

Table S2: Average number of deuterons incorporated in Sse1-strepII + ATP and in Sse1-Strep-Tag II in complex with Ssa1-NBD or Ssa1-His₁₀

PEPTIDE		Mass (exp) [Da]	DATASET 1				100%	DATASET 2						100%	
Start	End		HX time	10 s	30 s	2 min	2 h	10 s	30 s	2 min	10 min	30 min	1 h		
2	12	1133.5	Sse1 + ATP	0.3	0.3	0.5	3.8	5.2	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
			Ssa1-NBD complex	0.5	0.3	0.4	2.7		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	
			Ssa1 complex	0.3	0.3	0.5	2.0		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	
2	16	1546.8		0.3	0.4	0.9	6.9	8.3	0.3	0.5	1.0	2.9	5.3	6.8	8.8
				0.3	0.3	0.5	2.2		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	
				0.2	0.3	0.5	2.2		0.5	0.5	1.4	1.4	2.3	2.4	
2	17	1617.8		0.1	0.2	0.5	N.D.	9.4	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
				0.2	0.2	0.5	N.D.		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	
				0.0	N.D.	N.D.	N.D.		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	
2	25	2499.3		3.8	3.7	4.7	14.3	16.4	4.1	4.2	5.4	8.5	12.4	14.4	17.6
				3.1	3.6	4.0	6.7		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	
				2.5	3.1	3.5	6.1		3.0	3.5	4.3	5.3	5.8	6.3	
17	25	970.5		3.4	3.5	4.2	5.5	6.2	3.6	3.6	4.4	5.3	5.8	5.9	6.3
				3.2	3.6	3.7	5.0		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	
				2.6	3.3	3.5	4.2		2.8	3.3	3.6	3.9	4.2	4.4	
69	75	813.5		0.7	1.0	1.8	3.6	4.3	0.7	1.1	1.8	2.0	3.3	3.6	3.9
				0.7	1.1	1.7	2.6		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	
				0.8	1.1	1.9	2.5		0.5	1.1	1.7	1.6	2.4	2.5	
69	81	1609.8		0.7	1.2	1.8	5.3	5.8	1.1	1.6	2.1	3.0	4.8	5.3	6.2
				0.8	1.3	1.7	3.9		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	
				0.7	1.3	1.7	3.2		1.4	1.6	2.4	2.4	3.3	3.4	
75	92	2244.0		3.5	4.5	5.8	8.0	9.0	3.8	4.5	6.3	8.0	8.4	9.3	9.2
				3.5	4.4	5.4	8.0		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	
				3.6	4.4	5.5	7.6		4.0	4.9	6.3	7.8	8.3	8.2	
104	118	1688.9		4.2	5.2	6.6	9.2	9.9	4.3	5.2	7.0	8.3	9.6	9.7	10.4
				4.1	4.8	6.5	8.5		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	
				4.1	5.3	6.6	N.D.		4.5	4.9	6.7	8.0	8.0	8.1	
107	118	1286.7		2.6	3.1	4.3	7.1	7.5	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
				2.6	3.0	3.6	6.3		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	
				2.6	2.9	3.8	6.0		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	
122	140	2178.2		6.2	7.1	8.1	11.8	12.6	6.9	7.6	8.2	10.2	12.0	12.5	13.1
				6.3	6.9	7.1	9.9		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	
				5.4	7.2	7.6	9.3		6.1	7.1	8.2	8.7	9.0	9.6	
122	142	2380.2		6.3	7.4	8.0	12.0	19.2	7.0	7.7	8.4	10.3	11.9	12.5	12.7
				6.0	7.0	7.8	9.7		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	
				5.2	6.7	7.6	9.5		6.0	7.4	8.1	8.9	9.5	9.9	
123	142	2233.2		6.5	7.2	7.9	11.4	20.0	6.9	7.5	8.6	9.9	11.5	12.0	12.1
				6.3	7.4	7.6	9.8		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	
				5.4	7.2	7.8	9.6		6.2	7.5	8.2	8.9	9.5	9.7	
143	152	1203.6		0.7	0.7	0.9	2.0	5.3	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
				0.6	0.7	0.9	2.1		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	

Table S2

Table S2

Table S2

			3.5	4.8	5.7	N.D.		N.D.								
534	550	1869.0		4.1	5.3	6.4	8.4	11.5	4.5	5.0	6.5	7.1	7.4	8.0	8.9	11.7
				4.1	5.3	6.3	N.D.		N.D.							
				N.D.	N.D.	N.D.	N.D.		5.0	5.0	6.8	6.9	7.5	7.6	8.2	
551	563	1559.8		0.1	0.3	1.3	7.9	8.2	0.3	0.4	1.2	4.8	7.3	8.2	8.1	9.1
				0.0	0.0	0.1	2.4		N.D.							
				0.1	0.0	0.1	1.5		0.3	0.2	0.3	0.5	0.9	1.2	N.D.	
557	563	817.4		0.1	0.2	N.D.	N.D.	N.D.	0.1	0.1	0.9	3.6	N.D.	4.3	4.3	4.2
				-0.2	0.1	N.D.	N.D.		N.D.							
				0.1	0.1	N.D.	N.D.		0.1	0.0	0.3	0.8	N.D.	N.D.	N.D.	
564	576	1532.7		6.3	6.4	6.7	7.3	8.2	5.3	5.3	5.1	6.8	5.8	6.4	6.0	6.8
				2.5	3.7	4.0	7.1		N.D.							
				1.8	2.0	2.5	6.4		1.5	1.6	2.7	5.0	5.2	6.0	6.2	
577	585	1125.7		0.3	1.5	1.6	6.0	6.4	3.0	1.1	4.9	5.3	6.2	6.1	6.1	6.4
				0.1	0.7	0.8	5.1		N.D.							
				0.1	0.7	0.7	N.D.		7.2	N.D.	7.4	N.D.	7.7	N.D.	N.D.	
577	587	1383.7		1.2	N.D.	5.0	N.D.	7.5	N.D.							
				0.5	1.2	2.5	N.D.		N.D.							
				0.7	1.1	2.0	N.D.		N.D.							
579	585	849.5		0.5	1.3	3.5	4.6	5.6	0.7	1.1	0.9	N.D.	0.6	N.D.	0.6	N.D.
				0.5	0.8	1.1	2.9		N.D.							
				0.4	0.6	1.0	3.9		0.5	0.3	1.1	1.7	1.9	N.D.	N.D.	
596	610	1688.9		0.9	2.9	7.9	10.3	10.5	N.D.							
				0.6	1.1	2.4	10.2		N.D.							
				0.6	0.8	1.9	N.D.		N.D.							
613	631	2281.1		8.3	10.6	12.0	12.3	12.6	N.D.							
				4.7	5.7	7.3	12.4		N.D.							
				3.8	4.6	6.1	11.8		N.D.							
618	631	1669.9		5.3	7.0	9.0	9.8	10.1	4.6	5.7	8.6	8.9	9.5	9.8	9.2	10.2
				3.2	3.7	5.8	9.4		N.D.							
				2.9	3.1	4.2	8.7		3.3	3.4	4.0	6.1	6.3	8.2	8.3	
625	631	864.5		1.2	2.2	3.6	4.0	4.3	1.2	1.8	2.6	3.6	3.2	3.4	3.2	3.6
				0.4	0.8	1.4	3.7		N.D.							
				0.4	0.8	1.0	3.2		0.8	0.9	1.0	2.1	2.4	3.2	3.2	
625	643	2178.2		4.8	6.5	8.1	10.9	13.8	5.5	6.9	8.5	9.4	10.2	10.9	12.3	N.D.
				2.7	4.9	6.9	10.0		N.D.							
				2.5	4.0	5.5	9.6		2.7	3.8	5.8	7.5	8.5	8.9	9.9	
632	642	1218.7		2.1	4.2	6.8	7.8	8.2	2.7	3.6	7.2	8.0	8.1	8.2	7.7	8.2
				1.8	2.5	4.1	7.7		N.D.							
				1.7	2.8	4.0	7.6		1.9	2.8	4.1	6.8	7.1	7.6	7.8	
632	646	1659.9		3.4	6.4	N.D.	11.2	11.8	N.D.							
				2.9	4.0	N.D.	N.D.		N.D.							
				2.6	3.9	N.D.	N.D.		N.D.							
692	703	1461.6		2.5	3.0	3.5	N.D.									
				2.7	2.6	3.2	N.D.		N.D.							
				2.4	2.6	3.1	N.D.		N.D.							
695	703	1128.5		4.7	4.9	4.8	4.9	N.D.	5.0	4.8	4.9	4.9	5.0	5.1	5.1	N.D.
				4.6	4.9	4.7	4.6		N.D.							
				4.7	5.0	N.D.	5.0		4.8	4.7	4.8	4.9	5.0	4.9	5.3	