

Electronic supplementary Information

Characterization of mercury-containing protein in human plasma

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Table S1 Summary report of the peptide hits for HSA (human serum albumin) following the SwissProt database searching. The peptides were identified by HPLC-LTQ-FT after the tryptic digestion of the human plasma.

Peptide	Observed	Mr(expt)	Mr(calc)	Score
K.AACLLPK.L	386.72	771.4254	771.4313	47
K.LVTDLTK.V	395.2399	788.4652	788.4644	56
R.LSQRFPK.A	438.2588	874.5031	874.5025	25
K.AEFAEVSK.L	440.7245	879.4344	879.4338	56
K.YLYEIAR.R	464.2514	926.4883	926.4861	19
K.DDNPNLPR.L	470.7278	939.4411	939.441	47
R.LKCASLQK.F	474.2725	946.5305	946.527	14
K.DLGEENFK.A	476.22	950.4254	950.4345	44
K.FQNALLVR.Y	480.7861	959.5576	959.5552	51
K.TYETTLEK.C	492.7489	983.4833	983.4811	30
K.QTALVELVK.H	500.8066	999.5986	999.5964	86
K.LVAASQAALGL.-	507.3042	1012.5939	1012.5917	97
K.SLHTLFGDK.L	509.273	1016.5315	1016.5291	20
R.AFKAWAVAR.L	510.2942	1018.5738	1018.5712	46
K.CCKHPEAK.R	515.2655	1028.5165	1028.4532	8
K.LDELRDEGK.A	537.7758	1073.5371	1073.5353	50
R.NECFLQHK.D	538.2543	1074.4941	1074.4917	18
K.YLYEIARR.H	542.3024	1082.5902	1082.5872	20
K.KQTALVELVK.H	564.8531	1127.6917	1127.6914	70
K.KQTALVELVK.H	376.9051	1127.6935	1127.6914	63
K.KQTALVELVK.H	1128.7036	1127.6963	1127.6914	31
K.CCTESLVNR.R	569.7538	1137.493	1137.4907	39
K.KLVAASQAALGL.-	571.3525	1140.6905	1140.6866	85
R.DAHKSEVAHR.F	575.2931	1148.5716	1148.5686	63
K.LVNEVTEFAK.T	575.3097	1148.6048	1148.6077	24

K.CASLQKFGER.A	598.43	1194.8454	1194.5815	11
K.DVCKNYAEAK.D	399.8578	1196.5517	1196.5495	24
K.DVCKNYAEAK.D	599.2839	1196.5533	1196.5495	43
R.FKDLGEENFK.A	409.5	1225.4782	1225.5979	2
R.FKDLGEENFK.A	613.8075	1225.6004	1225.5979	39
R.FPKAEFAEVSK.L	626.79	1251.5654	1251.6499	3
R.FPKAEFAEVSK.L	418.22	1251.6382	1251.6499	25
K.ECCEKPLLEK.S	653.31	1304.6054	1304.6104	51
R.HPDYSVVLRL.L	656.38	1310.7454	1310.7347	45
K.AVMDDFAAFVEK.C	671.8239	1341.6333	1341.6275	51
K.AVMDDFAAFVEK.C	679.8203	1357.6259	1357.6224	49
R.LKCASLQKFGER.A	479.74	1436.1982	1435.7605	19
K.YICENQDSISSK.L	722.3261	1442.6377	1442.6347	61
R.ETYGEMADCCAK.Q	725.7689	1449.5233	1449.521	45
R.RHPDYSVVLRL.L	489.9536	1466.839	1466.8358	62
K.QTALVELVKHKPK.A	497.6409	1489.9009	1489.898	21
K.QTALVELVKHKPK.A	745.9609	1489.9073	1489.898	25
R.QIKKQTALVELVK.H	499.9847	1496.9323	1496.929	27
R.QIKKQTALVELVK.H	749.4739	1496.9333	1496.929	48
K.TCVADESAENCDK.S	749.7927	1497.5709	1497.5712	112
K.ADDKETCFAEEGK.K	750.3217	1498.6288	1498.6246	72
K.VPQVSTPTLVEVSR.N	504.6206	1510.84	1510.8355	35
K.VPQVSTPTLVEVSR.N	756.4281	1510.8417	1510.8355	66
K.LDELRDEGKASSAK.Q	506.9312	1517.7717	1517.7685	21
K.LDELRDEGKASSAK.Q	759.8942	1517.7738	1517.7685	43
K.LKECCEKPLLEK.S	516.2715	1545.7928	1545.7894	25
K.LKECCEKPLLEK.S	773.9044	1545.7943	1545.7894	57
K.DVFLGMFLYEYAR.R	812.396	1622.7774	1622.7803	54
K.ADDKETCFAEEGKK.L	543.2519	1626.7338	1626.7195	41
K.DVFLGMFLYEYAR.R	820.3968	1638.779	1638.7752	46

K.KVPQVSTPTLVEVSR.N	820.4727	1638.9308	1638.9305	104
K.KVPQVSTPTLVEVSR.N	547.3185	1638.9338	1638.9305	76
K.AEFAEVSKLVTDLTK.V	825.9526	1649.8906	1649.8876	99
K.AEFAEVSKLVTDLTK.V	550.9708	1649.8906	1649.8876	59
K.QNCELFEQLGEYK.F	829.3822	1656.7499	1656.7453	86
R.YKAAFTECCQAADK.A	831.8684	1661.7223	1661.7178	49
K.QEPERNECFLQHK.D	572.2722	1713.7946	1713.7893	26
K.QEPERNECFLQHK.D	857.91	1713.8054	1713.7893	44
R.HPYFYAPELLFFAK.R	581.6383	1741.8931	1741.8868	54
K.AACLLPKLDEL RDEGK.A	610	1826.9782	1826.956	44
K.EQLKAVMDDFAAFVEK.C	928.9585	1855.9024	1855.9026	29
K.EQLKAVMDDFAAFVEK.C	619.6448	1855.9125	1855.9026	21
R.RHPYFYAPELLFFAK.R	633.6727	1897.9964	1897.9879	58
R.HPYFYAPELLFFAKR.Y	633.6733	1897.998	1897.9879	49
R.RHPYFYAPELLFFAK.R	950.012	1898.0094	1897.9879	40
R.RPCFSALEVDETYVPK.E	637.6506	1909.9301	1909.9244	24
R.RPCFSALEVDETYVPK.E	955.9728	1909.931	1909.9244	37
K.SLHTLFGDKLCTVATLR.E	644.6868	1931.0387	1931.0299	37
K.SLHTLFGDKLCTVATLR.E	966.5276	1931.0406	1931.0299	75
R.NECFLQHKDDNPNLPR.L	666.32	1995.9382	1995.9221	36
R.NECFLQHKDDNPNLPR.L	999.19	1996.3654	1995.9221	1
R.FPKAEFAEVSKLVTDLTK.V	675.0466	2022.1179	2022.1037	61
R.YTKKVPQVSTPTLVEVSR.N	678.055	2031.1432	2031.1364	41
R.YTKKVPQVSTPTLVEVSR.N	1016.5795	2031.1445	2031.1364	71
K.VFDEFKPLVEEPQNLIK.Q	682.3723	2044.0949	2044.0881	44
K.VFDEFKPLVEEPQNLIK.Q	1023.0574	2044.1003	2044.0881	49
K.KVPQVSTPTLVEVSRNLGK.V	684.7344	2051.1813	2051.1739	32
R.RHPYFYAPELLFFAKR.Y	685.7084	2054.1033	2054.089	63
K.VHTECCHGDLLECADDR.A	696.39	2086.1482	2085.8303	7
K.EFNAETFTFHADICTLSEK.E	1130.5181	2259.0216	2259.0154	94

K.EFNAETFTFHADICTLSEK.E	754.0192	2259.0357	2259.0154	20
R.YKAAFTECCQAADKAACLLPK.L	806.0515	2415.1327	2415.1385	5
K.ALVLIAFAQYLQQCPFEDHVK.L	830.7728	2489.2967	2489.2777	50
K.EFNAETFTFHADICTLSEKER.Q	849.0629	2544.167	2544.1591	65
K.QNCELFEQLGEYKFQNALLVR.Y	867.1073	2598.3001	2598.29	22
K.QEPERNECFLQHKDDNPNLPR.L	879.4161	2635.2264	2635.2197	52
K.LVTDLTKVHTECCHGDLLECADDR.A	953.01	2856.0082	2856.2841	0
K.CCTESLVNRRPCFSALEVDETYVPK.E	1010.8114	3029.4124	3029.4045	8
K.TCVADESAENCCKSLHTLFGDKLCTVATLR.E	683.1272	3410.5996	3410.5905	6

Table S2 Amino acid sequence of HSA (human serum albumin) following the SwissProt database searching. The peptides identified by HPLC-LTQ-FT after the tryptic digestion of the human plasma are underlined and in red color. Sequence coverage of 77% could be obtained (471 identified of 609 known amino acids).

1-50

MKWVTFISLL FLSSAYSRG VFRRDAHKSE VAHRFKDLGE ENFKALVLIA

51-100

FAQYLQQCPE EDHVKLVNEV TEFAKTCVAD ESAENCCKSL HTLFGDKLCT

101-150

VATLRETYGE MADCCAKQEP ERNECFLOHK DDNPNLPRLV RPEVDVMCTA

151-200

FHDNEETFLK KYLYEIARRH PYFYAPELLE FAKRYKAAFT ECCQAADKAA

201-250

CLLPKLDELRL DEGKASSAKQ RLKCASLOKE GERAFKAWAV ARLSQRFPKA

251-300

EFAEVSKLVT DLTKVHTECC HGDLLECADD RADLAKYICE NQDSISSKLL

301-350

ECCEKPLLEK SHCIAEVEND EMPADLPSLA ADFVESKDVC KNYAEAKDVF

351-400

LGMFLYEYAR RHPDYSVLL LRLAKTYETT LEKCCAAADP HECYAKVFDE

401-450

FKPLVEEPQN LIKQNCLEFE QLGEYKFQNA LLVRYTKKVP QVSTPTLVEV

451-500

SRNLGKVGSK CCKHPEAKRM PCAEDYLSVV LNQLCVLHEK TPVSDRVTKC

501-550

CTESLVNRRP CFSALEVDET YVPKEFNAET FTFHADICTL SEKERQIKKQ

551-600

TALVELVKHK PKATKEQLKA VMDDEAAFE KCKKADDKET CFAEEGKKLV

601-609

AASQAALGL

Effects of Hg^{2+} to the free -SH in HSA

To study the effects of Hg^{2+} to the free -SH in HSA, different amount of Hg^{2+} ($0 - 2 \text{ mmol}^{-1}$) was added to 1 mmol^{-1} HSA in 100 mmol^{-1} PBS. Then the mixture was incubated at 37°C for one hour. The free -SH in the HSA was determined with hydrosulfuryl detection kit (A063, Nanjing jiancheng bioengineering institute, China), which was based on the Ellman's reagent, 5,5'-dithiobis(2-nitrobenzoic acid) (DTNB).