

Table S5: Average number of deuterons incorporated in Ssa1-NBD, and in Ssa1-NBD or Ssa1-His₁₀ in complex with Sse1-Strep-Tag II

PEPTIDE			AVERAGE NUMBER OF DEUTERONS INCORPORATED											
			DATASET 1						DATASET 2					
Start	End	Mass (exp) [Da]	HX time	10 s	30 s	2 min	2 h	100%	10 s	30 s	2 min	10 min	2 h	100%
1	8	819.4	Ssa1-NBD	2.5	2.7	2.6	2.8	4.7	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
			Ssa1-NBD-Sse1	2.8	3.5	2.8	2.5		N.D.	N.D.	N.D.	N.D.	N.D.	
			Ssa1-Sse1	N.D.	N.D.	N.D.	N.D.		N.D.	N.D.	N.D.	N.D.	N.D.	
2	15	1413.7		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
				N.D.	N.D.	N.D.	N.D.		N.D.	N.D.	N.D.	N.D.	N.D.	
				N.D.	N.D.	N.D.	N.D.		N.D.	N.D.	N.D.	N.D.	N.D.	
16	39	2657.3		4.9	7.6	9.5	11.6	N.D.	4.8	7.5	10.0	12.2	11.0	N.D.
				4.8	6.2	7.8	11.8		N.D.	N.D.	N.D.	N.D.	N.D.	
				3.6	N.D.	7.3	11.3		3.5	4.6	7.8	N.D.	N.D.	
23	39	1903.0		4.3	5.8	6.4	8.0	10.4	4.7	5.6	6.8	7.9	7.3	9.0
				4.2	4.9	5.6	8.3		N.D.	N.D.	N.D.	N.D.	N.D.	
				4.0	4.4	5.2	8.0		4.1	4.6	5.3	N.D.	7.2	
40	45	652.3		2.0	1.9	1.9	2.7	3.8	1.8	1.9	1.9	2.5	2.6	3.4
				2.0	2.2	2.1	2.6		N.D.	N.D.	N.D.	N.D.	N.D.	
				1.9	2.1	2.2	2.7		1.9	1.8	2.0	2.6	2.5	
40	48	1050.5		3.5	3.6	3.3	4.5	5.9	3.5	3.7	3.6	4.2	4.5	5.7
				3.7	3.8	3.7	4.4		N.D.	N.D.	N.D.	N.D.	N.D.	
				3.7	3.6	3.6	4.5		3.6	3.6	3.9	4.2	4.3	
46	66	2246.1		7.5	8.6	8.9	11.7	14.2	8.0	8.5	9.6	10.9	10.4	13.0
				6.7	7.8	8.6	10.4		N.D.	N.D.	N.D.	N.D.	N.D.	
				6.1	8.1	8.6	10.9		7.3	7.5	9.0	9.7	10.4	
49	63	1500.7		6.4	7.7	7.4	8.8	8.7	6.0	N.D.	7.5	N.D.	8.3	8.6
				4.9	5.8	6.6	8.2		N.D.	N.D.	N.D.	N.D.	N.D.	
				4.5	5.5	6.1	8.5		4.0	4.9	5.5	N.D.	6.1	
49	66	1847.9		6.5	7.6	7.9	10.0	11.6	6.5	7.4	7.8	9.4	8.3	10.3
				4.9	5.9	6.7	9.0		N.D.	N.D.	N.D.	N.D.	N.D.	
				5.5	5.8	6.8	9.2		3.7	4.0	5.7	N.D.	7.8	
67	83	1942.0		2.2	4.4	4.7	7.8	11.1	N.D.	N.D.	5.0	N.D.	N.D.	N.D.
				2.6	4.5	5.0	7.9		N.D.	N.D.	N.D.	N.D.	N.D.	
				2.7	5.4	5.8	8.7		N.D.	N.D.	N.D.	N.D.	N.D.	
76	92	2062.0		3.7	4.8	6.0	9.0	10.4	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
				3.5	4.5	5.8	8.6		N.D.	N.D.	N.D.	N.D.	N.D.	
				3.5	4.8	6.6	8.7		N.D.	N.D.	N.D.	N.D.	N.D.	
83	92	1232.6		1.6	2.0	2.3	3.9	5.0	1.4	0.9	2.0	2.9	2.0	3.5
				1.8	2.0	2.4	3.5		N.D.	N.D.	N.D.	N.D.	N.D.	
				1.9	2.2	2.7	3.5		1.8	2.1	2.2	2.9	2.2	
83	104	2554.3		2.2	2.9	3.9	8.9	13.3	7.9	0.1	12.8	N.D.	N.D.	N.D.
				2.3	3.0	3.8	8.1		N.D.	N.D.	N.D.	N.D.	N.D.	
				2.2	2.9	3.8	9.4		N.D.	N.D.	N.D.	N.D.	N.D.	
93	102	1111.6		0.8	1.0	1.1	1.9	5.4	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
				0.8	1.0	1.1	1.8		N.D.	N.D.	N.D.	N.D.	N.D.	
				0.9	1.0	1.2	1.9		N.D.	N.D.	N.D.	N.D.	N.D.	

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93	104	1339.7	0.9	1.1	1.3	3.5	7.2	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
			0.8	0.8	1.1	3.0		N.D.	N.D.	N.D.	N.D.	N.D.	
			N.D.	1.0	1.1	3.8		N.D.	N.D.	N.D.	N.D.	N.D.	
105	119	1711.8	2.4	3.1	3.3	5.9	9.4	2.1	2.5	3.1	N.D.	5.6	9.1
			2.4	3.0	3.4	5.7		N.D.	N.D.	N.D.	N.D.	N.D.	
			2.5	3.2	3.6	6.3		2.2	N.D.	3.2	N.D.	5.9	
105	120	1842.9	2.3	3.0	3.2	6.0	10.4	2.4	N.D.	3.3	N.D.	N.D.	10.0
			2.4	3.2	3.3	5.9		N.D.	N.D.	N.D.	N.D.	N.D.	
			2.5	3.2	3.4	6.2		N.D.	N.D.	3.6	N.D.	N.D.	
106	119	1564.8	1.9	2.5	2.7	5.2	8.7	1.8	2.3	3.4	3.5	5.5	7.9
			1.9	2.3	2.6	5.1		N.D.	N.D.	N.D.	N.D.	N.D.	
			1.9	2.5	2.6	5.8		2.1	2.4	2.8	N.D.	5.3	
120	133	1598.8	0.2	0.2	0.7	4.9	10.4	0.1	0.2	0.4	1.7	4.7	10.2
			0.4	0.3	0.4	2.3		N.D.	N.D.	N.D.	N.D.	N.D.	
			0.1	0.4	0.4	2.0		0.5	0.7	0.8	0.8	N.D.	
121	130	1104.6	0.1	0.1	0.2	1.7	6.2	0.0	0.2	0.1	N.D.	1.5	5.5
			0.1	0.1	0.2	0.8		N.D.	N.D.	N.D.	N.D.	N.D.	
			0.1	0.1	0.2	1.0		0.2	0.1	0.0	N.D.	1.3	
123	133	1255.6	0.2	0.3	0.7	3.8	7.2	0.1	0.0	0.4	N.D.	N.D.	7.2
			0.2	0.2	0.3	1.7		N.D.	N.D.	N.D.	N.D.	N.D.	
			0.1	0.2	0.3	1.8		0.1	N.D.	0.2	N.D.	N.D.	
140	147	818.4	0.3	0.2	0.7	1.1	3.8	0.0	-0.1	0.2	2.1	1.4	4.2
			0.3	0.7	0.8	0.8		N.D.	N.D.	N.D.	N.D.	N.D.	
			N.D.	0.6	1.1	1.4		0.1	0.3	0.6	N.D.	1.3	
140	165	2692.4	2.0	2.5	3.5	8.8	18.2	1.9	1.9	3.9	6.2	8.7	18.3
			2.3	3.2	4.4	8.9		N.D.	N.D.	N.D.	N.D.	N.D.	
			2.6	3.8	4.8	9.2		2.3	2.9	4.6	6.7	8.8	
148	165	1892.0	1.4	1.8	2.1	5.0	12.1	1.1	1.3	1.8	N.D.	N.D.	11.7
			1.4	1.7	2.2	5.2		N.D.	N.D.	N.D.	N.D.	N.D.	
			1.4	1.8	2.2	5.0		1.0	1.2	1.8	N.D.	N.D.	
148	167	2105.1	2.2	2.8	3.4	6.8	13.8	N.D.	2.7	N.D.	5.3	N.D.	N.D.
			2.3	3.0	3.8	7.0		N.D.	N.D.	N.D.	N.D.	N.D.	
			2.2	3.0	3.7	6.2		N.D.	N.D.	N.D.	N.D.	N.D.	
149	165	1744.8	1.0	1.4	1.6	4.9	11.4	1.0	1.2	1.6	1.9	4.2	11.3
			1.0	1.3	1.9	4.8		N.D.	N.D.	N.D.	N.D.	N.D.	
			0.7	1.1	1.7	4.7		0.7	N.D.	1.7	N.D.	N.D.	
149	167	1958.0	1.8	2.3	2.9	6.6	12.9	N.D.	2.3	N.D.	N.D.	N.D.	N.D.
			1.8	2.3	3.2	6.8		N.D.	N.D.	N.D.	N.D.	N.D.	
			1.8	2.4	3.2	6.8		N.D.	1.8	N.D.	N.D.	N.D.	
168	178	1167.6	1.9	1.9	1.8	3.0	6.6	2.2	2.4	2.3	N.D.	3.3	5.7
			1.9	2.0	1.9	2.6		N.D.	N.D.	N.D.	N.D.	N.D.	
			2.0	2.1	2.0	2.9		2.5	2.6	2.7	N.D.	2.5	
169	178	1054.6	1.1	1.2	1.0	1.9	5.6	1.4	1.5	1.5	1.9	2.1	4.7
			1.0	1.2	1.0	1.4		N.D.	N.D.	N.D.	N.D.	N.D.	
			1.1	1.4	1.2	2.0		2.1	2.1	2.3	2.9	2.0	
207	214	892.4	1.8	2.4	2.9	4.1	4.4	1.8	1.2	2.9	3.5	2.7	3.7
			1.8	2.3	2.9	4.1		N.D.	N.D.	N.D.	N.D.	N.D.	
			1.9	2.4	3.0	4.2		1.9	2.2	2.7	3.4	3.0	
215	229	1498.7	3.4	4.7	5.2	8.0	8.4	2.5	3.6	4.5	6.6	7.0	6.5
			4.9	5.8	5.8	7.9		N.D.	N.D.	N.D.	N.D.	N.D.	
			5.2	5.7	6.2	7.4		4.2	4.8	5.6	6.9	5.1	
216	229	1369.6	2.6	3.8	4.6	6.7	6.8	2.4	3.1	4.0	5.3	6.3	5.7
			4.7	5.3	5.4	6.6		N.D.	N.D.	N.D.	N.D.	N.D.	
			4.7	5.3	5.4	6.6		3.9	4.6	5.0	N.D.	N.D.	

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230	241	1530.7	0.3	0.7	1.8	5.2	7.7	0.5	0.5	1.9	3.9	4.2	7.8
			1.3	1.7	2.2	4.9		N.D.	N.D.	N.D.	N.D.	N.D.	
			1.3	1.6	2.2	5.3		1.3	1.7	2.6	3.7	4.3	
242	254	1605.9	5.2	6.4	6.1	6.7	6.9	3.8	6.0	5.1	6.7	6.3	6.6
			4.3	5.7	6.2	6.5		N.D.	N.D.	N.D.	N.D.	N.D.	
			N.D.	5.7	6.1	6.4		3.5	4.6	5.3	6.3	6.6	
242	256	1833.0	6.2	8.0	8.0	8.3	8.4	5.4	7.4	7.8	8.2	8.0	8.0
			4.8	6.5	7.6	8.1		N.D.	N.D.	N.D.	N.D.	N.D.	
			5.0	6.7	7.8	8.1		4.4	5.9	7.5	7.9	6.9	
265	280	1748.9	5.2	6.4	7.6	10.4	17.0	4.7	N.D.	7.6	N.D.	10.3	N.D.
			5.8	7.1	8.2	10.2		4.5	6.2	9.3	N.D.	6.0	
			5.7	7.0	8.4	10.4		N.D.	N.D.	N.D.	N.D.	N.D.	
266	280	1619.9	5.2	6.3	7.5	9.7	N.D.	4.5	4.4	6.4	8.1	9.2	N.D.
			5.4	6.8	7.6	9.4		N.D.	N.D.	N.D.	N.D.	N.D.	
			5.7	6.8	7.8	9.4		4.5	5.6	6.8	8.0	5.7	
307	323	1986.1	0.4	0.7	1.3	6.5	11.2	0.4	0.5	1.1	2.8	3.4	6.4
			0.4	0.6	0.9	5.1		N.D.	N.D.	N.D.	N.D.	N.D.	
			0.4	0.6	0.9	5.3		0.5	0.6	0.9	2.5	3.8	
307	330	2787.5	1.9	2.4	3.1	10.4	15.4	1.7	2.2	3.2	5.6	N.D.	N.D.
			2.0	2.3	2.7	8.6		N.D.	N.D.	N.D.	N.D.	N.D.	
			1.9	2.3	2.8	8.9		1.7	2.0	2.7	4.7	6.9	
316	323	941.6	0.2	0.2	0.5	2.6	4.9	0.6	0.3	0.7	N.D.	2.6	4.3
			0.1	0.2	0.5	2.1		N.D.	N.D.	N.D.	N.D.	N.D.	
			N.D.	0.2	N.D.	2.7		0.3	0.2	N.D.	N.D.	1.3	
316	330	1742.9	1.7	1.9	2.2	6.2	8.9	1.3	1.9	2.0	4.1	5.7	8.3
			1.7	1.9	2.2	5.4		N.D.	N.D.	N.D.	N.D.	N.D.	
			1.7	1.9	2.4	5.8		1.6	1.6	2.2	N.D.	3.6	
331	346	1707.1	1.6	2.9	3.8	7.5	11.2	1.8	2.1	3.8	5.6	4.9	10.5
			2.9	3.6	5.1	7.8		N.D.	N.D.	N.D.	N.D.	N.D.	
			2.9	3.5	5.0	8.2		2.5	3.0	5.0	N.D.	N.D.	
331	348	1907.2	1.7	2.9	3.9	7.7	13.2	1.4	2.5	3.5	N.D.	4.8	11.2
			N.D.	N.D.	N.D.	N.D.		N.D.	N.D.	N.D.	N.D.	N.D.	
			N.D.	N.D.	N.D.	N.D.		3.8	3.9	5.7	N.D.	N.D.	
331	349	2022.2	1.7	2.9	3.9	7.7	13.8	1.5	2.4	3.7	N.D.	5.2	13.4
			2.9	3.6	5.3	8.3		N.D.	N.D.	N.D.	N.D.	N.D.	
			2.9	3.4	5.2	8.7		2.2	N.D.	4.8	N.D.	N.D.	
334	346	1381.8	1.5	2.7	3.6	6.3	8.1	1.4	N.D.	3.3	N.D.	5.6	6.9
			2.6	3.4	4.7	6.9		N.D.	N.D.	N.D.	N.D.	N.D.	
			N.D.	3.3	5.2	7.0		2.2	2.8	N.D.	N.D.	N.D.	
334	348	1582.0	1.5	2.7	3.7	6.4	10.2	0.0	0.9	1.8	N.D.	4.5	6.8
			2.7	3.5	4.8	N.D.		N.D.	N.D.	N.D.	N.D.		
			N.D.	2.9	N.D.	N.D.		0.8	1.0	N.D.	N.D.	N.D.	
334	349	1697.0	1.5	2.6	3.5	6.7	10.8	1.5	2.5	3.5	N.D.	N.D.	10.1
			2.5	3.4	4.5	7.3		N.D.	N.D.	N.D.	N.D.	N.D.	
			2.9	3.1	4.6	7.6		2.3	2.6	4.1	N.D.	N.D.	
347	364	2094.0	4.8	6.2	6.6	8.0	10.0	4.7	5.9	6.8	N.D.	8.1	9.9
			4.2	5.6	6.3	7.4		N.D.	N.D.	N.D.	N.D.	N.D.	
			N.D.	5.8	6.8	7.8		4.1	N.D.	7.3	N.D.	N.D.	
350	364	1778.8	4.9	6.4	6.8	7.7	8.3	4.7	6.3	6.8	N.D.	7.5	6.7
			4.3	5.7	6.6	7.6		N.D.	N.D.	N.D.	N.D.	N.D.	
			N.D.	5.9	6.7	7.6		4.4	5.3	N.D.	N.D.	5.2	
365	373	848.4	0.1	0.1	0.2	0.7	5.7	0.1	0.0	0.1	0.4	0.7	5.3
			0.2	0.1	0.2	0.6		N.D.	N.D.	N.D.	N.D.	N.D.	
			0.2	0.2	0.3	0.2		0.1	0.0	0.1	0.5	0.4	

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366	373	777.4	-0.1	0.0	0.1	0.4	4.9	0.1	0.1	0.1	0.4	0.8	4.5
			0.1	0.0	0.1	0.2		N.D.	N.D.	N.D.	N.D.	N.D.	
			0.1	-0.1	0.1	0.1		0.2	0.1	0.2	N.D.	0.5	