

Pattern-based Identification of Protein Structural Variations by Mass Spectrometry

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	Overview
0	Mass spectrometry is widely used for characterization of protein primary structure and structural changes, such as sequence mutations and post-translational modifications.
0	MALDI-TOF MS is effective for peptide mass mapping, and LC-MS/MS is a powerful technique for protein/peptide sequencing and for localizing the site of structural changes.
0	For human hemoglobin, many mutations and post- or co- translational modifications have been found associated to biological functions and disease states.
0	In this presentation, we demonstrate the pattern-based identification of peptide structural changes for MALDI-TOF MS data. These pattern changes can be in intensity or in isotopic peak distribution, or both.
0	LC-MS/MS measurements of these samples confirmed their identification based on the MS results.



	Amino A	cid Seque	ences of I	Human He	emoglobir	าร
	VLSPADKTNV	KAAWGKVGAH	AGEYGAEALE	RMFLSFPTTK	TYFPHFDLSH	GSAOVKGHGK
Ь	VHLTPEEKSA	VTALWGKVNV	DEVGGEALGR	LLVVYPWTOR	FFESFGDLST	PDAVMGNPKV
d	VHLTPEEKTA	VNALWGKVNV	DAVGGEALGR	LLVVYPWTOR	FFESFGDLSS	PDAVMGNPKV
g	VHLTPEEKSA	VTALWGKVNV	DEVGGEALGR	LLVVYPWTQR	FFESFGDLST	PDAVMGNPKV
61	K VADALTNAV	AHVDDMPNAL	SALSDLHAHK	L <mark>R</mark> VDPVNF <mark>K</mark> L	LSHCLLVTLA	AHLPAEFTPA
	KAHGKKVLGA	FSDGLAHLDN	LKGTFATLSE	LHCDKLHVDP	ENFRLLGNVL	VCVLAHHFG <mark>K</mark>
	KAHGKKVLGA	FSDGLAHLDN	LKGTF <mark>SQ</mark> LSE	LHCDKLHVDP	ENFRLLGNVL	VCVLARNFGK
	KAHGKKVLGA	FSDGLAHLDN	LKGTFATLSE	LHCDKLHVDP	ENFRLLGNVL	VCVLAHHFGK
121	VHASLDKFLA	SVSTVLTSKY	ર			
	EFTPPVQAAY	Q <mark>K</mark> VVAGVANA	LAHKYH			
	EFTP <mark>QM</mark> QAAY	QKVVAGVANA	LAHKYH			
	EFTPPVQAAY	QKVVAGVANA	LAHKYH			
Sma hen and the	all "single prot noglobin. Tryp gamma chain beta chain.	ein database" sin sites are s s are shown ir	of the 4 predo hown in red an blue. The sic	ominantly exp nd amino acid kle cell mutati	ressed chains differences in on E6V is loca	of human the delta tted in
For data fals	our proteomic abase search a e negatives/pc	es approach w approaches fai psitives and lin	e search agair I due to high c nits % coverag	ast these datal legree of hom ge.	bases as stand ology which re	lard esult in







click for	normalized	144	natched			natched	protein		nerg	
STORE STORE AND	0.925091	00001h.22	pepuses 11	20	25	preca(am)	Hamatohio hata zhaio	P02021	100	
	0.533420	38 835952	7	31	27		Henosdobin gamma-A and gamma-O chains.	P02096		Alpha: ~ 85%
	0.442625	31,998439	5	27	22		Hemoglobin alpha chain	P01922	1	
	0.440832	34 423548	7	31	26		Hemoglobin delta chain.	P02042	2	Beta: ~ 95%
ATPR HUMAH	0.261142	23.660857	4	35	27	-	ATP synthese coupling factor 6, mitochondeial p	P18859		
SYUR HUMAN	0.217761	22.611110	3	33	26	,	Synoretin (SR).	Q9N230		Delta: ~ 60%
2013 HUMAN	0.187658	12.702982	3	17	15	41	Zinc finger protein 18 (Zinc finger protein KOX	P17022		
KADA RUMAN	0.132759	29.403922	5	53	43	40	A denyinte kinase isoenzyne 4, mitochondrial (EC	P27144		Gamma: ~ 72
YEXS HUMAN	0.106000	13.834866	3	25	19	+:	Hypothetical 9.7 kDa protein DJ34821.3.	Q9Y530		
EFTI HUMAN	0.088882	18 142410	3	39	27		Eppin precurate	095925		_
ICA HUMAR	0.085066	17.315803	3	29	24	÷)	Alpha-locialbumn precursor (Lactose synthase B	P00709		
2N15 HUMAN	0.079493	9.941772	2	15	11		Zanc finger protein 15 (Zinc finger protein KOX	P17019		
REIL HUMAN	0.078647	32.583479	7	79	65		Phosphatidylinositol transfer protein alpha iso	Q00169		
APRI HIIMAN	0.073882	11.167204	2	15	12	-	Apoptosis related protein APR-2.	Q9Y5M1		
TEM4 HUMAN	0.069333	28,931924	5	87	69		Tropomyorin, fibroblast non-muscle type (Tropom	P07226		
KICO HUMAH	0.066771	40.321.497	7	89	78	÷.	Kernlin, type I cytoslotletal 15 (Cytoloratin 15	P19012		95% coverage
FILA HUMAN	0.063989	37.216181	6	83	70		Filaggin precursor (Fragment).	P20930		beta sickle E6
3R21 HUMAN	0.065035	24 257 501	4	59	49	+	Synaptoromal associated protein 25 (SNAP-25) (S	P13795		
HER BURGH	0.0551.52	16.341271	э	31	27	÷).	Henoglobin epsilon chain.	P02100		
SYUE HUMAN	0.046700	13.645227	4	25	18.	•	Beta-synaclein	Q16143		
								Trypein		
									Re-PI	ot



































