

EC & potential mess-shift & XIC overlap		Q->LVP55	Q->LVP55 & LVP59	Q->LVP55	Solvent outlier		Peptide		VP55 alone										VP55 + VP39									
VP55 expts	VP39 expts	VP55 expts	VP55 is solvent outlier	VP55 expts	VP39 expts	VP55 expts	Theor. RMs	Pos	Seq	#exp	Max mean %Deu	Mean SASA value	%SASA residues	Propn Exchangeable Hbonded	Tot Hbonds as Propn of Exchangeable	Max mean SASA %Deu/mean	Max mean proton free %Deu/mean	#exp	Max mean %Deu	Mean SASA value	%SASA residues	Propn Exchangeable Hbonded	Tot Hbonds as Propn of Exchangeable	Shared peptide	Max mean %Deu/ VP55 + VP39			
							636.34	59.63	FNKDFV	1	48.71	1.09	25	0.75	1.25	44.69	1.95	1	19.09	0	0	1.00	2.00	x	1.38			
							651.38	88.92	DRLSYF	3	26.38	0	0	1.00	2	infinite	infinite	1	7.24	1.38	75	0.60	0.75	x	1.63			
							654.33	446.450	EYKDSLS	2	45.27	0.62	33.33	0.5	0.75	79.47	0.99	1	7.54	0.36	20	0.60	1.00	x	1.65			
							689.31	187.202	CYGSYSLY	2	11.94	0.36	20	0.60	1.00	33.17	0.30	1	7.65	0	0	1.00	2.00	x	1.23			
							691.35	286.291	YKPTDF	1	3.91	0	0	0	0	infinite	infinite	2	35.57	0.87	40	0.80	1.20	x	0.93			
							718.39	148.153	ELARDMLN	3	9.40	0	0	1.00	2.00	infinite	infinite	1	45.51	NA	NA	NA	NA					
							737.39	220.225	TNSRTFLI	3	33.17	0.48	22.22	0.8	1.2	69.10	1.66	2	57.57	0.87	40	0.80	1.20	x	0.93			
							765.44	14.20	GLVPRGSHLM	1	58.63	2.41	40	0.60	1.00	24.33	1.47	1	53.38	0	0	0.60	0.60					
							783.4	58.63	VFNKDFV	1	7.06	NA	NA	NA	NA	NA	NA	1	43.09	0	0	0.67	0.83					
							784.34	408.413	MYTYSNTI	1	22.64	1.03	20	0.60	1.00	53.23	0.76	1	22.64	1.03	20	0.60	1.00	x	1.34			
							788.34	2.8	MGSRRHHH	1	7.06	NA	NA	NA	NA	NA	NA	1	43.09	0	0	0.67	0.83					
							816.5	274.280	MNVVPKFI	2	30.34	0.57	11.11	0.6	1	53.23	0.76	1	22.64	1.03	20	0.60	1.00	x	1.34			
							855.44	401.407	YLHNNMY	4	14.27	3.2	50	0.50	0.50	4.46	2.29	1	43.09	0	0	0.67	0.83					
							857.44	410.416	TYFSNTLL	3	42.39	3.24	42.86	0.29	0.29	13.50	0.60	1	43.09	0	0	0.67	0.83					
							869.46	198.175	MGRHVSLLV	1	48.83	3.14	42.86	0.29	0.29	13.50	0.60	1	43.09	0	0	0.67	0.83					
							877.42	267.273	FNRQDTMN	3	56.30	0.86	22.22	0.83	1	65.47	3.31	2	24.04	1.29	33.33	0.83	1.00	x	2.34			
							878.47	300.308	MFSGDRL	1	31.21	0	0	0.83	1.00	infinite	1.84	4	32.68	0	0	0.83	1.00	x	0.96			
							878.52	27.33	LKMETYGL	1	22.66	0.4	0	1.00	2.00	infinite	infinite	2	5.77	0	0	0.67	0.87	x	8.55			
							895.38	408.414	MYTYSNTI	1	49.36	0	0	0.67	0.67	infinite	1.84	1	26.86	NA	NA	NA	NA					
							909.49	12.20	S.SGLVPRGSHM	3	31.20	0	0	0.83	1.50	infinite	1.84	1	26.86	NA	NA	NA	NA					
							928.41	438.445	LYOMLTSGEY	1	55.56	0	0	1.00	1.33	infinite	infinite	2	48.04	0	0	1.00	1.57					
							932.51	286.293	YKPTDFLI	1	55.56	0	0	1.00	1.33	infinite	infinite	2	48.04	0	0	1.00	1.57					
							935.4	2.9	MGSRRHHH	1	55.56	0	0	1.00	1.33	infinite	infinite	2	48.04	0	0	1.00	1.57					
							935.4	2.9	MGSRRHHH	1	55.56	0	0	1.00	1.33	infinite	infinite	2	48.04	0	0	1.00	1.57					
							976.48	146.153	MEELARDMLN	2	16.12	0	0	0.86	1.57	infinite	1.15	1	17.27	0	0	0.86	1.57	x	0.93			
							980.57	243.260	LSKPYLNLV	3	62.69	0	0	0.67	0.67	infinite	1.91	2	46.43	0	0	0.67	0.67	x	1.36			
							986.52	11.20	H.SSGLVPRGSHM	1	40.67	NA	NA	NA	NA	NA	NA	1	40.67	NA	NA	NA	NA					
							1007.59	85.92	E.KDRLSYF	2	27.73	0	0	1.00	2	infinite	infinite	1	47.20	2.74	42.86	0.57	0.57	x	0.27			
							1018.5	404.407	YLHNNMY	1	12.95	2.74	42.86	0.57	0.57	4.73	0.30	1	23.99	0	0	1.00	1.63					
							1019.59	231.239	FLKPTGNLI	1	12.95	2.74	42.86	0.57	0.57	4.73	0.30	1	23.99	0	0	1.00	1.63					
							1024.49	325.302	LEYRYTHGI	1	26.74	2.25	50	0.13	0.13	11.44	0.30	1	30.67	0	0	0.86	1.57					
							1029.59	127.158	L.TKAPNVSRLK	2	21.29	0	0	1.00	2.00	infinite	infinite	1	32.73	2.25	50	0.13	0.13	x	0.79			
							1051.47	149.157	LARDMLNSMN	1	4.79	NA	NA	NA	NA	NA	NA	1	4.79	NA	NA	NA	NA					
							1072.46	2.10	MGSRRHHH	1	4.79	NA	NA	NA	NA	NA	NA	1	4.79	NA	NA	NA	NA					
							1090.58	482.496	INEXDIVF	3	34.55	0.05	12.5	0.63	1.13	691.00	0.93	1	39.01	0.44	25	0.00	0.00					
							1091.6	327.335	YRYTHGVDF	2	38.12	0.11	22.22	0.78	1.11	346.55	1.73	1	25.97	0.11	22.22	0.78	1.11	x	1.47			
							1096.57	286.293	YKPTDFLI	2	38.12	0.11	22.22	0.78	1.11	346.55	1.73	1	25.97	0.11	22.22	0.78	1.11	x	1.47			
							1107.54	357.365	TYTQDYFSEK	1	22.54	0.54	12.5	0.63	0.63	41.74	0.61	1	34.96	0.54	12.5	0.63	0.63	x	0.64			
							1117.57	398.407	EYKRONALY	1	21.91	2.4	37.5	0.63	0.63	9.13	0.59	4	35.15	0	0	0.88	1.25	x	1.11			
							1122.54	300.308	MFSGDRL	2	38.15	0	0	0.88	1.25	infinite	3.26	4	35.15	0	0	0.88	1.25	x	1.11			
							1133.59	32.41	TYLGRVPSVNEV	4	57.30	0.03	14.29	0.57	0.57	191.00	1.33	2	30.71	1.21	37.5	0.75	1.13					
							1153.64	243.261	L.SKPYLNLV	3	30.76	NA	NA	NA	NA	NA	NA	2	12.99	NA	NA	NA	NA	x	2.37			
							1159.49	2.11	MGSRRHHH	3	30.76	NA	NA	NA	NA	NA	NA	2	12.99	NA	NA	NA	NA	x	2.37			
							1165.63	203.211	YLNNRNYG	1	42.11	1.78	37.5	0.50	0.75	23.66	0.84	1	41.95	1.78	37.5	0.50	0.75	x	1.00			
							1174.62	204.213	YLNNRNYG	3	42.11	1.78	37.5	0.50	0.75	23.66	0.84	1	41.95	1.78	37.5	0.50	0.75	x	1.00			
							1186.64	347.356	CIDENRNYTV	3	28.80	0.59	22.22	0.78	1	50.51	1.35	2	30.32	0.59	22.22	0.78	1.00	x	0.98			
							1192.67	216.225	D.LKOTNSRTFLI	1	37.88	0.48	22.22	0.78	1.00	77.88	0.78	1	36.58	0.48	22.22	0.78	1.00	x	1.02			
							1203.64	176.185	L.NNNKMLEEY	1	34.74	0	0	0.89	1.67	infinite	3.16	1	19.77	0.4	22.22	0.00	0.00	x	1.76			
							1208.56	284.293	N.YTYSNTI	2	31.13	1.08	33.33	0.78	1.22	28.82	1.42	1	30.60	1.08	33.33	0.78	1.22	x	1.02			
							1234.64	31.41	E.TYGRVPSVNEV	3	37.92	0	0	0.89	1.33	infinite	3.45	1	30.74	NA	NA	NA	NA	x	1.46			
							1235.63	300.308	MFSGDRL	3	37.92	0	0	0.89	1.33	infinite	3.45	1	30.74	NA	NA	NA	NA	x	1.46			
							1246.52	2.12	MGSRRHHH	2	38.12	0.11	22.22	0.78	1.11	346.55	1.73	1	25.97	0.11	22.22	0.78	1.11	x	1.47			
							1247.63	42.51	E.YHMKSGARLI	2	38.12	0.11	22.22	0.78	1.11	346.55	1.73	1	25.97	0.11	22.22	0.78	1.11	x	1.47			
							1250.69	287.308	M.MKFSQDRL	2	27.68	0	0	0.86	1.57	infinite	2.56	1	30.74	NA	NA	NA	NA	x	1.24			
							1254.66	325.305	E.YRYTHGVDF	3	43.70	0.04	11.11	0.87	1.22	1092.50	1.32	4	26.40	0.04	11.11	0.87	1.22	x	1.66			
							1263.62	148.158	ELARDMLNSMN	1	16.74	0	0	1.00	1.80	infinite	infinite	2	22.66	0	0	0.86	1.57					
							1266.69	297.308	M.MKFSQDRL	2	22.66	0	0	0.86	1.57	infinite	infinite	2	22.66	0	0	0.86	1.57					
							1271.74	274.284	MNVVPKFI	1	28.58	2.72	44.44	0.56	0.78	10.51	0.65	4	42.65	0.02	12.5	0.63	0.63	x	1.05			
							1284.68	243.262	LSKPYLNLV	2	44.72	0.02	12.5	0.63	0.63	2236.00	1.21	4	27.36	1.58	33.33	0.44	0.56					
							1289.65	205.215	LYNNRNYG	4	53.78	3.67	55.56	0.44	0.44	14.65	0.96	3	49.25	3.67	55.56	0.44	0.44	x	1.09			
							1293.59	336.345	FDGKRNINPMKCI	4	53.78	3.67	55.56	0.44	0.44	14.65	0.96	3	49.25	3.67	55.56	0.44	0.44	x	1.09			