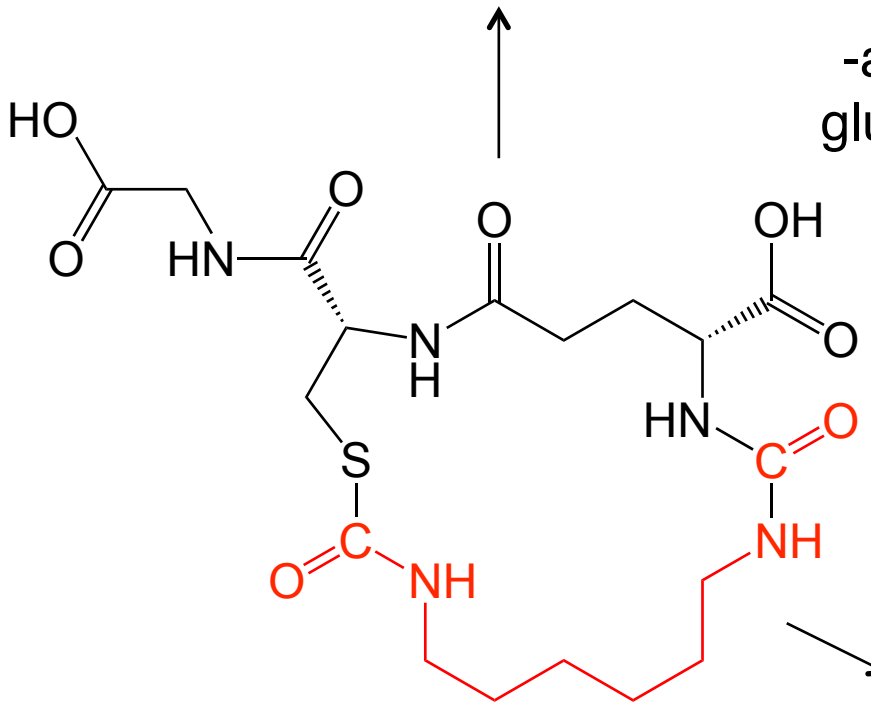
Chemical Formula: $C_5H_7NO_3$
Exact Mass: 129.0426

-gly

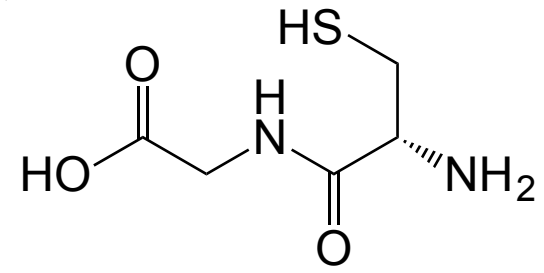


Chemical Formula: $C_2H_5NO_2$
Exact Mass: 75.0320

-anhydrous glutamic acid 129.0426

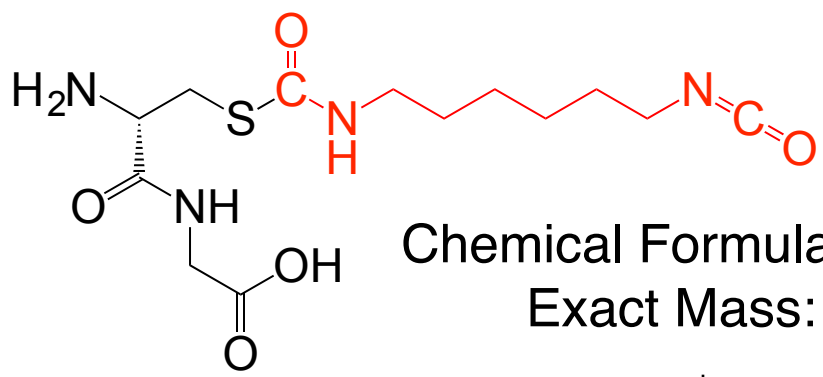


Chemical Formula: $C_{18}H_{29}N_5O_8S$
Exact Mass: 475.1737



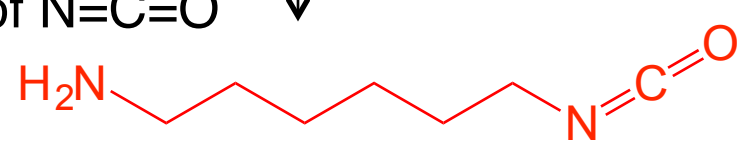
Chemical Formula: $C_5H_{10}N_2O_3S$
Exact Mass: 178.0412

-anhydrous glutamic acid 129.0426



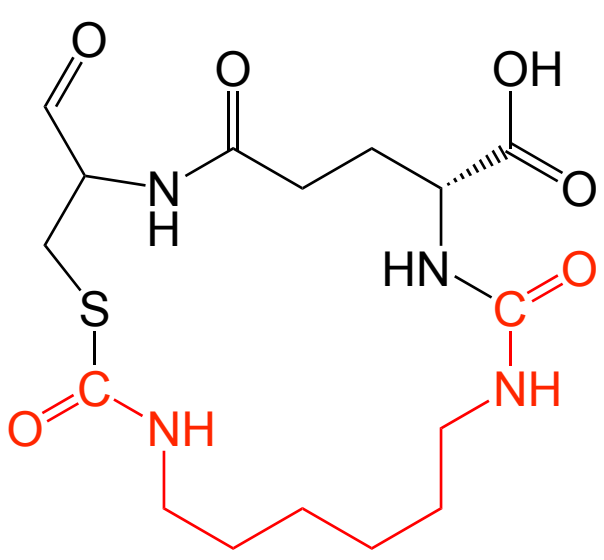
Chemical Formula: $C_{13}H_{22}N_4O_5S$
Exact Mass: 346.1311

-(cys-gly)/hydrolysis of N=C=O



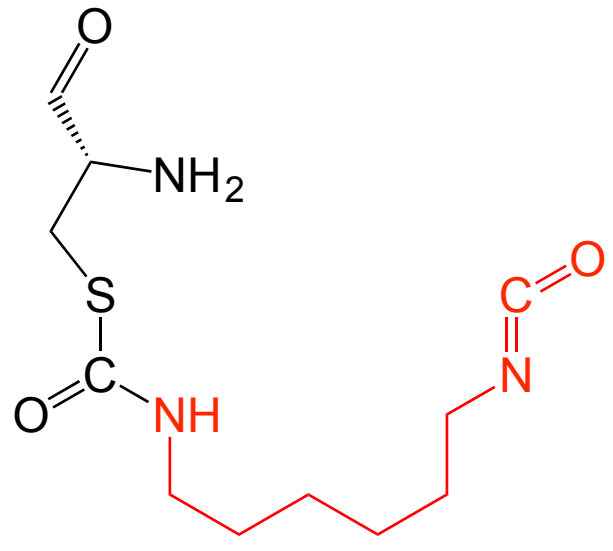
Chemical Formula: $C_7H_{14}N_2O$
Exact Mass: 142.1106

-gly
75.0320



Chemical Formula: $C_{16}H_{24}N_4O_6S$
Exact Mass: 400.1417

-anhydrous glutamic acid 129.0426



Chemical Formula: $C_{11}H_{17}N_3O_3S$
Exact Mass: 271.0991

Figure S5. Predicted HCD Fragments of mono(GSH)-HDI

Fig. S6

YPED

LCMS Peptides

Proteomic Analysis of Airway Fluid from Exposed Rabbit #1 (E1): Peptides matching uteroglobin including those with HDI modification

* note start / end peptide numbering includes 21 aa signal peptide

Protein ID	splP02779IUTER_RABIT
Protein Name	Uteroglobin OS=Oryctolagus cuniculus GN=SCGB1A1 PE=1 SV=1
Percent Coverage	71.4

26 peptides identified with score greater than identity score

Score	Expectation	Peptide Sequence	Start	End	M/Z	Ion Mass	Ion Mass(calc)	Delta	ppm	Charge
91.05	2.7E-7	R.FAHVIENLLLGTPSSYETSLK.E **BOLD RED**	27	47	1160.1155	2318.2164	2318.2158	0.0006	0.3	2
85.58	7.4E-8	K.EFEPDDTMKDAGMQMK.K **BOLD RED**	48	63	936.8953	1871.7761	1871.774	0.0021	1.1	2
72.44	0.000049	R.FAHVIENLLLGTPSSYETSLKEFEPDDTMK.D **BOLD RED**	27	56	1137.8954	3410.6643	3410.6592	0.0052	1.5	3
67.84	0.000013	K.KVLDSLPQTTR.E **BOLD RED**	64	74	629.3619	1256.7092	1256.7088	0.0004	0.3	2
64.15	0.0000064	K.EFEPDDTMKDAGMQMK.K + Oxidation (M) **BOLD RED**	48	63	944.892	1887.7694	1887.7689	0.0005	0.3	2
62.68	0.00018	R.FAHVIENLLLGTPSSYETSLK.E **BOLD RED**	27	47	773.7495	2318.2265	2318.2158	0.0107	4.6	3
58.86	0.00011	K.KVLDSLPQTTR.E **BOLD RED**	64	74	419.9114	1256.7123	1256.7088	0.0035	2.8	3
53.28	0.0016	R.FAHVIENLLLGTPSSYETSLK.E **BOLD RED**	27	47	580.5614	2318.2165	2318.2158	0.0007	0.3	4
50.85	0.009	R.FAHVIENLLLGTPSSYETSLKEFEPDDTMKDAGMQMK.K **BOLD RED**	27	63	1391.6679	4171.9817	4171.9792	0.0025	0.6	3
50.74	0.0071	R.FAHVIENLLLGTPSSYETSLKEFEPDDTMK.D **BOLD RED**	27	56	853.673	3410.663	3410.6592	0.0039	1.1	4
50.32	0.0078	R.FAHVIENLLLGTPSSYETSLKEFEPDDTMK.D + Oxidation (M) **BOLD RED**	27	56	1143.227	3426.6593	3426.6541	0.0052	1.5	3
49.23	0.00099	R.ENIMKLTEK.I **BOLD RED**	75	83	553.2999	1104.5853	1104.5849	0.0005	0.5	2
47.69	0.00012	K.EFEPDDTMK.D **BOLD RED**	48	56	556.2355	1110.4565	1110.4539	0.0026	2.3	2
46.2	0.0018	K.VLDSLPQTTR.E **BOLD RED**	65	74	565.3143	1128.6141	1128.6139	0.0002	0.2	2
43.55	0.0026	K.KVLDSLPQTTR.E + HDI_142 (HKN) **BOLD RED**	64	74	467.2804	1398.8195	1398.8195	0	0	3
43.46	0.0017	K.IVKSPLCM.- + Carbamidomethyl (C) **BOLD RED**	84	91	474.2565	946.4984	946.498	0.0004	0.4	2
39.94	0.0065	K.IVKSPLCM.- + Carbamidomethyl (C); HDI_142 (HKN) **BOLD RED**	84	91	545.3115	1088.6085	1088.6086	-0.0001	-0.1	2
39.86	0.0066	K.VLDSLPQTTR.E **BOLD RED**	65	74	377.2115	1128.6126	1128.6139	-0.0013	-1.2	3
38.32	0.00074	K.EFEPDDTMK.D + Oxidation (M) **BOLD RED**	48	56	564.2316	1126.4486	1126.4489	-0.0003	-0.3	2
37.8	0.0028	K.EFEPDDTMKDAGMQMK.K + Oxidation (M) **BOLD RED**	48	63	630.2639	1887.7699	1887.7689	0.0011	0.6	3
35.89	0.0039	K.EFEPDDTMKDAGMQMK.K + 2 Oxidation (M) **BOLD RED**	48	63	952.8906	1903.7666	1903.7638	0.0028	1.5	2
35.39	0.0077	K.EFEPDDTMKDAGMQMK.K **BOLD RED**	48	63	624.9321	1871.7744	1871.774	0.0004	0.2	3
33.63	0.0021	K.DAGMQMK.K + Oxidation (M) **BOLD RED**	57	63	398.6686	795.3227	795.3255	-0.0028	-3.5	2
32.74	0.0063	K.LTEKIVK.S **BOLD RED**	80	86	415.7705	829.5265	829.5273	-0.0008	-1	2
30.24	0.014	K.EFEPDDTMKDAGMQMK.K + 2 Oxidation (M) **BOLD RED**	48	63	635.5957	1903.7653	1903.7638	0.0015	0.8	3
23.35	0.02	K.DAGMQMK.K **BOLD RED**	57	63	390.6718	779.3291	779.3306	-0.0015	-1.9	2

Export options: CSV | Excel

Fig. S7

YPED

LCMS Peptides

Proteomic Analysis of Airway Fluid from Exposed Rabbit #2 (E2): Peptides matching uteroglobin including those with HDI modification

* note start / end peptide numbering includes 21 aa signal peptide

Protein ID	sp|P02779|UTER_RABIT
Protein Name	Uteroglobin OS=Oryctolagus cuniculus GN=SCGB1A1 PE=1 SV=1
Percent Coverage	100

31 peptides identified with score greater than identity score

Score	Expectation	Peptide Sequence	Start	End	M/Z	Ion Mass	Ion Mass(calc)	Delta	ppm	Charge
102.55	1.9E-8	R.FAHVIENLLLGTPSSYETSLK.E **BOLD RED**	27	47	1160.1169	2318.2193	2318.2158	0.0035	1.5	2
73.74	0.000036	R.FAHVIENLLLGTPSSYETSLKEFEPDDTMK.D **BOLD RED**	27	56	1137.896	3410.6662	3410.6592	0.007	2.1	3
71.68	0.0000055	K.KVLDSLPQTTR.E **BOLD RED**	64	74	629.3643	1256.714	1256.7088	0.0051	4.1	2
68.1	0.0000043	K.EFEPDDTMKDAGMQMK.K **BOLD RED**	48	63	936.8959	1871.7772	1871.774	0.0032	1.7	2
65.85	0.000088	R.FAHVIENLLLGTPSSYETSLK.E **BOLD RED**	27	47	580.5612	2318.2158	2318.2158	0	0	4
62.27	0.00019	R.FAHVIENLLLGTPSSYETSLK.E **BOLD RED**	27	47	773.7508	2318.2305	2318.2158	0.0148	6.4	3
56.06	0.002	R.FAHVIENLLLGTPSSYETSLKEFEPDDT**M**K.D + Oxidation (M) **BOLD RED**	27	56	1143.2262	3426.6568	3426.6541	0.0027	0.8	3
55.53	0.0024	R.FAHVIENLLLGTPSSYETSLKEFEPDDTMK.D **BOLD RED**	27	56	853.6727	3410.6616	3410.6592	0.0024	0.7	4
53.21	0.004	R.FAHVIENLLLGTPSSYETSLKEFEPDDTMK.D **BOLD RED**	27	56	683.1398	3410.6625	3410.6592	0.0033	1	5
51.66	0.0073	R.FAHVIENLLLGTPSSYETSLKEFEPDDTMKDAGMQ**M**K.K + Oxidation (M) **BOLD RED**	27	63	838.6031	4187.9791	4187.9741	0.005	1.2	5
50.4	0.00068	K.VLDSLPQTTR.E **BOLD RED**	65	74	565.3144	1128.6142	1128.6139	0.0003	0.3	2
50.18	0.00016	K.EFEPDDT**M**KDAGMQMK.K + Oxidation (M) **BOLD RED**	48	63	944.8923	1887.7701	1887.7689	0.0012	0.6	2
49.56	0.0092	R.FAHVIENLLLGTPSSYETSLKEFEPDDT**M**K.D + Oxidation (M) **BOLD RED**	27	56	686.338	3426.6537	3426.6541	-0.0004	-0.1	5
48.7	0.011	R.FAHVIENLLLGTPSSYETSLKEFEPDDT**M**K.D + Oxidation (M) **BOLD RED**	27	56	857.6709	3426.6545	3426.6541	0.0004	0.1	4
48.33	0.00094	K.VLDSLPQTTR.E **BOLD RED**	65	74	377.2115	1128.6126	1128.6139	-0.0013	-1.2	3
48	0.00011	K.EFEPDDTMK.D **BOLD RED**	48	56	556.236	1110.4574	1110.4539	0.0034	3.1	2
47.66	0.0013	R.ENIMKLTEK.I **BOLD RED**	75	83	553.3008	1104.5871	1104.5849	0.0023	2.1	2
45.29	0.0015	K.IV**K**SPL**C**M.- + Carbamidomethyl (C); HDI_142 (HKN) **BOLD RED**	84	91	545.3116	1088.6087	1088.6086	0.0002	0.2	2
40.86	0.00041	K.EFEPDDT**M**K.D + Oxidation (M) **BOLD RED**	48	56	564.2316	1126.4487	1126.4489	-0.0001	-0.1	2
40.6	0.0034	K.IVKSPL**C**M.- + Carbamidomethyl (C) **BOLD RED**	84	91	474.2564	946.4983	946.498	0.0003	0.3	2
39.89	0.018	K.VLDSLPQTTRENIMK.L **BOLD RED**	65	79	872.967	1743.9195	1743.9189	0.0006	0.3	2
38.58	0.00066	K.DAGMQ**M**K.K + Oxidation (M) **BOLD RED**	57	63	398.6699	795.3253	795.3255	-0.0002	-0.3	2
38.56	0.0038	K.EFEPDDTMKDAGMQMK.K **BOLD RED**	48	63	624.9324	1871.7755	1871.774	0.0015	0.8	3
38	0.012	K.KVLDSLPQTTR.E **BOLD RED**	64	74	419.9111	1256.7115	1256.7088	0.0026	2.1	3
35.01	0.019	K.IV**K**SPL**C**M.- + Oxidation (M); Carbamidomethyl (C); HDI_142 (HKN) **BOLD RED**	84	91	553.3101	1104.6057	1104.6035	0.0022	2	2
34.41	0.006	K.EFEPDDTMKDAGMQ**M**K.K + Oxidation (M) **BOLD RED**	48	63	630.2637	1887.7694	1887.7689	0.0005	0.3	3
33.02	0.013	K.LTE**K**IVK.S + HDI_168_KNH (HKN) **BOLD RED**	80	86	499.8157	997.6168	997.6172	-0.0004	-0.4	2
32.46	0.04	K.IV**K**SPL**C**M.- + Oxidation (M); Carbamidomethyl (C); HDI_168_KNH (HKN) **BOLD RED**	84	91	566.2985	1130.5825	1130.5828	-0.0003	-0.3	2
28.5	0.007	K.DAGMQMK.K **BOLD RED**	57	63	390.6725	779.3303	779.3306	-0.0002	-0.3	2
26.28	0.013	K.LTE**K**IVK.S + HDI_142 (HKN) **BOLD RED**	80	86	486.8264	971.6383	971.6379	0.0004	0.4	2
23.14	0.012	K.DAG**M**Q**M**K.K + 2 Oxidation (M) **BOLD RED**	57	63	406.6674	811.3202	811.3204	-0.0003	-0.4	2

Export options: CSV | Excel

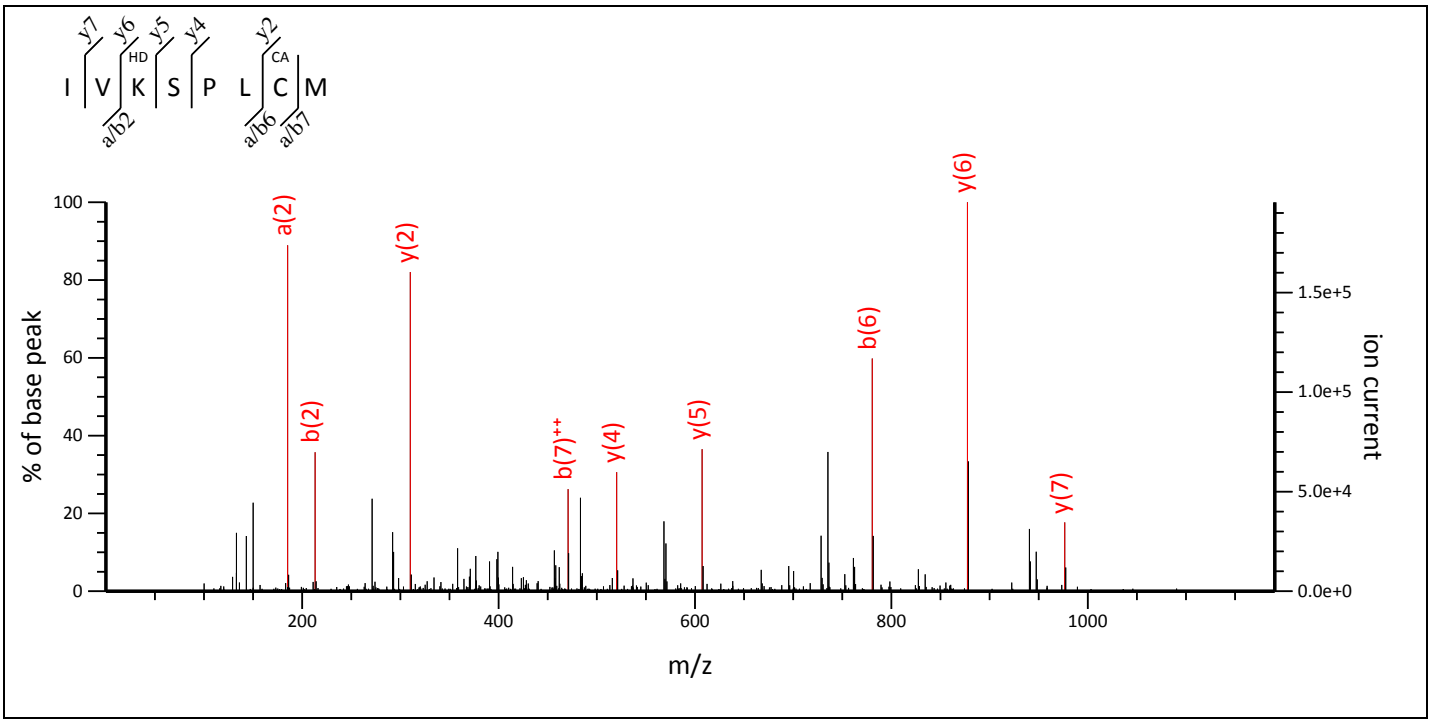
Fig. S8. LC-MS/MS analysis of ion with m/z matching that predicted for uteroglobin peptide + partially hydrolyzed HDI. MASCOT analysis is shown.

MATRIX SCIENCE **Mascot Search Results**

Peptide View

MS/MS Fragmentation of **IVKSPLCM**
Found in **sp|P02779|UTER_RABIT** in **Uniprot_Rabbit**, Uteroglobin OS=Oryctolagus cuniculus GN=SCGB1A1 PE=1 SV=1

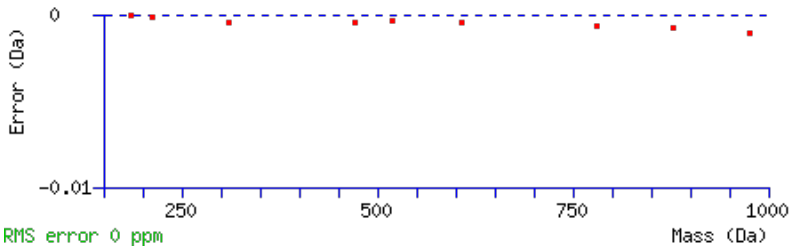
Match to Query 5724: 1088.608748 from(545.311650,2+) index(17227)
Title: Spectrum17277 scans:20882,
Data file File Name: OTF16-2691.raw

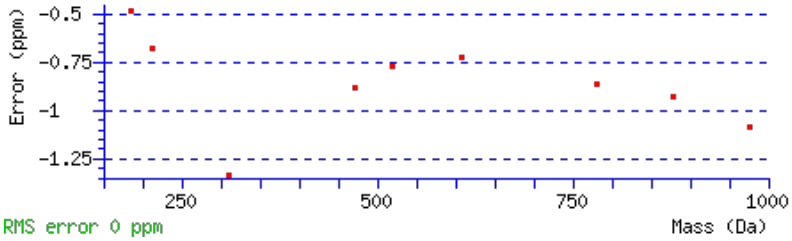


Label all possible matches ○ Label matches used for scoring ◉

Monoisotopic mass of neutral peptide Mr(calc): 1088.6086
Variable modifications:
K3 : HDI_142 (HKN)
C7 : Carbamidomethyl (C)
Ions Score: 45 **Expect:** 8.8e-05
Matches : 9/66 fragment ions using 10 most intense peaks (help)

#	a	a++	a*	a*++	b	b++	b*	b*++	Seq.	y	y++	y*	y*++	#
1	86.0964	43.5519			114.0913	57.5493			I					8
2	**185.1648**	93.0861			**213.1598**	107.0835			V	***976.5318***	488.7695	959.5053	480.2563	7
3	455.3704	228.1888	438.3439	219.6756	483.3653	242.1863	466.3388	233.6730	K	***877.4634***	439.2353	860.4369	430.7221	6
4	542.4024	271.7049	525.3759	263.1916	570.3974	285.7023	553.3708	277.1890	S	***607.2578***	304.1326			5
5	639.4552	320.2312	622.4287	311.7180	667.4501	334.2287	650.4236	325.7154	P	***520.2258***	260.6165			4
6	752.5393	376.7733	735.5127	368.2600	**780.5342**	390.7707	763.5076	382.2575	L	423.1730	212.0902			3
7	912.5699	456.7886	895.5434	448.2753	940.5648	**470.7861**	923.5383	462.2728	C	***310.0890***	155.5481			2
8									M	150.0583	75.5328			1





NCBI **BLAST** search of IVKSPLCM
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

Score	Mr(calc)	Delta	Sequence
45.3	1088.6086	0.0002	IVKSPLCM
1.9	1088.6165	-0.0077	LVQFMKR
0.1	1088.6012	0.0075	IVQTLCTVR
0.1	1088.6012	0.0076	IVRLTECQK
0.1	1088.6077	0.0010	IVSETLQATK
0.1	1088.6091	-0.0003	LVHIEHSVR

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

Fig. S9

Proteomic Analysis of Rabbit Airway Fluid: Peptides matching albumin including those with HDI modification *note start/end peptide numbering includes 24 aa leader sequence

YPED

LCMS Peptides

Protein ID	trIG1U9S2IG1U9S2_RABIT
Protein Name	Serum albumin OS=Oryctolagus cuniculus GN=ALB PE=1 SV=1
Percent Coverage	90.8

93 peptides identified with score greater than identity score

Score	Expectation	Peptide Sequence	Start	End	M/Z	Ion Mass	Ion Mass(calc)	Delta	ppm	Charge
93.95	1.5E-7	K.QNCELYEQLGDYNFQNALLVR.Y + Carbamidomethyl (C) **BOLD RED**	414	434	863.08	2586.2181	2586.2173	0.0008	0.3	3
90.38	1.5E-7	R.LPCVEDYLSVVLNR.L + Carbamidomethyl (C) **BOLD RED**	470	483	838.9384	1675.8621	1675.8603	0.0018	1.1	2
90.18	2.3E-8	K.CCSAEDKEACFAVEGPK.L + 3 Carbamidomethyl (C) **BOLD RED**	582	598	979.4078	1956.8011	1956.8016	-0.0004	-0.2	2
86.3	8.8E-7	K.QNCELYEQLGDYNFQNALLVR.Y + Carbamidomethyl (C) **BOLD RED**	414	434	1294.1178	2586.221	2586.2173	0.0038	1.5	2
85.28	5.9E-7	R.RPCFSALGPDETYVPK.E + Carbamidomethyl (C) **BOLD RED**	509	524	918.9513	1835.888	1835.8876	0.0004	0.2	2
81.27	7.5E-7	K.AFFGHYLYEVAR.R **BOLD RED**	157	168	736.87	1471.7254	1471.7248	0.0006	0.4	2
79.76	2.7E-8	K.ECCHGDLLECADDR.A + 3 Carbamidomethyl (C) **BOLD RED**	268	281	875.3359	1748.6573	1748.6553	0.0021	1.2	2
79.41	7.5E-7	K.YMCEHQETISSHLK.E + Carbamidomethyl (C) **BOLD RED**	287	300	881.8983	1761.7821	1761.7814	0.0007	0.4	2
78.98	0.0000012	K.KVPQVSTPTLVEISR.S **BOLD RED**	438	452	827.4806	1652.9466	1652.9461	0.0005	0.3	2
73.91	0.0000021	K.YMCEHQETISSHLK.E + Oxidation (M); Carbamidomethyl (C) **BOLD RED**	287	300	889.8954	1777.7762	1777.7763	-0.0001	-0.1	2
71.64	0.0000027	K.VHKECCHGDLLECADDR.A + 3 Carbamidomethyl (C) **BOLD RED**	265	281	1057.4468	2112.879	2112.8775	0.0015	0.7	2
70.46	0.000012	K.VLDEFQPLVDEPK.N **BOLD RED**	397	409	764.8991	1527.7837	1527.7821	0.0016	1	2
69.69	0.00001	K.KVPQVSTPTLVEISR.S **BOLD RED**	438	452	551.9899	1652.948	1652.9461	0.0018	1.1	3
68.93	0.00001	K.TVVGEFTALLDK.C **BOLD RED**	570	581	646.8586	1291.7026	1291.7024	0.0002	0.2	2
68.17	0.000016	K.VPQVSTPTLVEISR.S **BOLD RED**	439	452	763.4338	1524.8531	1524.8512	0.002	1.3	2
68.07	0.000019	R.PCFSALGPDETYVPK.E + Carbamidomethyl (C) **BOLD RED**	510	524	840.9008	1679.787	1679.7865	0.0005	0.3	2
67.8	0.000039	R.HPYFYAPELLYYAQK.Y **BOLD RED**	170	184	951.9755	1901.9365	1901.9352	0.0013	0.7	2
67.24	0.000017	K.NYEEAKDLFLGK.F **BOLD RED**	342	353	713.8644	1425.7142	1425.714	0.0002	0.1	2
65.84	0.000011	K.KQTALVELVK.H **BOLD RED**	549	558	564.8537	1127.6928	1127.6914	0.0015	1.3	2
65.2	0.000069	K.SLHDIFGDKICALPSLR.D + Carbamidomethyl (C) **BOLD RED**	89	105	971.5148	1941.015	1941.0142	0.0008	0.4	2
64.74	0.000008	K.CCSAEDKEACFAVEGPK.L + 3 Carbamidomethyl (C) **BOLD RED**	582	598	653.2744	1956.8014	1956.8016	-0.0002	-0.1	3
64.28	0.000032	R.RHPDYSVVLLLR.L **BOLD RED**	361	372	489.9531	1466.8374	1466.8358	0.0016	1.1	3
62.94	0.000021	K.AILTECCEAADK.G + 2 Carbamidomethyl (C) **BOLD RED**	187	198	690.8115	1379.6084	1379.6061	0.0023	1.7	2
62.73	0.00011	R.RPCFSALGPDETYVPK.E + Carbamidomethyl (C) **BOLD RED**	509	524	612.9719	1835.8938	1835.8876	0.0061	3.3	3
61.79	0.000037	K.ECCHGDLLECADDRADLAK.Y + 3 Carbamidomethyl (C) **BOLD RED**	268	286	1124.4757	2246.9369	2246.9354	0.0014	0.6	2
61.72	6.7E-7	R.DTYGDVADCCEK.K + 2 Carbamidomethyl (C) **BOLD RED**	106	117	716.7724	1431.5302	1431.5283	0.002	1.4	2
60.44	0.000043	K.KQTALVELVK.H **BOLD RED**	549	558	376.9045	1127.6917	1127.6914	0.0003	0.3	3
60.43	0.00018	K.AILTECCEAADKGACLTPK.L + 3 Carbamidomethyl (C) **BOLD RED**	187	205	1054.4959	2106.9771	2106.9748	0.0024	1.1	2
60.31	0.000047	K.ALISAAQER.L **BOLD RED**	213	221	479.7703	957.526	957.5243	0.0017	1.8	2
60.01	0.00021	K.EFNAETFTFHADICTLPETER.K + Carbamidomethyl (C) **BOLD RED**	525	545	1264.5745	2527.1344	2527.1326	0.0018	0.7	2

59.54	0.0000051	K.ACVADESAANCDK.S + 2 Carbamidomethyl (C) BOLD RED	76	88	705.7836	1409.5527	1409.5551	-0.0024	-1.7	2
59.48	0.00001	K.CCSESLVDR.R + 2 Carbamidomethyl (C) BOLD RED	500	508	563.2374	1124.4603	1124.459	0.0013	1.2	2
58.16	0.00006	K.SLHDIFGDK.I BOLD RED	89	97	516.2623	1030.5101	1030.5084	0.0017	1.6	2
56.46	0.00012	K.YMCEHQETISSHLK.E + Oxidation (M); Carbamidomethyl (C) BOLD RED	287	300	593.5999	1777.7779	1777.7763	0.0016	0.9	3
54.27	0.000058	K.ADFTDISK.I BOLD RED	250	257	448.7217	895.4288	895.4287	0.0001	0.1	2
53.92	0.00085	K.EFNAETFTFHADICTLPETER.K + Carbamidomethyl (C) BOLD RED	525	545	843.3856	2527.135	2527.1326	0.0025	1	3
53.76	0.0003	R.HPDYSVVLLLR.L BOLD RED	362	372	656.3746	1310.7346	1310.7347	-0.0001	-0.1	2
53.49	0.003	K.AHCIYGLHNDETPAGLPAVAEEFVEDKDVCK.N + 2 Carbamidomethyl (C) BOLD RED	311	341	1162.2111	3483.6114	3483.6075	0.0039	1.1	3
53.25	0.00013	K.QTALVELVK.H BOLD RED	550	558	500.8056	999.5966	999.5964	0.0002	0.2	2
52.96	0.00066	R.LCVLHEKTPVSEK.V + Carbamidomethyl (C) BOLD RED	484	496	770.4139	1538.8133	1538.8127	0.0007	0.5	2
52.96	0.00034	K.YMCEHQETISSHLK.E + Carbamidomethyl (C) BOLD RED	287	300	588.2682	1761.7827	1761.7814	0.0013	0.7	3
51.42	0.00018	K.KQTALVELVK.H + HDI_142 (HKN) BOLD RED	549	558	635.9086	1269.8026	1269.802	0.0006	0.5	2
50.56	0.00089	K.AFFGHYLYEVAR.R BOLD RED	157	168	491.5827	1471.7262	1471.7248	0.0014	1	3
50.26	0.00081	R.RHPDYSVVLLLR.L BOLD RED	361	372	734.4257	1466.8369	1466.8358	0.0011	0.7	2
49.72	0.000011	R.DTYGDVADCCEK.K + 2 Carbamidomethyl (C) BOLD RED	106	117	478.1833	1431.528	1431.5283	-0.0002	-0.1	3
48.96	0.00011	R.DTYGDVADCCEKK.E + 2 Carbamidomethyl (C) BOLD RED	106	118	780.8195	1559.6245	1559.6232	0.0013	0.8	2
48.84	0.0037	R.RHPYFYAPELLYYAQK.Y BOLD RED	169	184	687.02	2058.0382	2058.0363	0.0019	0.9	3
48.8	0.0037	R.RHPYFYAPELLYYAQK.Y BOLD RED	169	184	1030.0264	2058.0382	2058.0363	0.0019	0.9	2
48.75	0.00034	K.IVTDLTK.V BOLD RED	258	264	395.2394	788.4643	788.4644	0	0	2
48.06	0.00074	K.LVKEVTDLAK.A BOLD RED	66	75	372.5605	1114.6597	1114.6598	0	0	3
46.98	0.00003	K.CCATDDPHACYAK.V + 3 Carbamidomethyl (C) BOLD RED	384	396	784.7989	1567.5833	1567.5854	-0.002	-1.3	2
46.25	0.016	K.AHCIYGLHNDETPAGLPAVAEEFVEDKDVCK.N + 2 Carbamidomethyl (C) BOLD RED	311	341	871.9109	3483.6145	3483.6075	0.007	2	4
46.15	0.0016	K.YMCEHQETISSHLK.E + Carbamidomethyl (C) BOLD RED	287	300	441.4529	1761.7824	1761.7814	0.001	0.6	4
45.32	0.00075	K.KQTALVELVK.H + HDI_142 (HKN) BOLD RED	549	558	424.2747	1269.8022	1269.802	0.0001	0.1	3
45.03	0.0012	K.AILTECCEAADK.G + 2 Carbamidomethyl (C) BOLD RED	187	198	460.8754	1379.6044	1379.6061	-0.0017	-1.2	3
44.06	0.013	K.EFNAETFTFHADICTLPETERK.I + Carbamidomethyl (C) BOLD RED	525	546	886.083	2655.2272	2655.2275	-0.0003	-0.1	3
43.78	0.011	K.AFHDDEKAFFGHYLYEVAR.R BOLD RED	150	168	772.3675	2314.0806	2314.0807	-0.0001	0	3
43.66	0.0014	K.EVTDLAK.A BOLD RED	69	75	388.2127	774.4109	774.4123	-0.0015	-1.9	2
43.59	0.00011	K.ECCHGDLLECADDR.A + 3 Carbamidomethyl (C) BOLD RED	268	281	583.8931	1748.6574	1748.6553	0.0021	1.2	3
41.74	0.0013	R.PEADVLCK.A + Carbamidomethyl (C) BOLD RED	142	149	466.2314	930.4483	930.4481	0.0002	0.2	2
41.6	0.049	K.AHCIYGLHNDETPAGLPAVAEEFVEDKDVCK.N + 2 Carbamidomethyl (C) BOLD RED	311	341	697.7319	3483.623	3483.6075	0.0155	4.4	5
41.02	0.039	R.FNDVGEEHFIGLVLITFSQYLQK.C BOLD RED	35	57	899.8027	2696.3864	2696.385	0.0014	0.5	3
40.73	0.0015	K.AYEATLK.K BOLD RED	376	382	398.2156	794.4166	794.4174	-0.0008	-1	2
39.57	0.006	K.ECCDKPILEK.A + 2 Carbamidomethyl (C) BOLD RED	301	310	646.3051	1290.5957	1290.5948	0.0009	0.7	2
39.27	0.031	K.AFHDDEKAFFGHYLYEVAR.R BOLD RED	150	168	579.5272	2314.0798	2314.0807	-0.0009	-0.4	4
39.24	0.0046	K.EACFAVEGPK.L + Carbamidomethyl (C) BOLD RED	589	598	554.2609	1106.5073	1106.5066	0.0006	0.5	2
38.66	0.031	K.SLHDIFGDKICALPSLR.D + Carbamidomethyl (C) BOLD RED	89	105	648.0126	1941.0159	1941.0142	0.0017	0.9	3
38.45	0.039	R.RHPYFYAPELLYYAQK.Y BOLD RED	169	184	515.5161	2058.0353	2058.0363	-0.0009	-0.4	4
38.04	0.012	K.EKALISAAQER.L BOLD RED	211	221	405.8946	1214.662	1214.6618	0.0002	0.2	3
37.99	0.0039	K.FLYEYSR.R BOLD RED	354	360	489.2397	976.4649	976.4654	-0.0005	-0.5	2

37.86	0.0091	K.LVKEVTDLAK.A **BOLD RED**	66	75	558.3379	1114.6613	1114.6598	0.0016	1.4	2
37.64	0.0093	K.Y**MC**EHQETISSHLK.E + Oxidation (M); Carbamidomethyl (C) **BOLD RED**	287	300	445.4518	1777.7781	1777.7763	0.0018	1	4
36.95	0.038	K.VHKE**CC**HGDLLE**C**ADDRADLAK.Y + 3 Carbamidomethyl (C) **BOLD RED**	265	286	871.3924	2611.1553	2611.1577	-0.0024	-0.9	3
36.59	0.052	K.SLHDIFGDKI**C**ALPSLR.D + Carbamidomethyl (C) **BOLD RED**	89	105	486.2613	1941.0161	1941.0142	0.0019	1	4
36.56	0.0088	K.VHKE**CC**HGDLLE**C**ADDR.A + 3 Carbamidomethyl (C) **BOLD RED**	265	281	705.3001	2112.8783	2112.8775	0.0008	0.4	3
36.53	0.038	K.ADFTDISKIVTDLTK.V **BOLD RED**	250	264	556.3014	1665.8823	1665.8825	-0.0002	-0.1	3
36.16	0.012	R.AYKAWALVR.L **BOLD RED**	234	242	359.8779	1076.6119	1076.6131	-0.0012	-1.1	3
36.15	0.023	K.NYEEAKDLFLGK.F **BOLD RED**	342	353	476.2448	1425.7125	1425.714	-0.0014	-1	3
36.04	0.059	R.HPYFYAPELLYYAQK.Y **BOLD RED**	170	184	634.9858	1901.9355	1901.9352	0.0003	0.2	3
35.38	0.018	K.I**C**ALPSLR.D + Carbamidomethyl (C) **BOLD RED**	98	105	465.266	928.5174	928.5164	0.001	1.1	2
34.49	0.0068	K.AYEATLKK.C **BOLD RED**	376	383	462.2633	922.5121	922.5123	-0.0002	-0.2	2
34.34	0.0045	R.NE**C**FLHHK.D + Carbamidomethyl (C) **BOLD RED**	123	130	542.7521	1083.4897	1083.492	-0.0023	-2.1	2
33.47	0.0053	K.SEIAHR.F **BOLD RED**	29	34	356.6888	711.3631	711.3664	-0.0032	-4.5	2
33.07	0.0054	K.AWALVR.L **BOLD RED**	237	242	358.2159	714.4173	714.4177	-0.0004	-0.6	2
32.14	0.0021	K.**C**PYEEHAK.L + Carbamidomethyl (C) **BOLD RED**	58	65	517.2224	1032.4303	1032.4335	-0.0032	-3.1	2
30.69	0.024	R.L**C**VLHEK.T + Carbamidomethyl (C) **BOLD RED**	484	490	449.7441	897.4737	897.4742	-0.0005	-0.6	2
30.28	0.056	K.E**CC**HGDLLE**C**ADDRADLAK.Y + 3 Carbamidomethyl (C) **BOLD RED**	268	286	749.9867	2246.9382	2246.9354	0.0028	1.2	3
28.74	0.05	K.LDALKEK.A **BOLD RED**	206	212	408.7437	815.4729	815.4752	-0.0023	-2.8	2
26.89	0.015	K.NYEEAK.D **BOLD RED**	342	347	377.173	752.3314	752.334	-0.0027	-3.6	2
26.12	0.022	R.DTYGDVAD**CC**EKK.E + 2 Carbamidomethyl (C) **BOLD RED**	106	118	520.8817	1559.6231	1559.6232	-0.0001	-0.1	3
24.83	0.012	K.AFHDDEK.A **BOLD RED**	150	156	431.1893	860.364	860.3664	-0.0025	-2.9	2
23.18	0.039	K.K**CC**ATDDPHA**C**YAK.V + 3 Carbamidomethyl (C) **BOLD RED**	383	396	566.2327	1695.6762	1695.6803	-0.0042	-2.5	3
20.2	0.014	K.**CC**ATDDPHA**C**YAK.V + 3 Carbamidomethyl (C) **BOLD RED**	384	396	523.5347	1567.5824	1567.5854	-0.003	-1.9	3

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