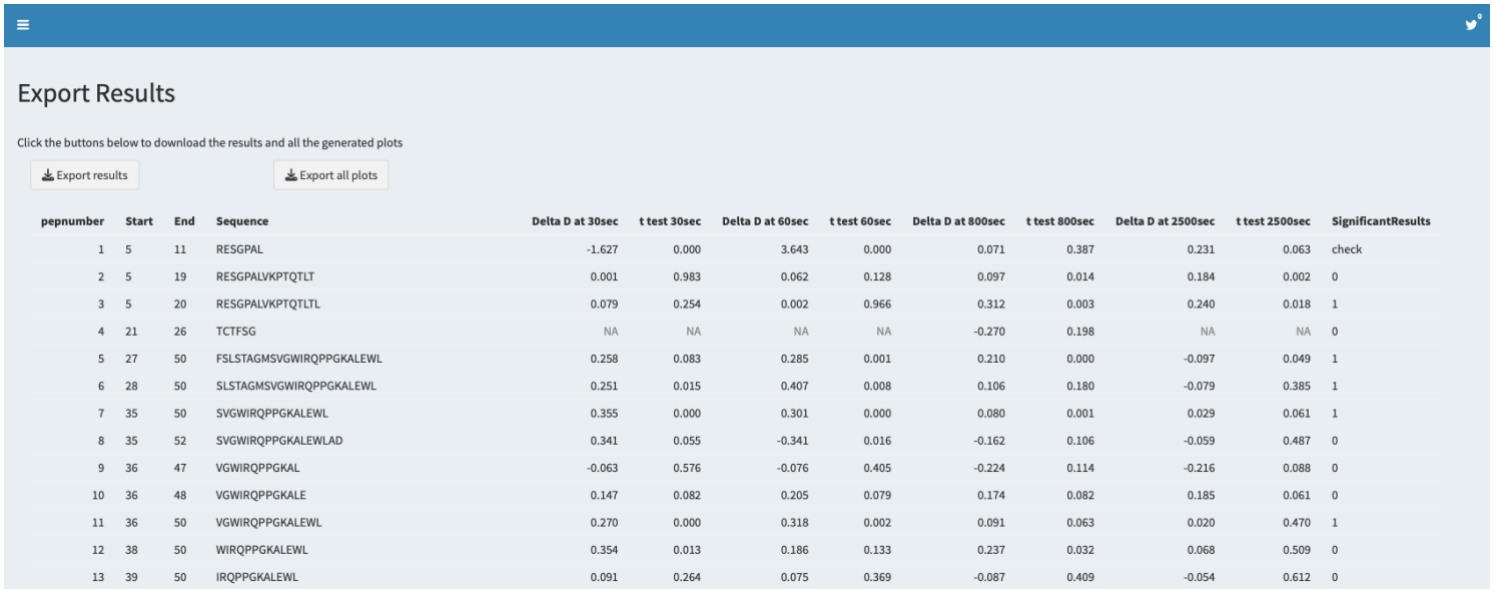
In the last tab, the user all the results can be exported.
First, a table show the basic results of the experiment with average deldaD values at each labeling timepoint and t-values from the Welch's t-test for each peptide. In the last column are the condensed results from the hybrid significant test. A number zero (0) means the peptide is non-significant. A number one means the peptide has at least one timepoint showing increased flexibility. Peptides with a negative number one are the ones with at least one timepoint showing increase in protection. Finally, if a peptide has the word "check" means is showing both increase and decrease flexibility at different timepoints.



Export Results

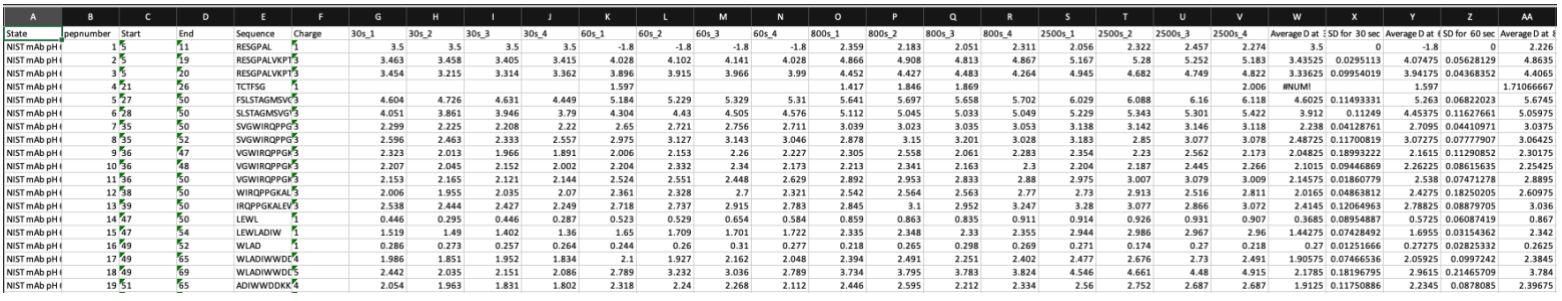
Click the buttons below to download the results and all the generated plots

Export results Export all plots

pepnumber	Start	End	Sequence	Delta D at 30sec	t test 30sec	Delta D at 60sec	t test 60sec	Delta D at 800sec	t test 800sec	Delta D at 2500sec	t test 2500sec	SignificantResults
1	5	11	RESGPAL	-1.627	0.000	3.643	0.000	0.071	0.387	0.231	0.063	check
2	5	19	RESGPALVKPTQTLT	0.001	0.983	0.062	0.128	0.097	0.014	0.184	0.002	0
3	5	20	RESGPALVKPTQTLTL	0.079	0.254	0.002	0.966	0.312	0.003	0.240	0.018	1
4	21	26	TCTFSG	NA	NA	NA	NA	-0.270	0.198	NA	NA	0
5	27	50	FSLSTAGMSVGWIRQPPGKALEWL	0.258	0.083	0.285	0.001	0.210	0.000	-0.097	0.049	1
6	28	50	SLSTAGMSVGWIRQPPGKALEWL	0.251	0.015	0.407	0.008	0.106	0.180	-0.079	0.385	1
7	35	50	SVGWIRQPPGKALEWL	0.355	0.000	0.301	0.000	0.080	0.001	0.029	0.061	1
8	35	52	SVGWIRQPPGKALEWLAD	0.341	0.055	-0.341	0.016	-0.162	0.106	-0.059	0.487	0
9	36	47	VGWIRQPPGKAL	-0.063	0.576	-0.076	0.405	-0.224	0.114	-0.216	0.088	0
10	36	48	VGWIRQPPGKALE	0.147	0.082	0.205	0.079	0.174	0.082	0.185	0.061	0
11	36	50	VGWIRQPPGKALEWL	0.270	0.000	0.318	0.002	0.091	0.063	0.020	0.470	1
12	38	50	WIRQPPGKALEWL	0.354	0.013	0.186	0.133	0.237	0.032	0.068	0.509	0
13	39	50	IRQPPGKALEWL	0.091	0.264	0.075	0.369	-0.087	0.409	-0.054	0.612	0

Two buttons are located at the top of the page. One ("Export all plots") will enable the user to download all the plots from the different tabs together in a compressed zip file, and the other ("Export results") button returns an excel spreadsheet with all the calculated results.

On the first sheet of the excel file, peptide number, start and end amino acid residue, sequence, charge, raw deuteration data, average deuteration and standard deviation for each labeling timepoint is displayed. Sheet two includes the same information but for protein state 2.



A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA
State	pepnumber	Start	End	Sequence	Charge	30s_1	30s_2	30s_3	30s_4	60s_1	60s_2	60s_3	60s_4	800s_1	800s_2	800s_3	800s_4	2500s_1	2500s_2	2500s_3	2500s_4	Average D at	SD for 30 sec	Average D at	SD for 60 sec	Average D at
NIST mAb pH	1	5	11	RESGPAL	1	3.5	3.5	3.5	3.5	-1.8	-1.8	-1.8	-1.8	2.359	2.183	2.051	2.311	2.056	2.322	2.457	2.274	3.5	0	-1.8	0	2.226
NIST mAb pH	2	5	19	RESGPALVKPT	3	3.463	3.458	3.405	3.415	4.028	4.102	4.141	4.028	4.866	4.908	4.813	4.867	5.167	5.28	5.252	5.183	3.43525	0.0295113	4.07475	0.05628129	4.8635
NIST mAb pH	3	5	20	RESGPALVKPT	3	3.454	3.215	3.314	3.362	3.896	3.915	3.966	3.99	4.452	4.427	4.483	4.264	4.945	4.682	4.749	4.822	3.33625	0.09954019	3.94175	0.04368352	4.4065
NIST mAb pH	4	21	26	TCTFSG	1					1.597				1.417	1.846	1.869					2.006	#NUM!		1.597		1.71066667
NIST mAb pH	5	27	50	FSLSTAGMSVG	3	4.604	4.726	4.631	4.449	5.184	5.229	5.329	5.31	5.641	5.697	5.658	5.702	6.029	6.088	6.16	6.118	4.6025	0.11493331	5.263	0.06822023	5.6745
NIST mAb pH	6	28	50	SLSTAGMSVG	3	4.051	3.861	3.946	3.79	4.304	4.43	4.505	4.576	5.112	5.045	5.033	5.049	5.229	5.343	5.301	5.422	3.912	0.11249	4.45375	0.11627661	5.05975
NIST mAb pH	7	35	50	SVGWIRQPPG	3	2.299	2.225	2.208	2.22	2.65	2.721	2.756	2.711	3.039	3.023	3.035	3.053	3.138	3.142	3.146	3.118	2.238	0.04128761	2.7095	0.04410971	3.0375
NIST mAb pH	8	35	52	SVGWIRQPPG	3	2.596	2.463	2.333	2.557	2.975	3.127	3.143	3.046	2.878	3.15	3.201	3.028	3.183	2.85	3.077	3.078	2.48725	0.11700819	3.07275	0.07777907	3.06425
NIST mAb pH	9	36	47	VGWIRQPPG	3	2.323	2.013	1.966	1.891	2.006	2.153	2.26	2.227	2.305	2.558	2.061	2.283	2.354	2.23	2.562	2.173	2.04825	0.18993222	2.1615	0.11290852	2.30175
NIST mAb pH	10	36	48	VGWIRQPPGK	3	2.207	2.045	2.152	2.002	2.204	2.332	2.34	2.173	2.213	2.341	2.163	2.3	2.204	2.187	2.445	2.266	2.1015	0.09446869	2.26225	0.08615635	2.25425
NIST mAb pH	11	36	50	VGWIRQPPGK	3	2.153	2.165	2.121	2.144	2.524	2.551	2.448	2.629	2.892	2.953	2.833	2.88	2.975	3.007	3.079	3.009	2.14575	0.01860779	2.538	0.07471278	2.8895
NIST mAb pH	12	38	50	WIRQPPGKAL	3	2.006	1.955	2.035	2.07	2.361	2.328	2.7	2.321	2.542	2.564	2.563	2.77	2.73	2.913	2.516	2.811	2.0165	0.04863812	2.4275	0.18250205	2.60975
NIST mAb pH	13	39	50	IRQPPGKALEW	3	2.538	2.444	2.427	2.249	2.718	2.737	2.915	2.783	2.845	3.1	2.952	3.247	3.28	3.077	2.866	3.072	2.4145	0.12064963	2.78825	0.08879705	3.036
NIST mAb pH	14	47	50	LEWL	1	0.446	0.295	0.446	0.287	0.523	0.529	0.654	0.584	0.859	0.863	0.835	0.911	0.914	0.926	0.931	0.907	0.3685	0.08954887	0.5725	0.06087419	0.867
NIST mAb pH	15	47	54	LEWLADIW	1	1.519	1.49	1.402	1.36	1.65	1.709	1.701	1.722	2.335	2.348	2.33	2.355	2.944	2.986	2.967	2.96	1.44275	0.07428492	1.6955	0.03154362	2.342
NIST mAb pH	16	49	52	WLAD	1	0.286	0.273	0.257	0.264	0.244	0.26	0.31	0.277	0.218	0.265	0.298	0.269	0.271	0.174	0.27	0.218	0.27	0.01251666	0.27275	0.02825332	0.2625
NIST mAb pH	17	49	65	WLADIWWDD	4	1.986	1.851	1.952	1.834	2.1	1.927	2.162	2.048	2.394	2.491	2.251	2.402	2.477	2.676	2.73	2.491	1.90575	0.07466536	2.05925	0.0997242	2.3845
NIST mAb pH	18	49	69	WLADIWWDD	5	2.442	2.035	2.151	2.086	2.789	3.232	3.036	2.789	3.734	3.795	3.783	3.824	4.546	4.661	4.48	4.915	2.1785	0.18196795	2.9615	0.21465709	3.784
NIST mAb pH	19	51	65	ADIWWDDKK	4	2.054	1.963	1.831	1.802	2.318	2.24	2.268	2.112	2.446	2.595	2.212	2.334	2.56	2.752	2.687	2.687	1.9125	0.11750886	2.2345	0.0878085	2.39675

Sheet 3 contains all the statistical parameters used during calculations, such as the pooled standard deviation, the standard error of the mean, the significance level, the t value used to calculate the threshold and the actual global statistical threshold. Additionally, contains a small reminder of the coloring scheme used in the representations to identify significant peptides.

A	B	C	D	E	F	G	H	I	J
PooledSD	StrdErrorMea	alpha	tValUsed	StatisticalThreshold					
0.105052309	0.0742832	0.01	3.70742802	0.27539962					
Positive deltaD values (State2-State ref) means increase in flexibility by state 2 compared to the reference (Peptides colored as red)									
Negative deltaD values (State2-State ref) means increase in protection by state 2 (Peptides colored as blue)									
Peptides presenting protection and deprotection at different labeling times are colored as yellow (Check data in HDExaminer)									

Sheet 4 contains the same table displayed at the beginning. Average deldaD values at each labeling timepoint and t-values from the Welch's t-test for each peptide plus the summary of the hybrid significance test. Additionally, peptides considered significant will be colored. Red for peptides with increased flexibility, blue for peptides with increased protection and peptides colored yellow are the ones showing mixed behavior. Note that for a peptide to be considered significant at least one the labeling timepoints must be significant. Numbers in bold are the ones that failed the hybrid significance test.

A	B	C	D	E	F	G	H	I	J	K	L	M	N
pepnumber	Start	End	Sequence	Delta D at 30s	t test 30sec	Delta D at 60s	t test 60sec	Delta D at 80(	t test 800sec	Delta D at 25(	t test 2500sec	SignificantResults	
1	5	11	RESGPAL	**-1.6265**	**0.00013307**	**3.64325**	**1.1978E-06**	0.071	0.38708572	0.2305	0.06265032	check	
2	5	19	RESGPALVKPT	0.0005	0.98338704	0.06175	0.12752003	0.09725	0.01420546	0.184	0.00221591	0	
3	5	20	RESGPALVKPT	0.0795	0.25375516	0.00225	0.96611825	**0.312**	**0.00301816**	0.23975	0.01801373	1	
4	21	26	TCTFSG					-0.2701667	0.19827077			0	
5	27	50	FSLSTAGMSVG	0.2585	0.08329361	**0.285**	**0.00093581**	0.2095	0.00027776	-0.09725	0.04912632	1	
6	28	50	SLSTAGMSVG	0.25125	0.01496914	**0.407**	**0.00752667**	0.10625	0.18034452	-0.079	0.38487604	1	
7	35	50	SVGWIRQPPG	**0.35475**	**5.1353E-05**	**0.30125**	**0.00019713**	0.07975	0.00085292	0.02875	0.06128473	1	
8	35	52	SVGWIRQPPG	0.341	0.05494845	-0.3415	0.01625308	-0.162	0.10596959	-0.05875	0.48740858	0	
9	36	47	VGWIRQPPGK	-0.0635	0.57605315	-0.076	0.40529894	-0.22425	0.114213	-0.2160833	0.08782909	0	
10	36	48	VGWIRQPPGK	0.14675	0.08241251	0.2055	0.07872732	0.174	0.08179632	0.18475	0.06126488	0	
11	36	50	VGWIRQPPGK	0.26975	1.684E-06	**0.318**	**0.00185362**	0.0905	0.06318118	0.01975	0.47000406	1	
12	38	50	WIRQPPGKAL	0.35425	0.01275498	0.1865	0.13333858	0.23675	0.0319014	0.06825	0.5089168	0	
13	39	50	IRQPPGKALEV	0.09075	0.26381961	0.075	0.36915329	-0.087	0.40858835	-0.05425	0.61224656	0	
14	47	50	LEWL	0.1335	0.05622341	0.1595	0.00711418	-0.069	0.01437324	-0.10425	0.05749376	0	
15	47	54	LEWLADIW	0.03375	0.45135739	0.0975	0.00603881	**0.2755**	**6.9897E-05**	0.1585	0.00607089	1	
16	49	52	WLAD	-0.0755	0.00431502	-0.115	0.00154843	-0.15175	0.00273822	-0.07575	0.12256706	0	
17	49	65	WLADIWWDD	0.03225	0.58889962	0.06625	0.40044404	0.0975	0.20479812	0.25675	0.02150135	0	
18	49	69	WLADIWWDD	0.2895	0.04538516	0.1975	0.18028856	**0.32175**	**8.5823E-05**	0.19725	0.14646982	1	
19	51	65	ADIWWDDKK	0.06325	0.38595028	0.03525	0.67708494	0.17675	0.11540635	0.16375	0.06690555	0	

Finally, in the last sheet are the k-means clustering results, average deuteration and t-value from the Welch's t-test at each labeling timepoint for all peptides. Timepoints in cluster 1 are considered insignificant, timepoints in cluster 2 are considered intermediate effects and timepoints located in cluster 3 are considered strong effects.

Additional information such as cluster sizes, cluster limits and number of iterations are also included here.

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V
pepnumber	Start	End	Sequence	Delta D at 30s	Cluster30sec	t test30sec	Delta D at 60s	Cluster60sec	t test60sec	Delta D at 80(	Cluster800sec	t test800sec	Delta D at 25(	Cluster2500si	t test2500sec						
1	5	11	RESGPAL	-1.6265	3	0.00013307	3.64325	3	1.1978E-06	0.071	1	0.38708572	0.2305	1	0.06265032	Cluster sizes					
2	5	19	RESGPALVKPT	0.0005	1	0.98338704	0.06175	1	0.12752003	0.09725	1	0.01420546	0.184	1	0.00221591	7113	2753	574			
3	5	0	RESGPALVKPT	0.0795	1	0.25375516	0.00225	1	0.96611825	0.312	1	0.00301816	0.23975	1	0.01801373	Cluster 1 (abs	From 0 to 0.0317				
4	1	6	TCTFSG		1			1		-0.2701667	1	0.19827077		1		Cluster 2 (abs	From 0.0317 to 0.0865				
5	7	0	FSLSTAGMSVG	0.2585	1	0.08329361	0.285	1	0.00093581	0.2095	1	0.00027776	-0.09725	1	0.04912632	Cluster 3 (abs	From 0.0865 to max value				
6	8	0	SLSTAGMSVG	0.25125	1	0.01496914	0.407	1	0.00752667	0.10625	1	0.18034452	-0.079	1	0.38487604	k-means clust	3				
7	5	0	SVGWIRQPPG	0.35475	1	5.1353E-05	0.30125	1	0.00019713	0.07975	1	0.00085292	0.02875	1	0.06128473	Datapoints in cluster 1 are considered insignificant or negligible within your dataset					
8	5	2	SVGWIRQPPG	0.341	1	0.05494845	-0.3415	1	0.01625308	-0.162	1	0.10596959	-0.05875	1	0.48740858	Datapoints in cluster 2 are intermediate effects within your dataset					
9	6	7	VGWIRQPPGK	-0.0635	1	0.57605315	-0.076	1	0.40529894	-0.22425	1	0.114213	-0.2160833	1	0.08782909	Datapoints in cluster 3 are strong effects within your dataset					
10	6	8	VGWIRQPPGK	0.14675	1	0.08241251	0.2055	1	0.07872732	0.174	1	0.08179632	0.18475	1	0.06126488						
11	6	0	VGWIRQPPGK	0.26975	1	1.684E-06	0.318	1	0.00185362	0.0905	1	0.06318118	0.01975	1	0.47000406						
12	8	0	WIRQPPGKAL	0.35425	1	0.01275498	0.1865	1	0.13333858	0.23675	1	0.0319014	0.06825	1	0.5089168						
13	9	0	IRQPPGKALEV	0.09075	1	0.26381961	0.075	1	0.36915329	-0.087	1	0.40858835	-0.05425	1	0.61224656						
14	7	0	LEWL	0.1335	1	0.05622341	0.1595	1	0.00711418	-0.069	1	0.01437324	-0.10425	1	0.05749376						
15	7	4	LEWLADIW	0.03375	1	0.45135739	0.0975	1	0.00603881	0.2755	2	6.9897E-05	0.1585	1	0.00607089						
16	9	2	WLAD	-0.0755	1	0.00431502	-0.115	1	0.00154843	-0.15175	1	0.00273822	-0.07575	1	0.12256706						
17	9	5	WLADIWWDD	0.03225	1	0.58889962	0.06625	1	0.40044404	0.0975	1	0.20479812	0.25675	1	0.02150135						
18	9	9	WLADIWWDD	0.2895	1	0.04538516	0.1975	1	0.18028856	0.32175	1	8.5823E-05	0.19725	1	0.14646982						
19	1	5	ADIWWDDKK	0.06325	1	0.38595028	0.03525	1	0.67708494	0.17675	1	0.11540635	0.16375	1	0.06690555						