

Table S1: Average number of deuterons incorporated in Sse1 in the presence and absence of nucleotide

PEPTIDE			DATASET 1				DATASET 2		
Start	End	Mass (exp) [Da]	HX time	10s	2 min	100%	HX time	2 min	100%
2	16	1546.8	nucl.-free	N.D.	N.D.	N.D.	nucl.-free	8.5	8.6
			ADP 1 mM ⁽¹⁾	N.D.	N.D.		ADP 1 mM ⁽¹⁾	4.9	
			ATP 100 uM	N.D.	N.D.		ATP 1 mM	1.3	
17	25	970.5		5.3	5.7	6.0		6.0	6.2
				4.4	4.8			5.3	
				3.5	4.3			4.8	
69	75	813.5		3.6	3.8	4.3		4.3	4.0
				1.9	2.7			N.D.	
				1.0	1.8			2.3	
69	81	1609.8		5.7	5.2	5.9		6.1	6.0
				2.3	3.6			3.5	
				0.9	2.1			2.4	
75	92	2244.0		9.4	9.4	10.4		9.6	9.7
				7.4	9.1			8.0	
				4.0	6.5			7.0	
76	81	814.3		0.9	3.6	3.5		N.D.	N.D.
				0.5	0.6			N.D.	
				0.2	0.5			N.D.	
93	106	1605.9		7.7	9.1	8.2		N.D.	N.D.
				5.0	5.2			N.D.	
				1.1	2.7			N.D.	
104	118	1688.9		9.2	8.9	9.6		10.9	N.D.
				8.6	7.6			10.0	
				3.9	6.6			9.3	
107	118	1286.7		6.9	7.2	7.6		N.D.	N.D.
				4.7	5.9			N.D.	
				2.7	4.6			N.D.	
122	140	2178.2		11.5	11.9	12.4		N.D.	N.D.
				8.4	9.8			N.D.	
				6.3	8.1			N.D.	
122	142	2380.4		11.3	11.8	19.5		13.0	N.D.
				7.0	9.6			10.8	
				6.3	8.2			9.2	
123	142	2233.2		10.8	11.8	21.3		12.5	N.D.
				8.6	9.8			10.5	
				6.6	8.4			9.5	
143	152	1203.6		0.7	1.7	5.5		N.D.	N.D.
				0.7	1.5			N.D.	
				0.8	1.1			N.D.	
143	159	2064.0		0.9	2.0	11.5		2.7	N.D.
				0.8	1.8			2.3	
				0.8	1.4			1.9	
153	159	878.4		0.1	0.3	4.2		0.7	N.D.
				0.1	0.2			0.2	

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			0.1	0.2		0.3	
160	174	1577.9	0.7	1.6	10.7	2.0	N.D.
			0.6	1.4		1.7	
			0.4	1.0		1.3	
160	177	1849.0	0.4	1.5	13.2	1.5	N.D.
			0.3	1.2		1.1	
			0.3	0.9		0.9	
160	182	2326.2	0.4	1.3	N.D.	N.D.	N.D.
			0.2	0.9		N.D.	
			0.0	0.6		N.D.	
186	200	1680.9	3.8	4.5	8.2	4.9	8.4
			3.8	4.3		4.7	
			3.9	4.5		4.8	
186	201	1828.0	3.6	4.2	8.8	4.5	8.9
			3.8	4.2		4.6	
			3.8	4.3		4.6	
201	214	1558.7	0.9	2.7	N.D.	2.9	N.D.
			0.4	0.5		0.3	
			0.3	0.4		0.2	
202	211	1080.5	1.0	2.3	N.D.	3.0	N.D.
			0.2	0.6		1.1	
			0.0	0.2		0.6	
202	212	1167.5	1.1	2.6	11.0	3.0	8.9
			0.5	0.6		0.8	
			0.2	0.3		0.3	
202	214	1411.6	0.9	2.5	N.D.	N.D.	N.D.
			0.2	0.7		N.D.	
			0.1	0.1		N.D.	
202	215	1482.7	1.0	2.3	9.4	3.0	N.D.
			0.4	0.7		1.4	
			0.1	0.2		1.1	
215	236	2375.3	5.2	6.5	N.D.	7.1	N.D.
			2.8	4.5		5.2	
			2.6	4.1		4.2	
215	239	2750.4	6.6	8.0	17.9	9.4	N.D.
			2.4	4.8		5.9	
			2.3	3.6		4.3	
216	236	2304.2	4.8	6.2	N.D.	7.3	N.D.
			2.6	4.4		4.9	
			2.3	3.5		4.1	
239	248	1144.6	4.6	5.0	5.6	6.5	N.D.
			0.2	2.1		2.2	
			0.1	0.5		0.5	
240	248	1031.5	3.6	3.9	4.3	4.4	4.4
			0.3	1.9		2.1	
			0.2	0.7		1.1	
240	249	1178.5	4.6	5.2	4.8	5.5	N.D.
			0.4	1.5		2.0	
			0.4	1.1		1.2	
241	248	960.4	2.7	2.8	3.2	3.4	3.3
			0.3	1.4		1.7	
			0.3	0.5		1.1	
249	269	2610.5	12.3	13.8	14.5	15.1	15.8

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			3.7	8.8		10.0	
			3.4	7.6		8.3	
270 289	2116.2		11.7	13.6	14.1	14.1	N.D.
			5.0	8.4		8.8	
			4.7	6.5		6.2	
290 301	1292.6		7.2	7.5	7.8	8.0	8.1
			4.0	6.0		6.3	
			3.8	5.3		5.6	
293 301	975.5		5.2	5.3	5.5	N.D.	N.D.
			2.2	4.0		N.D.	
			2.1	3.1		N.D.	
295 308	1618.8		6.6	8.8	9.6	9.9	N.D.
			2.7	4.7		4.9	
			2.6	3.8		4.0	
307 314	939.6		1.4	3.7	4.2	4.2	N.D.
			0.1	1.0		1.0	
			0.1	0.8		0.8	
307 315	1068.6		1.8	4.9	5.1	4.7	N.D.
			0.3	1.5		1.3	
			0.3	1.3		1.2	
308 / 314 / 309 315	810.5		1.6	3.3	3.6	3.5	3.6
			0.4	1.5		1.7	
			0.2	1.2		1.6	
315 330	1753.0		2.5	2.9	11.9	2.7	N.D.
			1.3	2.1		2.1	
			0.9	1.9		1.8	
315 332	1911.1		2.7	4.4	13.2	4.7	N.D.
			1.8	2.9		3.3	
			1.8	3.0		3.4	
315 337	2530.3		3.9	5.4	17.3	N.D.	N.D.
			2.7	4.2		N.D.	
			2.7	4.0		N.D.	
337 357	2259.2		9.9	11.0	15.1	12.4	15.1
			3.1	1.7		5.0	
			2.2	1.9		2.0	
338 357	2112.2		9.7	12.1	14.5	12.6	N.D.
			2.3	5.4		5.3	
			1.5	1.9		1.8	
358 366	962.5		3.9	5.0	5.2	5.4	5.4
			2.3	4.2		4.4	
			2.0	4.0		4.3	
358 377	2031.1		6.2	N.D.	N.D.	N.D.	N.D.
			4.8	N.D.		N.D.	
			4.6	N.D.		N.D.	
358 378	2178.1		7.3	10.6	15.0	N.D.	N.D.
			5.0	7.7		N.D.	
			4.7	7.6		N.D.	
367 377	1086.5		2.7	5.5	6.7	6.5	6.8
			1.7	3.5		3.7	
			1.4	2.5		2.6	
367 378	1233.6		2.5	6.0	7.6	7.0	7.6
			1.4	3.2		3.9	
			1.2	2.3		2.6	

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379	387	953.5	3.1	4.3	7.2	4.8	14.4
			2.9	3.4		3.8	
			2.9	3.2		3.6	
388	394	948.6	2.4	3.2	3.4	3.9	3.8
			2.5	3.2		3.6	
			2.5	3.3		4.0	
388	403	1976.0	3.3	4.9	9.2	5.3	N.D.
			3.2	5.0		5.3	
			3.3	5.4		5.7	
388	404	2139.1	3.1	4.9	10.0	N.D.	N.D.
			3.1	4.9		N.D.	
			3.2	5.3		N.D.	
395	403	1045.5	0.7	1.4	4.5	1.1	N.D.
			0.7	1.7		1.4	
			0.8	2.0		1.9	
395	404	1208.5	0.9	1.6	5.5	N.D.	N.D.
			0.6	1.8		N.D.	
			0.7	1.9		N.D.	
404	416	1680.7	4.6	5.7	7.4	6.3	8.0
			4.4	5.4		5.9	
			4.3	5.3		5.9	
405	416	1517.6	4.7	5.5	6.5	6.1	N.D.
			4.5	5.4		6.0	
			4.5	5.3		6.0	
417	430	1465.7	3.1	4.3	7.2	4.7	7.3
			3.1	4.1		4.5	
			3.1	4.3		4.8	
431	439	1035.5	1.1	2.3	5.5	2.5	5.7
			1.0	2.4		2.6	
			0.9	2.4		2.7	
431	444	1482.7	1.3	2.8	9.7	3.4	N.D.
			1.3	2.7		3.1	
			1.3	2.8		3.1	
434	441	926.4	0.9	1.8	4.6	2.1	4.6
			0.8	1.6		1.9	
			0.8	1.6		1.9	
434	442	997.4	0.7	1.7	5.6	1.8	N.D.
			0.6	1.6		1.9	
			0.6	1.6		2.1	
434	444	1155.5	0.8	1.8	6.8	2.0	6.6
			0.7	1.8		1.9	
			0.7	1.7		1.8	
445	458	1615.8	3.6	5.9	7.0	N.D.	N.D.
			3.5	5.7		N.D.	
			3.4	5.8		N.D.	
445	462	2100.0	3.8	6.3	9.8	5.9	10.1
			3.3	6.0		5.6	
			3.3	6.1		5.4	
446	462	1937.0	2.3	5.2	9.4	N.D.	N.D.
			2.2	4.8		N.D.	
			2.7	4.4		N.D.	
463	482	2149.2	3.5	5.1	12.8	5.7	8.4
			3.5	5.0		5.5	

Table S1

			3.5	5.0		5.4	
463	489	2877.5	4.0	6.2	13.8	N.D.	N.D.
			3.6	5.8		N.D.	
			3.8	5.7		N.D.	
501	516	1790.9	4.0	6.1	6.7	N.D.	N.D.
			4.0	5.9		N.D.	
			3.7	6.3		N.D.	
503	516	1548.7	3.0	4.7	5.0	N.D.	N.D.
			3.3	4.7		N.D.	
			3.1	4.8		N.D.	
503	519	1876.8	5.0	6.7	7.2	7.7	N.D.
			5.2	6.6		7.0	
			5.2	6.8		7.3	
521	533	1548.9	3.9	6.6	7.8	6.3	7.5
			4.5	6.4		7.2	
			4.6	6.6		7.2	
534	550	1869.0	4.8	9.9	11.6	8.2	11.7
			5.0	8.1		8.0	
			4.0	6.8		6.8	
551	563	1559.8	7.9	8.1	8.5	6.8	7.2
			4.0	5.0		6.3	
			0.9	1.6		N.D.	
557	563	817.4	4.0	3.8	3.7	N.D.	N.D.
			4.0	3.9		N.D.	
			0.6	1.6		N.D.	
564	576	1532.7	5.8	7.5	7.9	7.3	7.0
			5.8	6.9		7.5	
			5.9	6.8		7.4	
577	585	1125.7	1.3	6.0	6.4	6.4	6.6
			0.8	4.8		5.3	
			0.7	3.8		4.4	
579	585	849.5	1.2	5.4	5.7	5.7	N.D.
			0.9	4.1		4.7	
			0.7	3.4		4.0	
596	610	1688.9	5.4	10.3	10.6	N.D.	N.D.
			3.4	8.9		N.D.	
			1.2	8.0		N.D.	
613	631	2281.1	8.3	12.1	12.6	13.0	N.D.
			7.9	11.7		12.6	
			6.9	11.7		12.4	
618	631	1669.9	6.1	9.7	10.2	10.3	10.8
			5.6	9.1		9.9	
			4.7	8.8		9.8	
625	631	864.5	1.6	4.1	4.4	3.9	3.6
			1.4	3.7		3.9	
			0.9	3.5		3.8	
632	642	1218.7	4.3	7.9	8.4	N.D.	N.D.
			2.8	7.4		N.D.	
			2.1	6.9		N.D.	

(1) ATP-free ADP, purified as described in ref. 12