Cross sections for doubly-protonated peptides from tryptic digests[a]

Number of residues	Assigned sequence[b]	Peptide source[c]	MW[d]	Cross section (Å^2)[e]		Number of measurements[f]
4	IQDK	ubiq	502.58	174.97		1
4	YTKK	HSA	538.65	188.84		1
5	GITWK	cytc_horse	603.70	172.82		1
5	IDAMR	albu_sheep	604.73	205.17	(0.08)	2
5	IEHLR	albu_pig	666.79	199.48	(1.23)	2
5	KNQDK	kcas_bov	631.69	179.66		1
5	LRLQK	crephos_rab	656.83	188.79		1
5	TLTGK	ubiq	518.62	174.97		1
6	AKIQDK	ubiq	701.83	212.99		1
6	AWSVAR	albu_sheep	688.79	188.27		1
6	DWPDAR	crephos_rab	758.80	208.84		1
6	FVIEIR	albu_pig	775.95	211.25		1
6	GGVHVK	crephos_rab	595.71	179.46		1
6	HLDDLK	hb_bov	739.83	212.92	(1.16)	4
		hb_sheep				
6	HLDNLK	hb_pig	738.85	212.80	(0.72)	3
6	IEEIFK	crephos_rab	777.92	226.04		1
6	LIFAGK	ubiq	647.83	199.02		1
6	LNQLLR	enolase_yst	755.92	204.90		1
6	MQIFVK	ubiq	764.99	222.87		1
6	QLEDGR	ubiq	716.76	223.07		1
6	SEIAHR	albu_pig	711.78	193.99	(2.55)	5
		albu_sheep				
6	YIPGTK	cytc_horse	677.80	189.88	(3.56)	2
7	ASEDLKK	myo_horse	789.89	238.09		1
7	ATDEQLK	albu_sheep	803.87	205.29		1
7	ATKEQLK	HSA	816.96	215.40		1
7	AVPYPQR	bcas_bov	829.96	211.55		1
7	GDVAFVK	transfr_hum	734.86	194.38		1
7	GFFYTPK	ins_bov	859.00	225.36		1
7	GVLHAVK	enolase_yst	722.89	202.50		1
7	IATAIEK	enolase_yst	744.89	196.62		1
7	IVTDLAK	albu_pig	758.92	201.59	(1.94)	2
7	LGLVGSR	albu_pig	700.84	192.82	(2.40)	3
7	LMVEMEK	crephos_rab	879.10	225.09		1
7	LVTDLTK	BSA	788.95	210.68		1
7	MIFAGIK	cytc_horse	779.00	207.03	(1.25)	3
7	NPDPWAK	transfr_hum	826.91	213.72		1

7	Ac-SIPETQK	alcodehy_yst	843.94	214.09		1
7	VDPVNFK	hb_dog	817.95	203.64	(3.57)	7
		hb_bov				
		hb_hum				
		hb_pig				
7	VKAHGKK	hb_sheep	766.95	203.95		1
7	VLPVPQK	bcas_bov	779.99	215.38		1
7	VVTDLTK	albu_dog	774.92	205.05		1
7	WNMQNGK	conA	876.99	211.48	(0.37)	2
7	YLYEIAR	albu_pig	927.08	236.05	(0.46)	3
7	YLYEVAR	albu_sheep	913.05	230.94	(0.30)	3
8	ADFAEISK	albu_dog	879.97	213.59		1
8	ADFTDVTK	albu_sheep	895.97	213.10	(1.15)	2
8	ADFTEISK	albu_pig	910.00	219.23		1
8	DDHPNLPK	albu_horse	935.01	225.23		1
8	DDNPNLPR	HSA	939.99	229.08		1
8	DDTVCLAK	transfr_hum	863.99	213.30		1
8	DIPVPKPK	alcodehy_yst	893.10	231.34		1
8	DLGEENFK	HSA	951.01	238.58		1
8	DLGEQYFK	albu_pig	999.10	243.83	(0.55)	2
8	ELSDIAHR	aldol_rab	940.03	232.56	(3.58)	2
8	EYEATLEK	albu_dog	982.06	230.57	(2.63)	3
8	FGVNGSEK	conalb_chick	836.91	211.12	(1.97)	3
8	IDALNENK	blacto_bov	916.01	226.20	(1.73)	3
8	KLGLVGSR	albu_pig	829.02	227.76	(0.13)	3
8	KVSEALTK	hb_rab	875.04	211.32	(0.42)	2
8	LIVTQTMK	blacto_bov	933.18	234.72		1
8	SEVAHRFK	HSA	973.11	231.57		1
8	VHLSAEEK	hb_pig	912.02	226.77	(2.70)	3
8	VHLTAEEK	hb_dog	926.04	230.04	(2.15)	2
8	VLTPDLYK	crephos_rab	948.13	241.28	(2.73)	3
8	YLGEEYVK	transfr_hum	1000.12	244.85	(4.55)	2
8	YLYEIARR	HSA	1083.26	252.64		1
9	AAVTAFWGK	hb_bov	950.11	229.12	(3.11)	3
9	AAVTGFWGK	hb_sheep	936.09	229.67		1
9	ANELLINVK	alcodehy_yst	1013.21	252.18	(2.33)	3
9	APNHAVVTR	transfr_hum	964.10	231.13	(3.65)	3
9	EAVLGLWGK	hb_pig	972.16	232.31	(0.88)	2
9	EGIPPDQQR	ubiq	1039.12	252.51		1
9	EKVLASSAR	albu_sheep	960.11	229.84	(0.42)	3
9	LHDRNTYEK	transfr_hum	1175.27	261.21	(0.90)	2
9	LHVDPENFK	hb_bov	1098.23	252.51	(3.57)	3
		hb_dog				

9	LHVDPENFR	hb_hum	1126.24	255.74	(4.51)	2
		hb_sheep				
9	LRVDPVNFK	hb_bov	1087.29	261.06	(3.73)	5
		hb_hum				
		hb_sheep				
9	MFLGFPTTK	hb_pig	1041.28	248.32	(1.69)	5
		hb_rab				
9	MFLSFPTTK	hb_bov	1071.31	254.66	(2.89)	8
		hb_hum				
		hb_sheep				
9	QLLLTADDR	aldol_rab	1044.18	264.51		1
9	QSALAELVK	albu_horse	958.13	238.41		1
9	QTALVELLK	albu_sheep	1014.24	246.39	(2.50)	2
9	QTALVELVK	HSA	1000.21	247.90		1
9	SAVTALWGK	hb_hum	932.09	229.36	(1.54)	2
		hb_rab				
9	SKGGVVGIK	aldol_rab	844.03	227.29		1
9	SLVSGLWGK	hb_dog	946.12	236.87		1
9	TDLNHENLK	crephos_rab	1083.17	258.47	(2.16)	3
9	TFQSFPTTK	hb_dog	1056.19	244.10	(1.36)	2
9	TGAPARSER	enolase_yst	944.02	239.16		1
9	TLSDYNIQK	ubiq	1081.20	258.99		1
9	VAAHAVVAR	conalb_chick	893.06	224.58	(2.42)	2
9	YFGYTGALR	conalb_chick	1047.19	250.59	(4.81)	3
10	AWGGKKENLK	aldol_rab	1130.32	265.36		1
10	DLFDPIIQDR	crephos_rab	1231.38	275.32	(2.20)	3
10	EAYKSEIAHR	albu_dog	1203.33	270.89	(0.00)	2
10	ECCEKPLLEK	HSA	1191.43	267.09		1
10	EKDIVGAVLK	alcodehy_yst	1071.29	253.92	(2.96)	3
10	FKDLGEEHFK	BSA	1249.40	282.95		1
10	FKDLGEENFK	HSA	1226.36	275.66	(0.71)	3
10	FKDLGEQYFK	albu_pig	1274.45	286.80	(0.18)	3
10	GVIFYESHGK	alcodehy_yst	1136.28	259.73	(2.27)	3
10	IGSEVYHNLK	enolase_yst	1159.31	264.63	(1.78)	3
10	KQSALAELVK	albu_horse	1086.30	252.69		1
10	KQTALVELLK	albu_pig	1142.41	267.73	(2.24)	8
		albu_sheep				
		BSA				
10	KQTALVELVK	HSA	1128.38	264.46		1
10	LLVVYPWTQR	hb_hum	1274.54	287.97	(2.67)	4
		hb_pig				
		hb_rab				
10	LVNELTEFAK	BSA	1163.34	266.65		1

10	LVNEVTEFAK	albu_horse	1149.32	261.00	(1.56)	3
		HSA				
10	SEEEYPDLSK	crephos_rab	1196.24	261.41	(1.98)	2
10	VLNSFSDGLK	hb_dog	1079.23	249.32	(0.48)	3
10	VLQSFSDGLK	hb_pig	1093.25	255.01	(2.35)	3
10	YNDLGEEHFR	albu_dog	1279.34	270.41	(0.71)	3
11	HKPHATEEQLR	albu_pig	1345.49	284.51	(1.83)	3
11	HKTDLNHENLK	crephos_rab	1348.49	295.16		1
11	HLVDEPQNLIK	albu_sheep	1305.50	290.36	(0.83)	4
		BSA				
11	HPDYSVSLLLR	albu_horse	1299.50	287.44	(0.31)	3
11	HPEYAVSVLLR	albu_sheep	1283.50	287.75	(3.00)	2
11	HQTVPQNTGGK	transfr_hum	1166.27	256.68	(4.86)	2
11	KVLDSFSNGMK	hb_bov	1225.43	269.78	(4.85)	3
		hb_sheep				
11	KVLQSFSDGLK	hb_pig	1221.43	290.65		1
11	LAKEYEATLEK	albu_dog	1294.47	255.81		1
11	LEQWAEEAVAR	glox_aspgn	1301.43	279.51	(3.87)	2
11	LFTGHPETLEK	myo_horse	1271.44	286.20	(4.02)	2
11	SASDLTWDNLK	transfr_hum	1249.35	277.98		1
11	SCQAQPTTMAR	kcas_bov	1193.40	267.63		1
11	TGPNLHGLFGR	cytc_horse	1168.33	267.56	(0.72)	3
11	TPEVDDEALEK	blacto_bov	1245.31	269.64	(4.98)	2
11	VGLSASTGLYK	conA	1095.27	253.96	(0.20)	2
11	VLSPADKTNIK	hb_rab	1185.39	263.79	(2.50)	2
12	AAFTECCQAADK	HSA	1257.41	269.89	(5.22)	2
12	AVMDDFAAFVEK	HSA	1342.54	275.89		1
12	DTDFKLNELRGK	apotransf_bov	1435.61	308.04	(0.23)	2
12	EETLMEYLENPK	cytc_horse	1495.67	312.71	(0.80)	3
12	EFTPPVQAAYQK	hb_hum	1378.55	289.31	(0.95)	2
12	EFTPVLQADFQK	hb_bov	1422.61	300.31	(2.37)	4
12	ENLKAAQEEYVK	aldol_rab	1421.58	308.18		1
12	FLANVSTVLTSK	hb_rab	1279.51	287.78	(0.33)	3
		hb_sheep				
12	FLASVSTVLTSK	hb_hum	1252.48	289.60	(2.14)	2
12	GQSIDDMIPAQK	crephos_rab	1302.47	279.24	(2.24)	3
12	GTEFTVNDLQGK	conalb_chick	1308.42	284.14	(1.72)	3
12	RHPEYAVSVLLR	albu_sheep	1439.69	313.44	(2.35)	4
		BSA				
12	SIGGEVFIDFTK	alcodehy_yst	1312.49	282.95	(4.08)	3
12	SISIVGSYVGNR	alcodehy_yst	1251.41	278.59	(1.60)	2
12	TVDMESTEVFTK	acas_bov	1386.54	294.42	(2.64)	2
12	TVLGNFSAFVAK	albu_horse	1253.47	282.48		1

12	VNQIGTLSESIK	enolase_yst	1288.47	278.95		1
12	VVAGVANALAHK	hb_dog	1149.37	272.31	(2.65)	14
		hb_hum				
		hb_pig				
		hb_rab				
		hb_sheep				
12	VYGRCELAAAMK	lys_tew	1311.59	283.85		1
13	CASIQKFGERALK	BSA	1450.73	319.03		1
13	CLQDGAGDVAFVK	lactotrans_bov	1322.51	284.08		1
13	FDKALKALPMHIR	blacto_bov	1539.91	297.70		1
13	GNPTVEVELTTEK	enolase_yst	1416.56	301.98	(2.86)	2
13	KGTEFTVNDLQGK	conalb_chick	1436.59	298.50	(3.64)	3
13	KVYGRCELAAAMK	lys_tew	1439.76	305.24		1
13	LGEYGFQNALIVR	albu_pig	1479.71	313.94	(3.30)	2
		BSA				
13	RFYRQLLLTADDR	aldol_rab	1666.91	325.91		1
13	SFLVWVNEEDHLR	crephos_rab	1643.83	341.65	(2.24)	3
13	TCVADESHAGCEK	BSA	1349.46	283.88		1
13	VKVDEVGAEALGR	hb_sheep	1342.52	285.25	(0.03)	2
13	VKVDEVGGEALGR	hb_bov	1328.50	285.58	(1.90)	4
13	VNVDEVGGEALGR	hb_dog	1314.43	287.12	(1.80)	7
		hb_hum				
		hb_pig				
13	VNVEEVGGEALGR	hb_rab	1328.45	286.28	(3.03)	3
13	VVGLSTLPEIYEK	alcodehy_yst	1447.70	310.43	(1.85)	2
14	APQVSTPTLVEIGR	albu_horse	1467.69	306.85	(1.58)	2
14	GILAADESTGSIAK	aldol_rab	1332.48	289.61	(3.75)	2
14	HGTVVLTALGGILK	myo_horse	1378.79	312.22	(0.49)	3
14	LDELRDEGKASSAK	HSA	1518.65	309.42		1
14	LSVEALNSLTGEFK	crephos_rab	1507.71	318.15	(2.52)	3
14	SAGWNIPIGTLLHR	conalb_chick	1534.79	315.82		1
14	TGQAPGFTYTDANK	cytc_horse	1470.60	297.61	(2.24)	3
14	TPEVDDEALEKFDK	blacto_bov	1635.75	333.91	(1.43)	2
14	VGTAHIIYNSVDKR	conA	1572.79	343.52	(1.21)	3
14	VVAGVANALAHRYH	hb_bov	1477.70	325.95		1
15	ANGTTVLVGMPAGAK	alcodehy_yst	1386.64	302.28		1
15	AVDDFLISLDGTANK	enolase_yst	1578.75	316.45		1
15	HQGLPQEVLNENLLR	acas_bov	1759.99	353.86		1
15	IGGHAGDYGGEALDR	hb_dog	1487.56	298.65	(0.89)	2
15	IGSHGGEYGAEAVER	hb_rab	1531.61	299.00	(0.81)	2
15	KAPQVSTPTLVEIGR	albu_horse	1595.87	330.12	(1.17)	2
15	KAPQVSTPTLVEISR	albu_sheep	1625.89	331.49	(1.37)	3
15	LCMGSGLNLCEPNNK	transfr_hum	1592.87	320.80	(0.05)	3

15	LGANAILGVSLAASR	enolase_yst	1412.66	310.74	(6.42)	2
15	LGHDFNPNVQAAFQK	hb_pig	1685.87	333.24	(0.91)	2
15	VEADIAGHGQEVLIR	myo_horse	1606.81	340.95	(1.00)	3
15	VGAHAGEYGAEALER	hb_hum	1529.64	306.47	(1.16)	2
15	VGGNAGAYGAEALER	hb_sheep	1434.54	288.98	(1.80)	3
15	VGGQAGAHGAEALER	hb_pig	1422.53	300.48	(2.81)	3
15	VLGIDGGEGKEELFR	alcodehy_yst	1618.81	354.90	(1.40)	3
15	YSHEEIAMATVTALR	aldol_rab	1691.93	335.42	(0.90)	3
16	GLSDGEWQQVLNVWGK	myo_horse	1816.01	352.48	(0.52)	2
16	HGGTIPIVPTAEFQDR	gludehy_bov	1737.94	335.66		1
16	HHGNEFTPVLQADFQK	hb_sheep	1868.05	353.50	(1.14)	3
16	LLGNVLVCVLAHHFGK	hb_hum	1720.12	318.03		1
16	NTDGSTDYGILQINSR	lys_tew	1753.85	330.83		1
16	SISIVGSYVGNRADTR	alcodehy_yst	1694.87	334.59	(1.85)	3
16	TITLEVEPSDTIENVK	ubiq	1787.99	360.05	(0.47)	2
16	TYFPHFDFTHGSEQIK	hb_rab	1954.14	363.50	(2.18)	3
16	TYFPHFDLSHGSAQVK	hb_bov	1834.03	364.16	(1.49)	9
		hb_hum				
		hb_sheep				
16	TYFPHFDLSPGSAQVK	hb_dog	1794.00	350.32	(1.56)	3
16	TYFPHFNLSHGSDQVK	hb_pig	1877.05	369.15		1
16	VLAAFSEGLSHLDNLK	hb_rab	1713.96	375.98	(3.62)	3
16	VLGAFSDGLAHLDNLK	hb_hum	1669.91	365.62	(1.48)	2
16	WLTGPQLADLYHSLMK	enolase_yst	1873.21	372.93	(1.77)	2
16	YLEFISDAIIHVLHSK	myo_horse	1885.20	404.45	(0.04)	2
17	AAQDSFAAGWGVMVSHR	enolase_yst	1789.99	371.96	(3.71)	2
17	GHHEAELKPLAQSHATK	myo_horse	1854.06	361.52		1
17	HPYFYGPELLFHAEEYK	albu_horse	2140.39	397.72	(1.79)	3
17	SGETEDTFIADLVVGLR	enolase_yst	1822.01	354.32	(5.38)	2
17	STHETNALHFMFNQFSK	conA	2039.26	384.39	(3.28)	3
17	TAGIQIVADDLTVTNPK	enolase_yst	1755.99	357.02		1
18	AKIIAEGANGPTTPQADK	gludehy_bov	1781.99	341.97	(4.73)	2
18	KGHHEAELKPLAQSHATK	myo_horse	1982.24	374.41		1
18	MLTAEEKAAVTAFWGKVK	hb_bov	1980.36	379.02	(4.54)	2
18	MLTAEEKAAVTGFWGKVK	hb_sheep	1966.33	357.38		1
18	SIVPSGASTGVHEALEMR	enolase_yst	1841.08	394.66	(1.36)	3
19	AHELLNTKLEQWAEEAVAR	glox_aspgn	2208.47	390.65		1
19	DMPIQAFLLYQEPVLGPVR	bcas_bov	2186.60	400.67		1
19	EPMIGVNQELAYFYPELFR	acas_bov	2316.66	405.63		1
19	FFDSFGDLSTPDAVMSNAK	hb_dog	2049.25	385.30	(2.98)	2
19	FFEHFGDLSNADAVMNNPK	hb_sheep	2153.36	393.23	(0.93)	3
19	FFESFGDLSNADAVMGNPK	hb_pig	2046.25	377.85	(0.96)	2
19	FFESFGDLSSANAVMNNPK	hb_rab	2075.29	381.63	(5.56)	3

19	FFESFGDLSTADAVMNNPK	hb_bov	2090.30	388.79	(1.76)	4
19	FFESFGDLSTPDAVMGNPK	hb_hum	2059.29	378.16		1
19	TVDYIIAGGGLTGLTTAAR	glox_aspgn	1850.11	366.03	(2.52)	2
20	IGEHTPSALAIMENANVLAR	aldol_rab	2107.42	399.25		2
20	VYVEELKPTPEGDLEILLQK	blacto_bov	2313.68	426.75	(2.14)	2
21	AAANFFSASCVPCADQSSFPK	apotransf_bov	2148.40	389.55		1
21	GTGGVDTAAVGSVFDISNADR	crephos_rab	2009.12	363.68	(1.95)	2
22	AVEHLDDLPGALSELSDLHAHK	hb_bov	2367.61	437.19	(2.50)	4
22	AVGHLDDLPGALSALSDLHAHK	hb_pig	2237.51	418.64	(0.31)	2
22	AVGHLDDLPGALSTLSDLHAHK	hb_rab	2267.53	422.37	(2.90)	2
22	AVGHLDDLPGTLSDLSDLHAHK	hb_sheep	2311.54	438.43	(3.25)	3
22	RGTGGVDTAAVGSVFDISNADR	crephos_rab	2165.31	387.93	(4.68)	2
22	TVGGKEDVIWELLNHAQEHFGK	apotransf_bov	2507.80	432.00		1
22	YTPSGQAGAAASESLFISNHAY	aldol_rab	2242.39	404.01		1
23	GVVPLAGTNGETTTQGLDGLSER	aldol_rab	2272.46	396.30	(3.46)	3
23	WSGFSGGAIECETAENTEECIAK	apotransf_bov	2432.62	412.48		1
24	ATDGGAHGVINVSVSEAAIEASTR	alcodehy_yst	2312.49	415.18	(1.48)	3
24	NLCNIPCSALLSSDITASVNCAKK	lys_tew	2465.89	412.61		1

[a]All values were obtained using an injected-ion mobility/time-of-flight technique. For a description, see: Hoaglund, C. S.; Valentine, S. J.; Sporleder, C. R.; Reilly, J. P.; Clemmer, D. E. *Anal. Chem.* **1998**, *70*, 2236; Henderson, S. C.; Valentine, S. J.; Counterman, A. E.; Clemmer, D. E., *Anal. Chem.* **1999**, *71*, 291.

[b]Peptide sequences correspond to fragments expected from tryptic digests as obtained from peptide_mass.pl [http://expasy.hcuge.ch/sprot/peptide-mass.html]. N-terminal acetylation is indicated by the prefix Ac.

[c]All proteins were obtained from Sigma and used without further purification. Purities were typically ≥70%. Tryptic digests were performed by addition of 150 μL of a 0.2 mg/mL trypsin (Sigma, sequencing grade) solution in 0.2 M ammonium bicarbonate (EM Science) to 0.5 mL of a 20 mg/mL solution of each protein. Protein names are abbreviated as follows: albumin (albu), alcohol dehydrogenase (alcodehy), alpha-casein (acas), aldolase (aldol), apotransferrin (apotransf), beta-casein (bcas), beta-lactoglobulin (blacto), bovine serum albumin (BSA), carbonic anhydrase (canhyd), conalbumin (conalb), concanavalin A (conA), creatine phosphokinase (crephos), cytochrome c (cytc), glucose dehydrogenase (gludehy), glucose oxidase (glox), hemoglobin (hb), human serum albumin (HSA), kappa-casein (kcas), lactotransferrin (lactotrans), lysozyme (lys), myoglobin (myo), transferrin (transfr), and ubiquitin (ubiq). The sources of the proteins are separated from the protein name by an underscore, and are abbreviated as follows: aspergillus niger (aspgn), bovine (bov), chicken (chick), human (hum), rabbit (rab), sperm whale (sw), turkey egg white (tew), and yeast (yst).

[d]Molecular weights are reported as an isotopic average and were checked by comparison with http://expasy.hcuge.ch/sprot/peptide-mass.html.

[e]Cross sections correspond to the average of multiple data sets. Uncertainties are given in parentheses and correspond to one standard deviation when three or more measurements were made, or as the range when only two measurements were made.

[f]Total number of separate observations and cross section measurements for each peptide sequence.