

Operator: massmap1
 Date/time: 2018-10-04/8:52:11am
 hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

hdx_etd_riis-Files of the Projekts Used for Kinetics Analysis (7)

#	Path
1	C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\demo\2h.hdx_etd_riis
2	C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\demo\3min.hdx_etd_riis
3	C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\demo\9h_19h.hdx_etd_riis
4	C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\demo\12min.hdx_etd_riis
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6	C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\demo\40h.hdx_etd_riis
7	C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\demo\56min_4h.hdx_etd_riis

Peptide name: XBPlu wt
 Peptide sequence: KKKISPWILAVLTLQIQSLISCWAFKKK
 Variable name: Exchange Time
 Variable unit: min

Exchange Data Sets Used for Kinetics Analysis (29)

(Value=Exchange Time/min, #riis: number hdx_etd_riis-file)

#	#riis	Value	Path
1	1	120	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu 2h\160427W07.mmp
2	1	120	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu 2h\160427W08.mmp
3	1	120	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu 2h\160427W06.mmp
4	2	3	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu wt 3min\161130W08.mmp
5	2	3	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu wt 3min\161130W09.mmp
6	2	3	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu wt 3min\161130W16.mmp
7	2	3	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu wt 3min\161130W17.mmp
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9	2	3	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu wt 3min\161130W18.mmp
10	3	1140	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu wt 9h 19h\161109W05.mmp
11	3	1140	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu wt 9h 19h\161109W06.mmp
12	3	540	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu wt 9h 19h\161109W13.mmp
13	3	540	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu wt 9h 19h\161109W14.mmp
14	3	540	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu wt 9h 19h\161109W15.mmp
15	3	1140	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu wt 9h 19h\161109W04.mmp
16	4	12	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu wt 12min\160211W12.mmp
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18	4	12	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu wt 12min\160211W14.mmp
19	5	27	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu wt 27min\161108W08.mmp
20	5	27	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu wt 27min\161108W09.mmp
21	5	27	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu wt 27min\161108W10.mmp
22	6	2400	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu 40h\161116W02.mmp
23	6	2400	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu 40h\161116W03.mmp
24	7	56	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu 56 min 4h\160301W04.mmp
25	7	56	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu 56 min 4h\160301W05.mmp
26	7	56	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu 56 min 4h\160301W06.mmp
27	7	240	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu 56 min 4h\160302W07.mmp
28	7	240	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu 56 min 4h\160302W08.mmp
29	7	240	C:\massmap\tests\HDX-Fragmentierung\kinetics\XBPlu 56 min 4h\160302W09.mmp

Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Exchange type: Replacement of D by H
 File with chemical rate constants: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\...
 ...kinetics\lis_etc\wild_type_kex.txt
 Temperature exchange reaction [°C]: 20

hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBPlu wt

Peptide sequence: KKKISPWILAVLTLQIQSLISCWAFKKK

File with chemical rate constants: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\...
 ...kinetics\lis_etc\wild_type_kex.txt

Temperature exchange reaction [°C]: 20

RC_exp/RC_int: Experimental/chemical rate constant

OR: Opening rate, i.e. equilibrium fraction of exchange competent open conformation

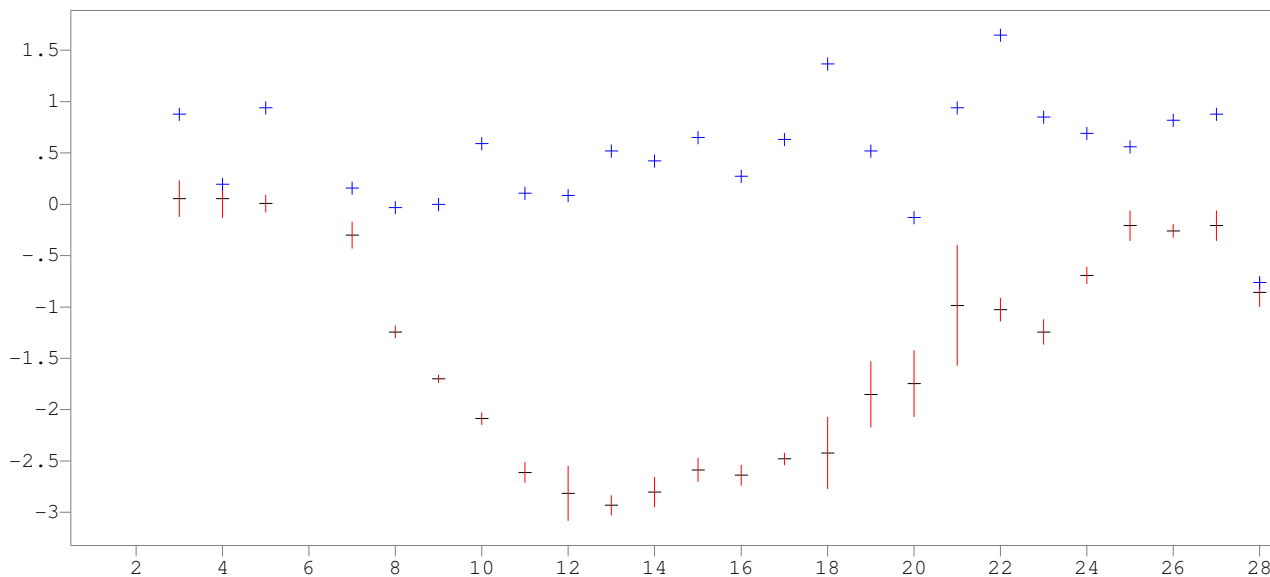
Delta_G, LL/UP: Difference of Gibbs Free Energy, lower/upper limit of delta_G confidence interval

#AA	AA	log(RC_exp*min)	log(RC_int*min)	OR [%]	Delta_G [kcal/mol]	LL [kcal/mol]	UL [kcal/mol]
3	K	0.0539 +/- 0.1766	0.8785	14.9763	1.0109	0.7202	1.2809
4	I	0.0539 +/- 0.1860	0.1948	72.2992	-0.5585	n.d.	0.0673
5	S	0.0082 +/- 0.0852	0.9395	11.7125	1.1759	1.0446	1.3037
7	W	-0.2994 +/- 0.1310	0.1565	35.0023	0.3603	0.0623	0.6123
8	I	-1.2435 +/- 0.0627	-0.0315	6.1385	1.5876	1.4976	1.6768
9	L	-1.6982 +/- 0.0385	-0.0017	2.0116	2.2621	2.2095	2.3147
10	A	-2.0872 +/- 0.0611	0.5911	0.2098	3.5888	3.5067	3.6708
11	V	-2.6114 +/- 0.1007	0.1065	0.1914	3.6421	3.5068	3.7773
12	L	-2.8151 +/- 0.2685	0.0878	0.1251	3.8903	3.5298	4.2505
13	T	-2.9319 +/- 0.0974	0.5209	0.0353	4.6280	4.4973	4.7586
14	L	-2.8028 +/- 0.1453	0.4216	0.0596	4.3217	4.1268	4.5166
15	Q	-2.5866 +/- 0.1160	0.6503	0.0580	4.3385	4.1829	4.4940
16	I	-2.6378 +/- 0.1014	0.2737	0.1226	3.9018	3.7658	4.0379
17	Q	-2.4801 +/- 0.0609	0.6306	0.0775	4.1693	4.0875	4.2510
18	S	-2.4215 +/- 0.3506	1.3681	0.0162	5.0796	4.6095	5.5496
19	L	-1.8508 +/- 0.3219	0.5209	0.4250	3.1765	2.7423	3.6093
20	I	-1.7465 +/- 0.3247	-0.1284	2.4095	2.1547	1.7032	2.5975
21	S	-0.9858 +/- 0.5881	0.9395	1.1875	2.5738	1.7651	3.3673
22	C	-1.0272 +/- 0.1164	1.6480	0.2113	3.5846	3.4282	3.7410
23	W	-1.2435 +/- 0.1241	0.8500	0.8063	2.8014	2.6336	2.9689
24	A	-0.6917 +/- 0.0836	0.6904	4.1491	1.8279	1.7104	1.9444
25	F	-0.2081 +/- 0.1471	0.5606	17.0339	0.9217	0.6742	1.1522
26	K	-0.2592 +/- 0.0666	0.8195	8.3414	1.3953	1.2971	1.4921
27	K	-0.2081 +/- 0.1471	0.8785	8.1925	1.4067	1.1882	1.6186
28	K	-0.8568 +/- 0.1392	-0.7625	80.4825	-0.8247	n.d.	-0.1976

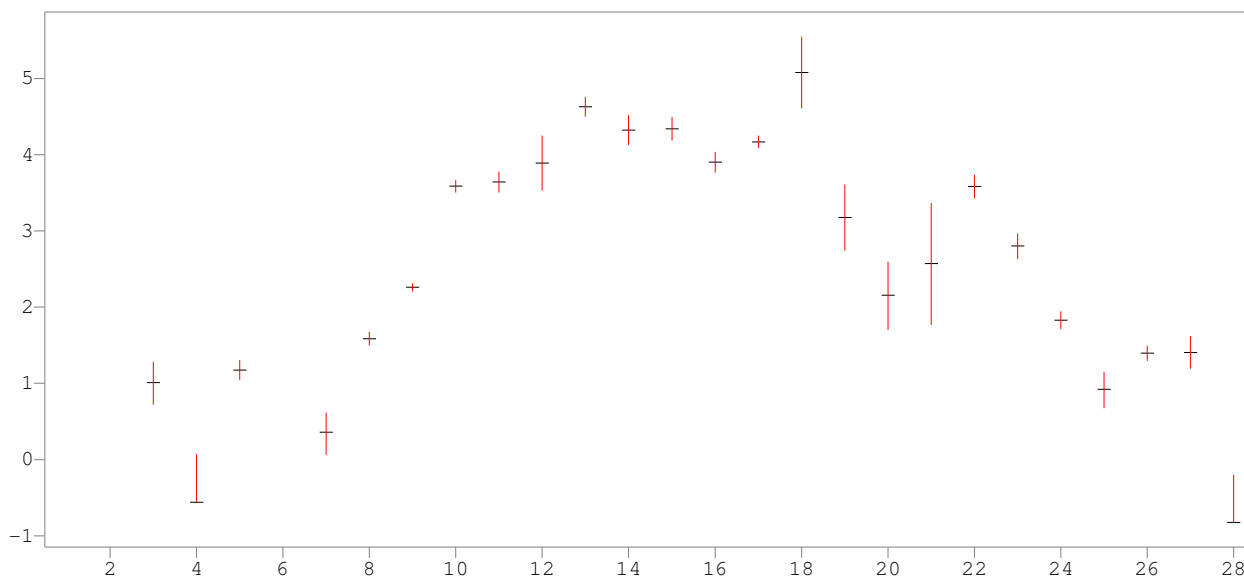
hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin
 Peptide name: XBP1u wt
 Peptide sequence: KKKISPWILAVLTLQIQLISCWAFKKK
 File with chemical rate constants: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\...
 ...kinetics\lis_etc\wild_type_kex.txt
 Temperature exchange reaction [°C]: 20

Black horizontal dash: Exp. rate constant (upper graphics), Delta_G (lower graphics)
 Red vertical line: Error range (top: rate constant, bottom: Delta_G)
 Blue +: chemical rate constant

Log(Rate Constant*min)



Delta_G [kcal/mol]



Number of Amino Acid

hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBPlu wt

Peptide sequence: KK <K> ISPWILAVLTLQIQSLISCWAFKKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 3)

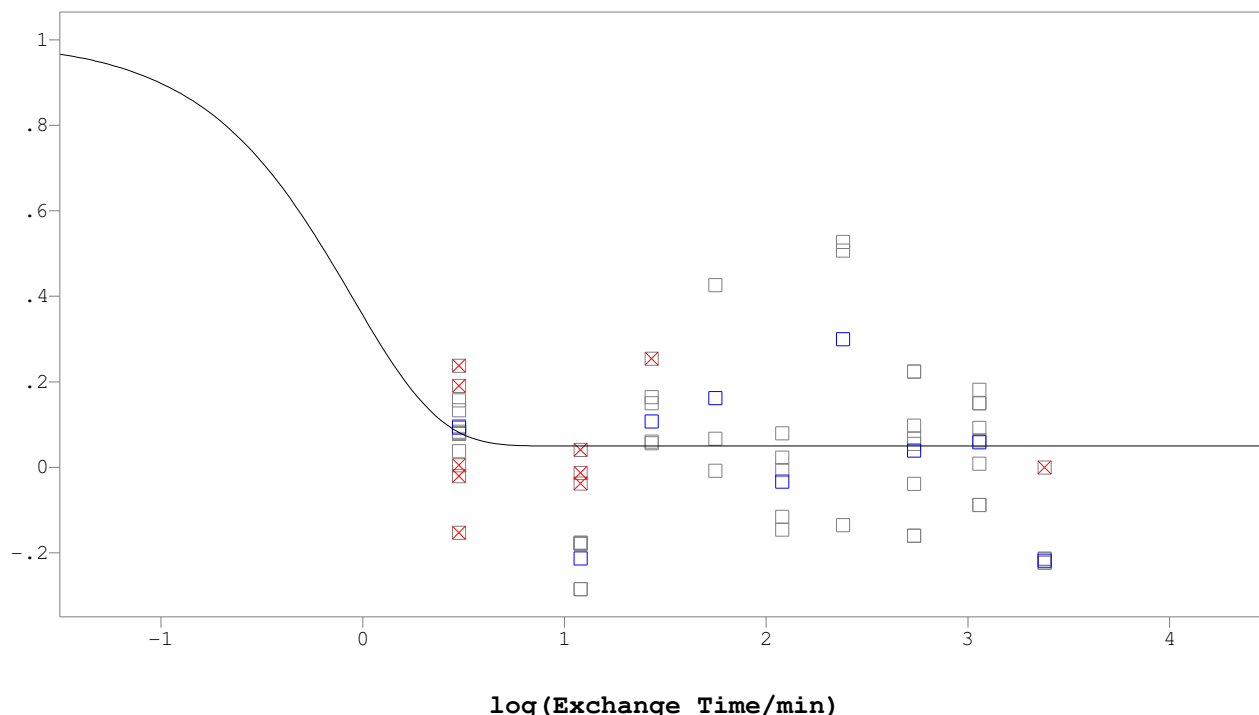
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: 1
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	0.0934	0.0787	0.0799	0.0799	(0.1906)	(-0.1527)	(0.2376)
		(0.0048)	0.0960	(-0.0204)	0.1567	0.1339	0.0834
		0.0382					
12	-0.2129	(-0.0378)	-0.1778	-0.1778	(0.0413)	-0.1761	-0.1761
		(-0.0130)	-0.2846	-0.2846			
27	0.1080	0.0604	0.1645	0.0569	0.1501	(0.2540)	
56	0.1621	0.4268	-0.0073	0.0668			
120	-0.0329	0.0231	-0.1157	-0.1456	0.0798	-0.0063	
240	0.3000	0.5273	0.5074	-0.1350			
540	0.0392	0.0554	-0.0379	0.0981	0.2242	0.2242	0.0678
		-0.1592	-0.1592				
1140	0.0591	0.0092	0.1500	0.1500	0.0631	0.1820	0.0930
		-0.0874	-0.0874				
2400	-0.2177	-0.2220	-0.2220	(0.0000)	-0.2133	-0.2133	

Fitted rate constant (RC): log(RC*min) = .0539 +/- .1766

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBPlu wt

Peptide sequence: KKK <I> SPWILAVLTLQIQSLISCWAFKKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 4)

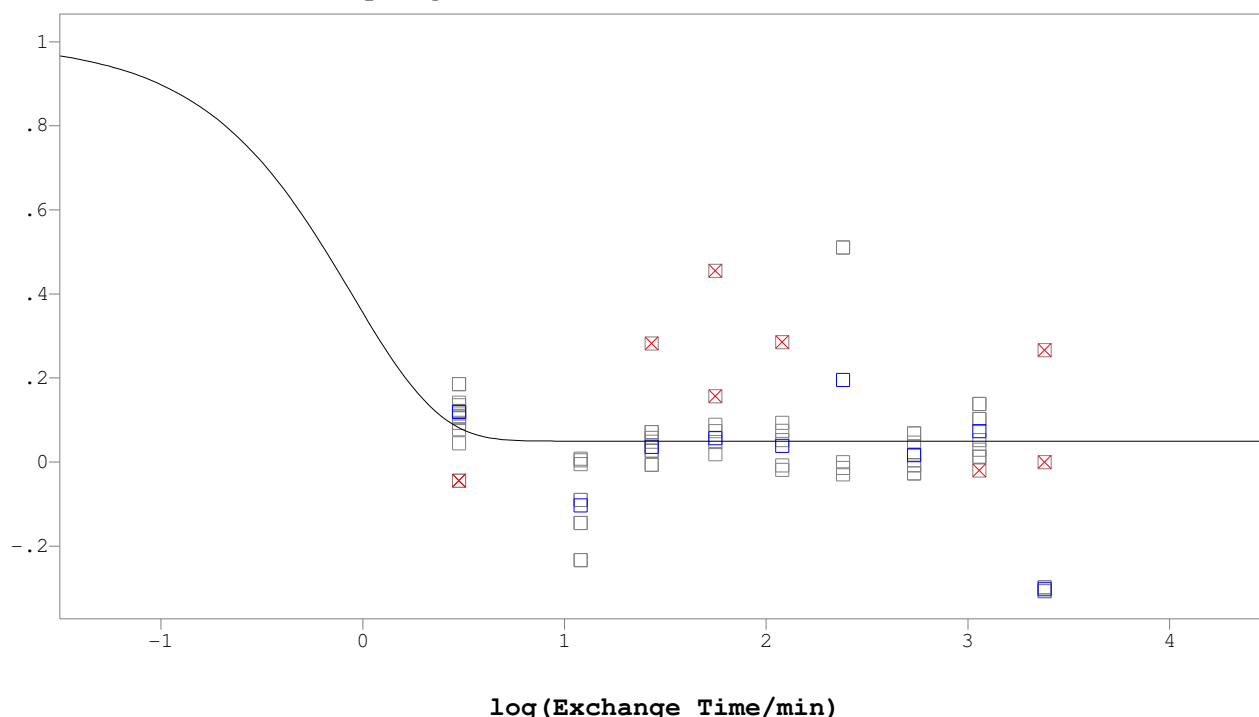
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: 1
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	0.1198	0.0935	0.1860	0.1860	0.1048	(-0.0444)	(-0.0444)
		0.0783	0.1218	0.1218	0.0450	0.1413	0.1082
		0.1188	0.1154	0.1358			
12	-0.1028	0.0048	-0.1442	-0.1442	0.0087	-0.2331	-0.2331
		(-0.0041)	(-0.0900)	(-0.0900)			
27	0.0366	0.0490	0.0274	0.0274	0.0576	-0.0062	-0.0062
		(0.2827)	0.0718	0.0718			
56	0.0573	0.0738	(0.4551)	0.0188	0.0477	(0.1572)	0.0888
120	0.0391	(0.2859)	0.0939	0.0746	-0.0075	0.0527	-0.0180
240	0.1961	-0.0136	0.5112	0.5113	0.0000	-0.0285	
540	0.0169	-0.0072	-0.0064	0.0467	0.0688	0.0688	0.0182
		(-0.0268)	(-0.0268)				
1140	0.0737	(-0.0197)	0.1028	0.1028	0.0294	0.1383	0.1383
		0.0526	0.0127	0.0127			
2400	-0.3023	(0.2663)	-0.3069	-0.3069	(0.0000)	-0.2977	-0.2977

Fitted rate constant (RC): log(RC*min) = .0539 +/- .186

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBPlu wt

Peptide sequence: KKKI <S> PWILAVLTLQIQSLISCWAFKKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 5)

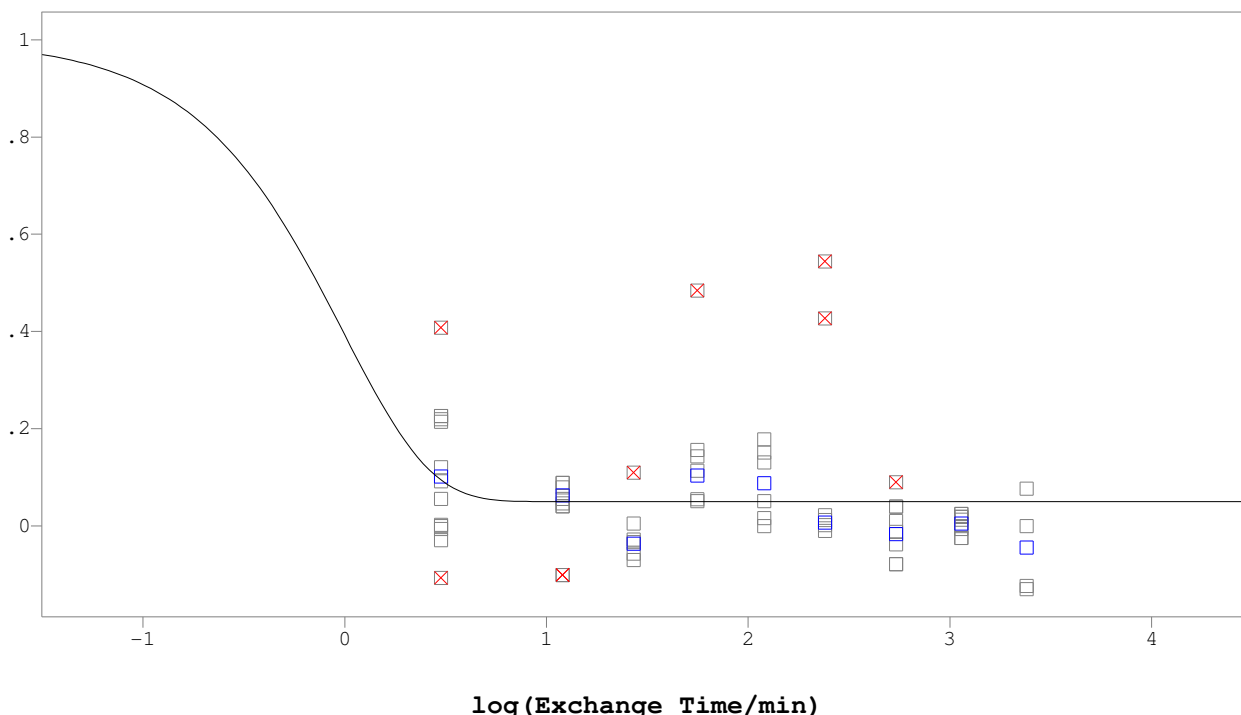
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: 1
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	0.1021	0.0024	0.2264	0.2264	-0.0060	0.2145	(-0.1070)
		0.0920	0.0000	(0.4082)	0.0556	-0.0290	0.1209
		0.2195					
12	0.0630	0.0794	0.0407	0.0407	0.0560	(-0.1008)	(-0.1008)
		0.0465	0.0887	0.0887			
27	-0.0364	-0.0279	-0.0699	-0.0327	-0.0566	(0.1101)	0.0049
56	0.1040	0.0549	(0.4845)	0.0510	0.1135	0.1567	0.1435
120	0.0880	0.0510	0.1512	0.1780	0.1311	0.0166	-0.0001
240	0.0068	0.0124	(0.4274)	-0.0096	(0.5446)	0.0021	0.0224
540	-0.0165	0.0105	(0.0898)	-0.0377	-0.0784	-0.0784	-0.0116
		0.0401	0.0401				
1140	0.0051	0.0000	0.0250	0.0250	-0.0058	-0.0242	-0.0242
		0.0128	0.0187	0.0187			
2400	-0.0441	0.0768	-0.1299	0.0000	-0.1232		

Fitted rate constant (RC): $\log(\text{RC} \cdot \text{min}) = .0082 \pm .0852$

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBPlu wt

Peptide sequence: KKKISP <W> ILAVLTLQIQSLISCWAFKKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 7)

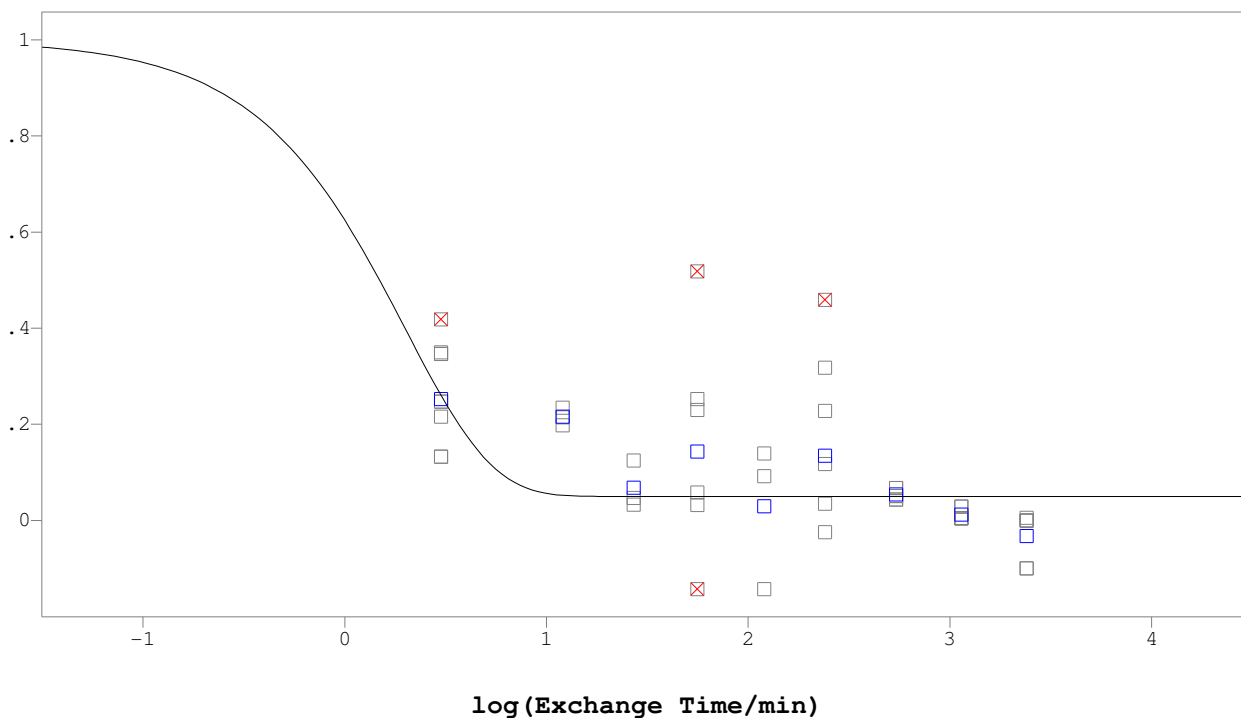
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: 1
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	0.2526	0.2159	0.3501	(0.4189)	0.1331	0.1331	0.2474
		0.2474	0.3468	0.3468			
12	0.2160	0.2351	0.1982	0.2145			
27	0.0683	0.0329	0.0469	0.1249			
56	0.1434	0.0584	(0.5182)	0.0321	0.2301	(-0.1428)	0.2529
120	0.0297	0.1394	-0.1424	0.0921			
240	0.1350	0.0349	0.3182	0.2280	(0.4593)	-0.0238	0.1173
540	0.0543	0.0437	0.0437	0.0679	0.0679	0.0511	0.0511
1140	0.0127	0.0289	0.0289	0.0049	0.0049	0.0043	0.0043
2400	-0.0320	-0.0991	-0.0991	0.0058	0.0000	0.0000	0.0001

Fitted rate constant (RC): $\log(\text{RC} \cdot \text{min}) = -0.2994 \pm 0.131$

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBPlu wt

Peptide sequence: KKKISPW <I> LAVLTLQIQSLISCWAFKKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 8)

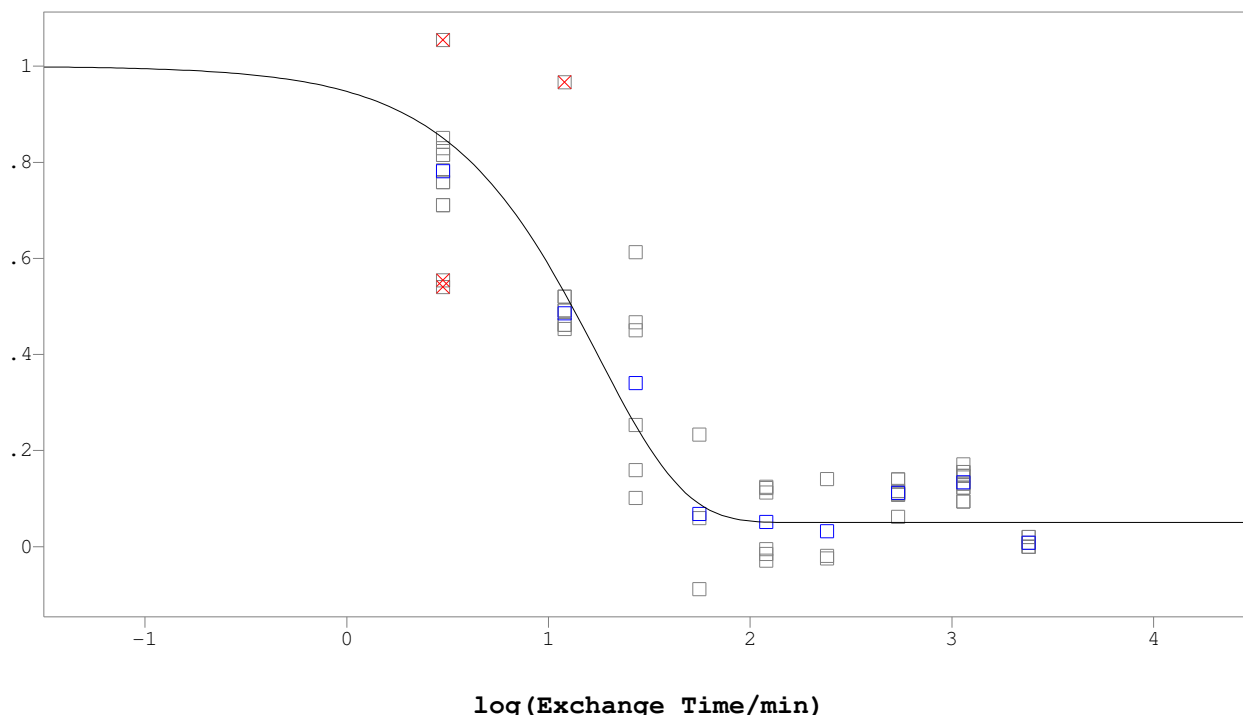
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: 1
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	0.7817	0.8294 (1.0549)	0.8506	0.8157	0.8157	(0.5406)	
		0.7589	0.7589	0.7840	0.7109	0.7109 (0.5548)	
12	0.4861	0.4919	0.4919	0.5208	0.5208	(0.9666) 0.4618	
		0.4618	0.4536				
27	0.3410	0.4676	0.6128	0.2536	0.4505	0.1595 0.1018	
56	0.0684	0.2337	0.0597	-0.0883			
120	0.0519	0.1126	-0.0047	-0.0287	-0.0148	0.1248 0.1221	
240	0.0326	-0.0187	0.1409	-0.0242			
540	0.1121	0.1081	0.1081	0.1162	0.1107	0.1107 0.1124	
		0.1400	0.1400	0.0621			
1140	0.1342	0.1227	0.1227	0.1314	0.1314	0.1478 0.1478	
		0.1717	0.1557	0.1557	0.0942	0.0942	
2400	0.0081	0.0201	0.0201	0.0081	0.0000	0.0000 0.0002	

Fitted rate constant (RC): log(RC*min) = -1.2435 +/- .0627

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBPlu wt

Peptide sequence: KKKISPWI <L> AVLTLQIQSLISCWAFKFKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 9)

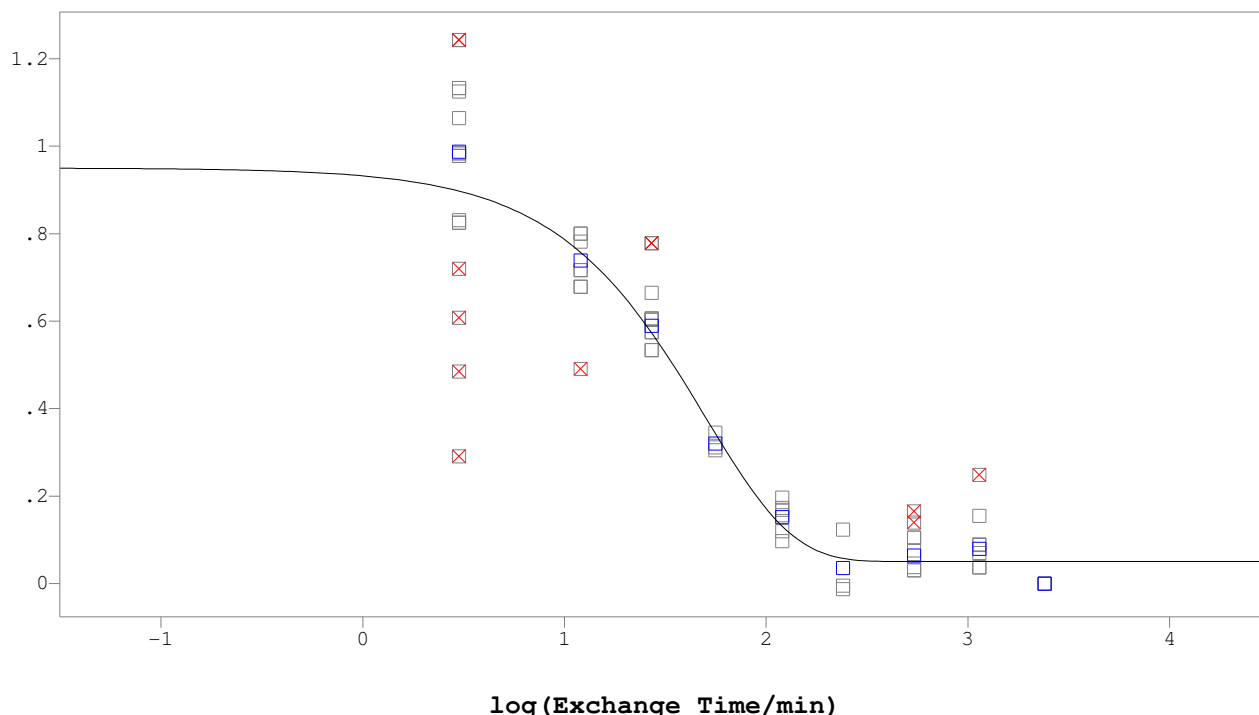
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: .95
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	0.9877	0.9785	0.9785	(0.4854)	(1.2434)	(1.2434)	(0.7197)
		1.1335	1.1335	(0.6081)	1.1251	(0.2910)	0.9840
		0.9840	1.0650	0.8256	0.8256	0.8312	
12	0.7393	0.7170	0.7170	0.8006	0.8006	(0.4909)	0.6787
		0.6787	0.7820				
27	0.5894	0.6034	0.6034	0.6651	0.6068	0.6068	(0.7782)
		(0.7782)	0.5342	0.5342	0.5750	0.5750	
56	0.3206	0.3451	0.3117	0.3047			
120	0.1519	0.1565	0.1195	0.1687	0.0969	0.1731	0.1966
240	0.0355	0.1236	-0.0044	-0.0127			
540	0.0642	0.0306	0.0306	0.0761	0.1049	0.1049	(0.1392)
		0.0376	(0.1654)				
1140	0.0796	0.0370	0.0370	0.0884	0.1550	(0.2485)	0.0900
		0.0700					
2400	0.0000	0.0000	0.0000	0.0000	0.0000		

Fitted rate constant (RC): log(RC*min) = -1.6982 +/- .0385

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBPlu wt

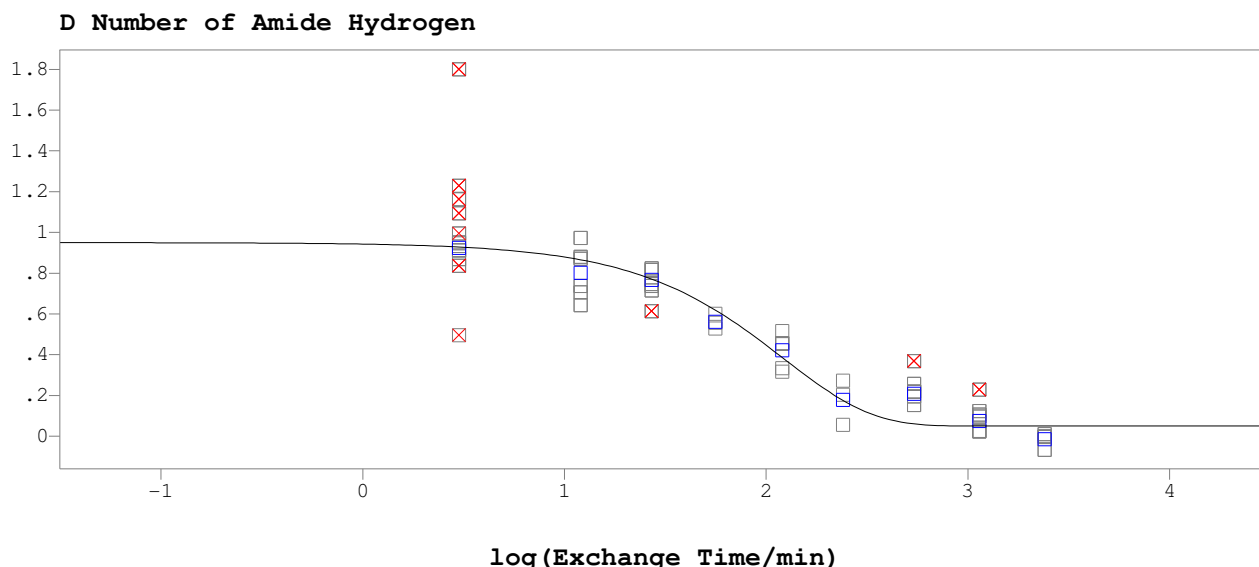
Peptide sequence: KKKISPWIL <A> VLTLLQIQSLISCWAFKKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 10)

Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: .95
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	0.9249	(0.9949)	0.9949	0.9513	0.9513	(0.8371)	(0.8371)
		(1.1638)	(1.1638)	(1.8004)	(1.8004)	(1.2298)	(1.2298)
		(1.0945)	(1.0945)	(0.4957)	0.8705	0.8705	0.9141
		0.9124	0.9124	0.9464			
12	0.8025	0.8718	0.8718	0.6442	0.6442	0.7064	0.7064
		0.7376	0.7376	0.9744	0.9744	0.8803	0.8803
27	0.7688	0.7375	0.7375	(0.6141)	(0.6141)	0.8173	0.8173
		0.7479	0.7479	0.8239	0.8239	0.7169	0.7169
56	0.5624	0.6012	0.5286	0.5572			
120	0.4227	0.3339	0.5167	0.4565	0.4572	0.3171	0.4545
240	0.1786	0.2737	0.0573	0.2047			
540	0.2098	0.2203	0.2203	0.1548	0.1548	0.2584	0.2584
		(0.3693)	(0.3693)	0.2192	0.2192	0.1961	0.1961
1140	0.0758	0.1243	0.1243	0.0263	0.0263	0.0232	0.0232
		(0.2294)	(0.2294)	0.0979	0.0979	0.1070	0.1070
2400	-0.0144	0.0000	0.0000	-0.0649	-0.0649	-0.0032	-0.0032
		0.0105	0.0105				

Fitted rate constant (RC): $\log(\text{RC} \cdot \text{min}) = -2.0872 \pm 0.0611$

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBP1u wt

Peptide sequence: KKKISPWILA <V> LTLQIQSLISCWAFKFKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 11)

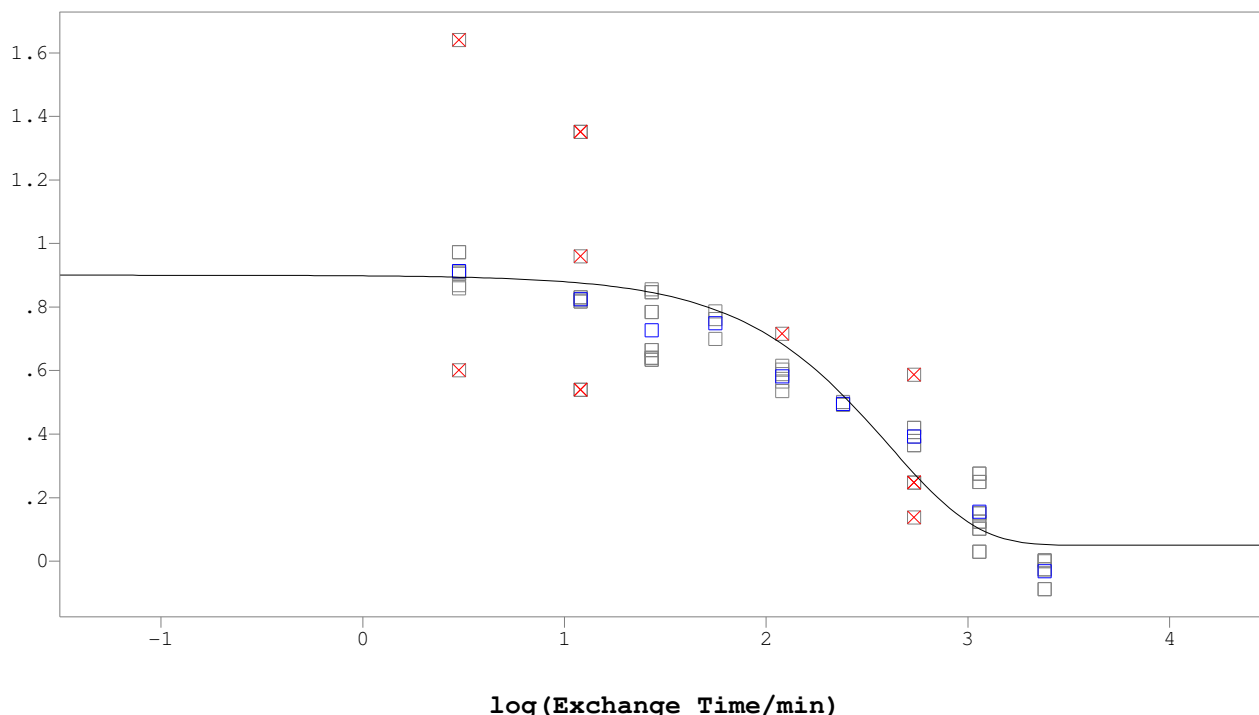
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: .9
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	0.9139	0.8692	0.9055	0.9055	(1.6411)	0.9734	0.9734
		0.8588	(0.6015)	0.9112			
12	0.8246	0.8243	0.8311	0.8311	(0.5396)	(0.5396)	(1.3522)
		(1.3522)	(0.9601)	0.8180	0.8180		
27	0.7276	0.6409	0.6409	0.6652	0.6652	0.8564	0.6350
		0.6350	0.7848	0.7848	0.8472	0.8472	
56	0.7499	0.6999	0.7867	0.7628			
120	0.5821	0.6158	0.5896	0.6030	(0.7163)	0.5661	0.5357
240	0.4961	0.4921	0.4942	0.5017			
540	0.3928	(0.2480)	(0.2480)	(0.1382)	0.3653	0.3653	(0.5872)
		0.4201	0.4201	0.3929			
1140	0.1557	0.1515	0.1515	0.1245	0.1245	0.0302	0.0302
		0.2760	0.2760	0.1023	0.1023	0.2494	0.2494
2400	-0.0314	0.0000	-0.0877	-0.0877	0.0035	0.0035	-0.0255
		-0.0255					

Fitted rate constant (RC): $\log(\text{RC} \cdot \text{min}) = -2.6114 \pm 0.1007$

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBP1u wt

Peptide sequence: KKKISPWILAV <L> TLQIQSLISCWAFKKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 12)

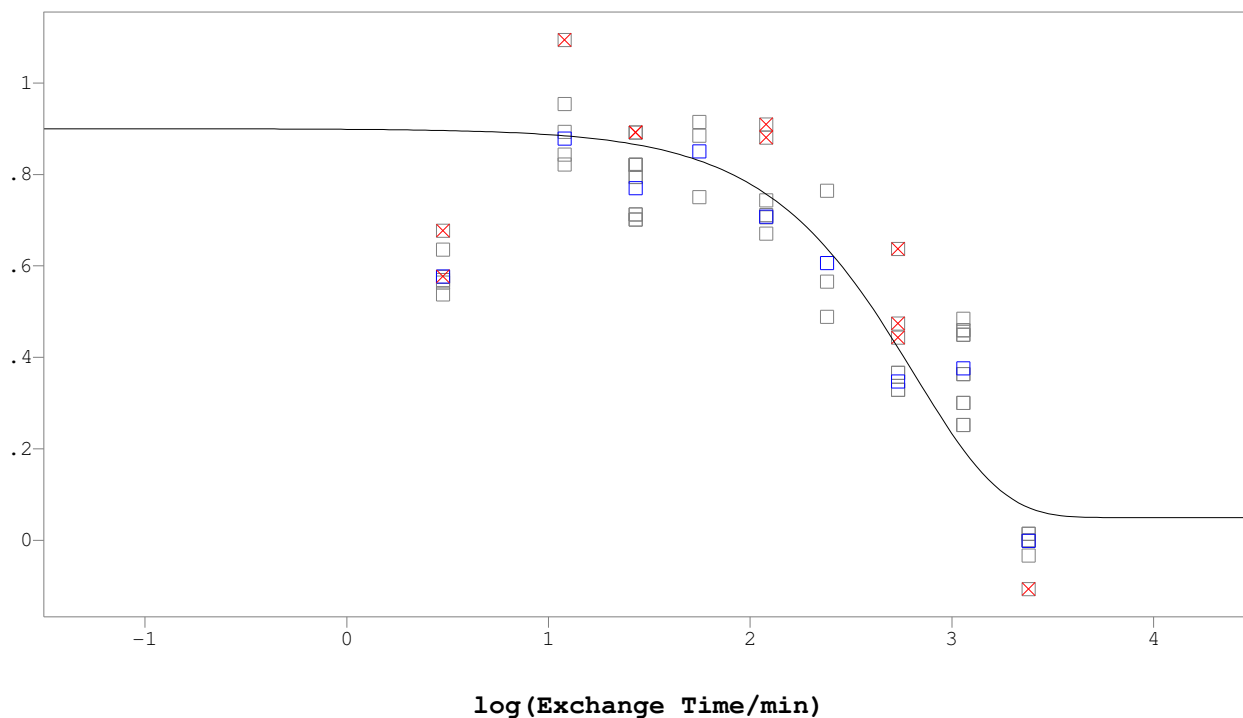
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: .9
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	(0.5770)	0.6363	0.5768	(0.6775)	0.5642	0.5378	0.5697
12	0.8784	0.8933	0.9542	(1.0943)	0.8219	0.8441	
27	0.7704	0.7945	0.7945	0.8212	0.8212	0.7131	0.7131
		0.8216	0.8216	0.7015	0.7015	(0.8920)	(0.8920)
56	0.8505	0.7508	0.8853	0.9154			
120	0.7080	0.7112	0.7067	0.6707	0.7434	(0.9094)	(0.8806)
240	0.6064	0.5657	0.7644	0.4889			
540	0.3481	0.3665	0.3665	0.3296	0.3296	(0.4438)	(0.4746)
		(0.6377)					
1140	0.3764	0.2529	0.2529	0.4598	0.4598	0.4496	0.4496
		0.3012	0.3012	0.3638	0.3638	0.4852	
2400	-0.0007	0.0000	0.0000	(-0.1063)	0.0145	0.0145	-0.0327

Fitted rate constant (RC): log(RC*min) = -2.8151 +/- .2685

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBPlu wt

Peptide sequence: KKKISPWILAVL <T> LQIQSLISCWAFKKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 13)

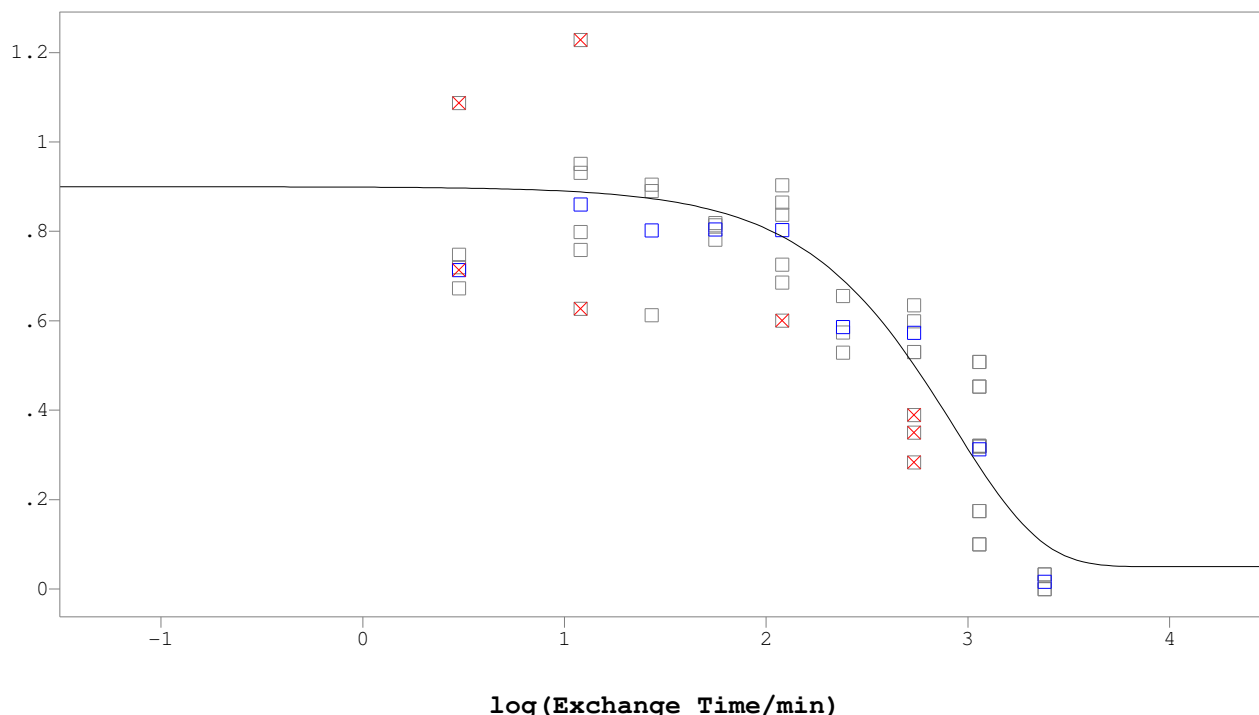
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: .9
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	(0.7136)	0.7202	0.6726	(1.0871)	0.7478		
12	0.8602	0.7590	0.9514	(1.2284)	(0.6269)	0.7992	0.9312
27	0.8026	0.8902	0.6124	0.9050			
56	0.8048	0.8189	0.7814	0.8139			
120	0.8033	0.7256	0.8644	(0.6008)	0.6857	0.9032	0.8373
240	0.5861	0.5739	0.6554	0.5289			
540	0.5737	0.6351	0.5994	(0.3501)	(0.3893)	(0.2839)	0.5301
1140	0.3128	0.1001	0.1001	0.4532	0.4532	0.3210	0.3210
		0.3194	0.3194	0.1749	0.1749	0.5082	0.5082
2400	0.0167	0.0000	0.0000	0.0333	0.0333		

Fitted rate constant (RC): $\log(\text{RC} \cdot \text{min}) = -2.9319 \pm 0.0974$

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBP1u wt

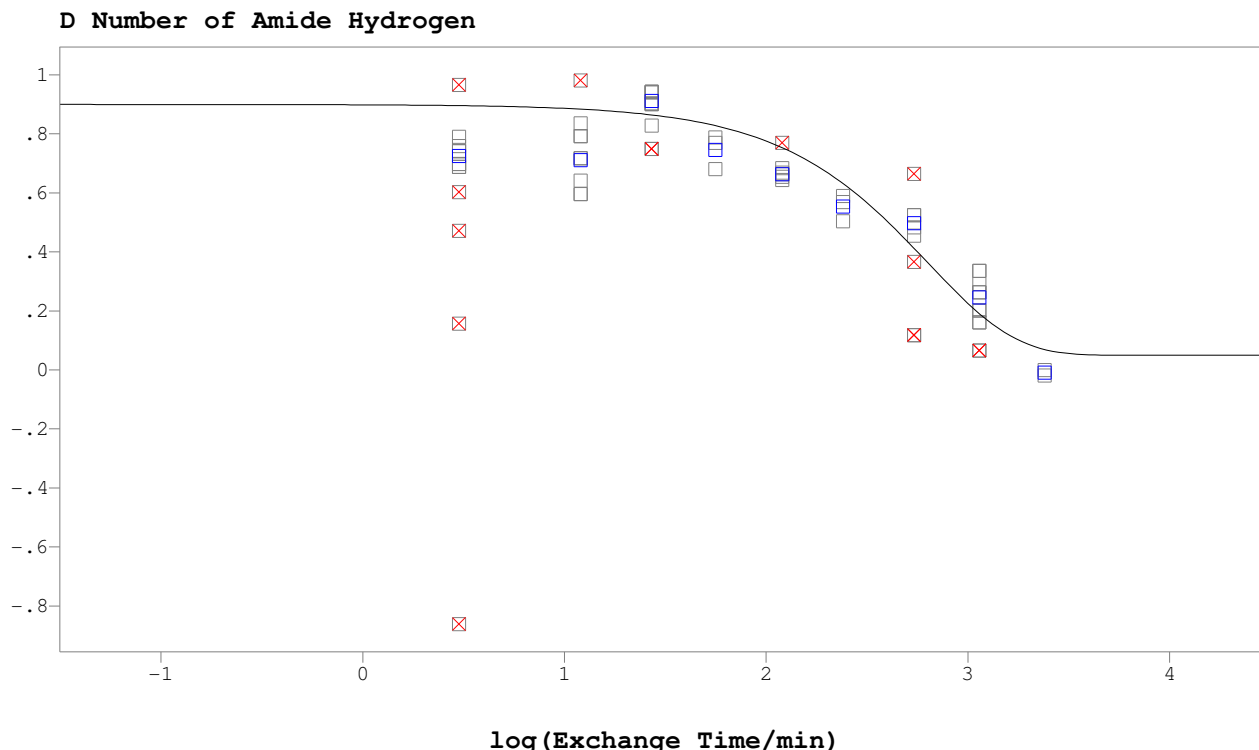
Peptide sequence: KKKISPWILAVLT <L> QIQSLISCWAFKKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 14)

Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: .9
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	0.7260	0.6988	0.6988	(0.9660)	0.7415	0.7415	0.6882
		0.6882	(-0.8611)	(0.6025)	0.7907	(0.4716)	0.7594
		(0.1569)					
12	0.7115	0.5963	0.5963	0.8360	0.7178	0.7178	0.6417
		0.7929	0.7929	(0.9809)			
27	0.9118	0.9034	0.9034	0.9411	0.9411	(0.7488)	(0.7488)
		0.9429	0.9429	0.8287	0.9013	0.9013	
56	0.7462	0.7696	0.7879	0.6809			
120	0.6634	(0.7703)	0.6552	0.6635	0.6843	0.6695	0.6445
240	0.5545	0.5899	0.5046	0.5688			
540	0.4975	(0.6651)	0.5253	0.5253	0.4835	(0.1182)	(0.1182)
		0.4558	(0.3660)				
1140	0.2466	0.3367	0.3367	0.2636	0.2636	(0.0666)	(0.0666)
		0.2018	0.2018	0.2918	0.1617	0.1617	
2400	-0.0091	0.0000	-0.0182				

Fitted rate constant (RC): $\log(\text{RC} \cdot \text{min}) = -2.8028 \pm 0.1453$

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBP1u wt

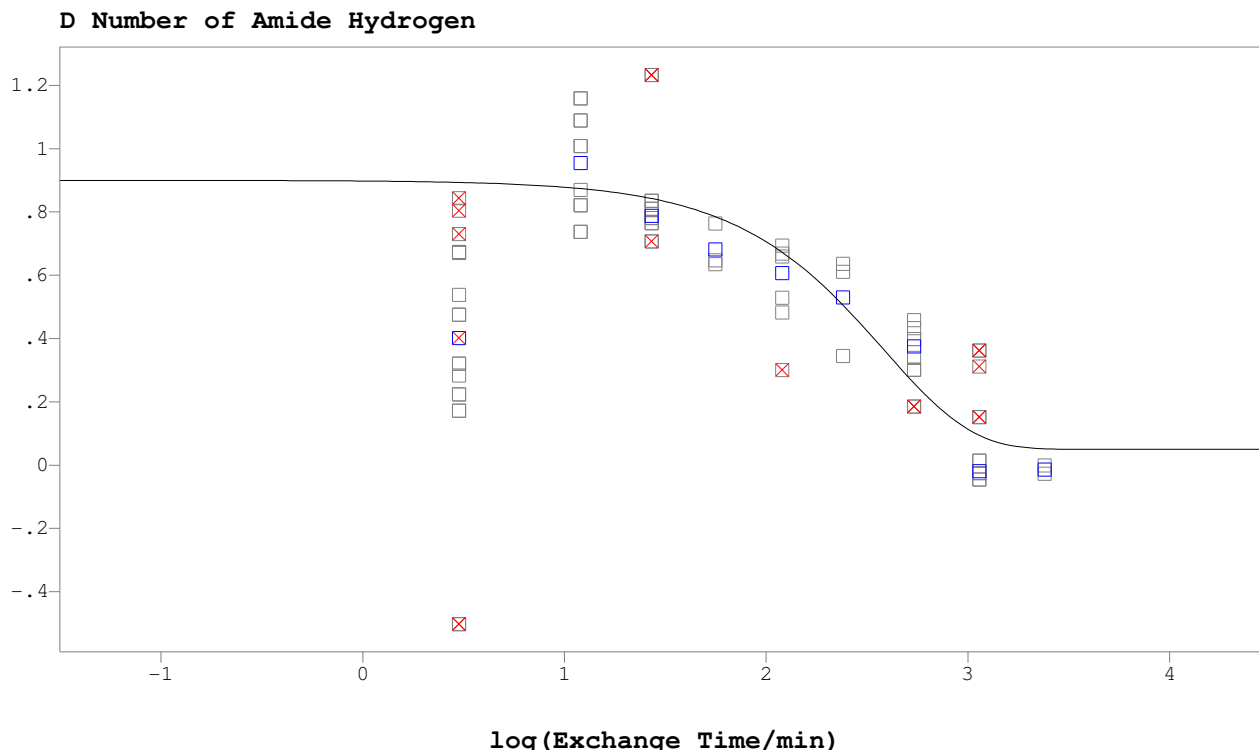
Peptide sequence: KKKISPWILAVLTL <Q> IQSLISCWAFKKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 15)

Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: .9
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	(0.4022)	0.4762	0.4762	0.1728	0.1728	0.6736	0.6736
		0.3215	0.3215	(-0.5020)	(-0.5020)	0.2237	0.2237
		(0.7302)	(0.8443)	(0.8040)	0.5382	0.6709	0.2836
12	0.9547	1.1591	1.1591	1.0891	1.0891	0.8697	0.8213
27	0.7879	0.8354	0.8354	0.8107	0.8107	(1.2333)	(1.2333)
		0.7808	0.7808	(0.7071)	0.7071	0.7647	0.7647
56	0.6824	0.6360	0.7637	0.6473			
120	0.6071	0.6943	0.4827	0.6689	0.6600	(0.3014)	0.5292
240	0.5309	0.6108	0.3450	0.6369			
540	0.3762	0.3391	0.3987	0.3987	0.4586	(0.1856)	(0.1856)
		0.4335	0.3024	0.3024			
1140	-0.0180	(0.3629)	(0.3629)	0.0153	0.0153	-0.0450	-0.0450
		(0.1527)	(0.1527)	(0.3119)	-0.0243	-0.0243	
2400	-0.0133	0.0000	-0.0266				

Fitted rate constant (RC): log(RC*min) = -2.5866 +/- .116

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBPlu wt

Peptide sequence: KKKISPWILAVLTLLQ <I> QSLISCWAFKKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 16)

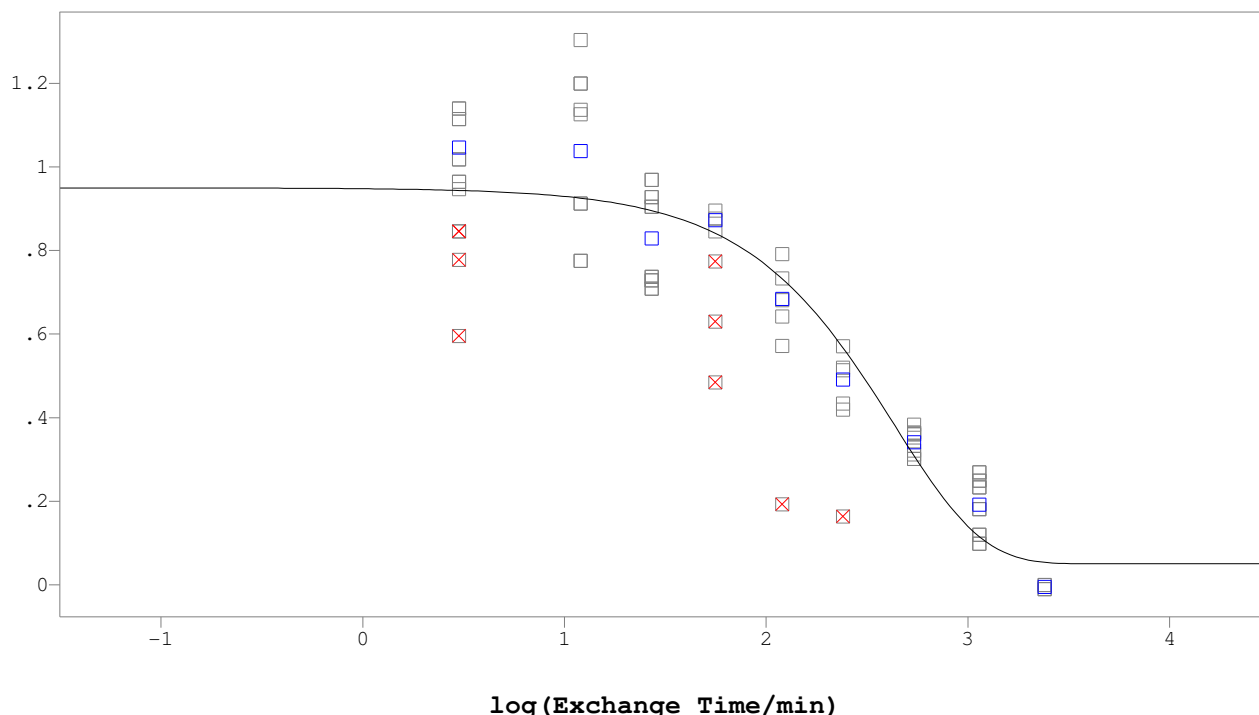
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: .95
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	1.0473	0.9477 (0.8464)	(0.8464)	1.0182	1.0182	(0.5955)	
		1.1403	1.1403	0.9653	0.9653	1.1149	1.1149
		(0.7780)					
12	1.0384	1.3045	1.2000	1.2000	1.1372	0.9128	0.9128
		1.1265	0.7757	0.7757			
27	0.8298	0.9052	0.9052	0.7290	0.7290	0.9696	0.9696
		0.7092	0.7092	0.9283	0.9283	0.7372	0.7372
56	0.8732	(0.6303)	(0.4850)	0.8962	0.8771	(0.7743)	0.8461
120	0.6844	0.6816	0.5719	0.7922	0.6425	(0.1930)	0.7338
240	0.4918	0.5138	0.4196	0.4341	(0.1636)	0.5199	0.5714
540	0.3414	0.3126	0.3609	0.3609	0.3838	0.3644	0.3644
		0.3217	0.3016	0.3016			
1140	0.1921	0.1815	0.1815	0.0984	0.0984	0.2495	0.2495
		0.2693	0.2693	0.2333	0.2333	0.1202	0.1202
2400	-0.0052	0.0000	0.0000	-0.0103	-0.0103		

Fitted rate constant (RC): $\log(\text{RC} \cdot \text{min}) = -2.6378 \pm .1014$

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBPlu wt

Peptide sequence: KKKISPWILAVLTLQI <Q> SLISCWAFKFKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 17)

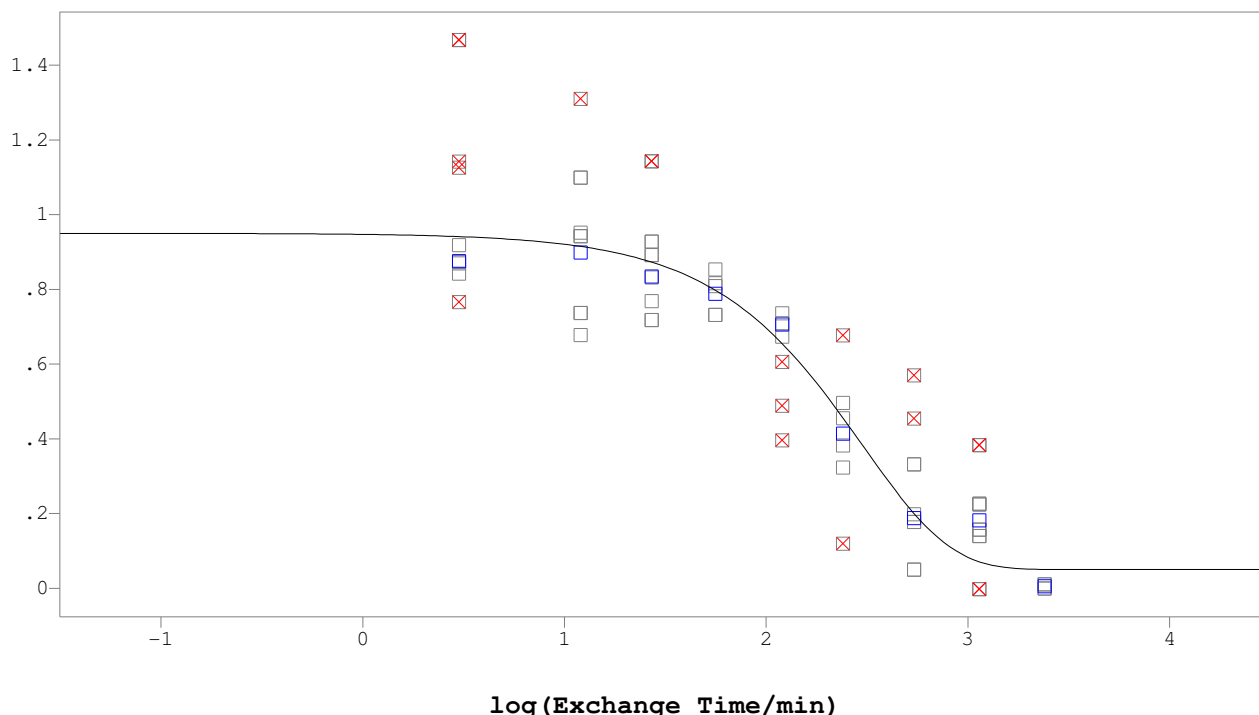
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: .95
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	0.8765	(1.4682)	(1.4682)	(1.1261)	0.8701	(0.7662)	0.8737
		(1.1423)	0.9191	0.8427			
12	0.8988	0.9432	0.9432	0.6783	1.0994	1.0994	0.9524
		0.7372	0.7372	(1.3108)			
27	0.8348	0.8921	0.8921	0.7691	0.7182	0.7182	0.9283
		0.9283	(1.1429)	(1.1429)	0.8319		
56	0.7888	0.7320	0.8095	0.8540	0.7320	0.8165	
120	0.7066	(0.4887)	0.7363	0.7096	(0.6061)	(0.3963)	0.6738
240	0.4145	0.4555	0.3232	(0.6769)	(0.1192)	0.3822	0.4969
540	0.1883	0.0500	0.0500	(0.5703)	0.3319	0.3319	(0.4544)
		0.1779	0.1779	0.1981			
1140	0.1818	(-0.0022)	(-0.0022)	0.1573	0.1573	(0.3835)	(0.3835)
		0.1402	0.1402	0.2265	0.2265	0.2241	
2400	0.0054	0.0000	0.0000	0.0107	0.0107		

Fitted rate constant (RC): log(RC*min) = -2.4801 +/- .0609

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBP1u wt

Peptide sequence: KKKISPWILAVLTLQIQ <S> LISCWAFKKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 18)

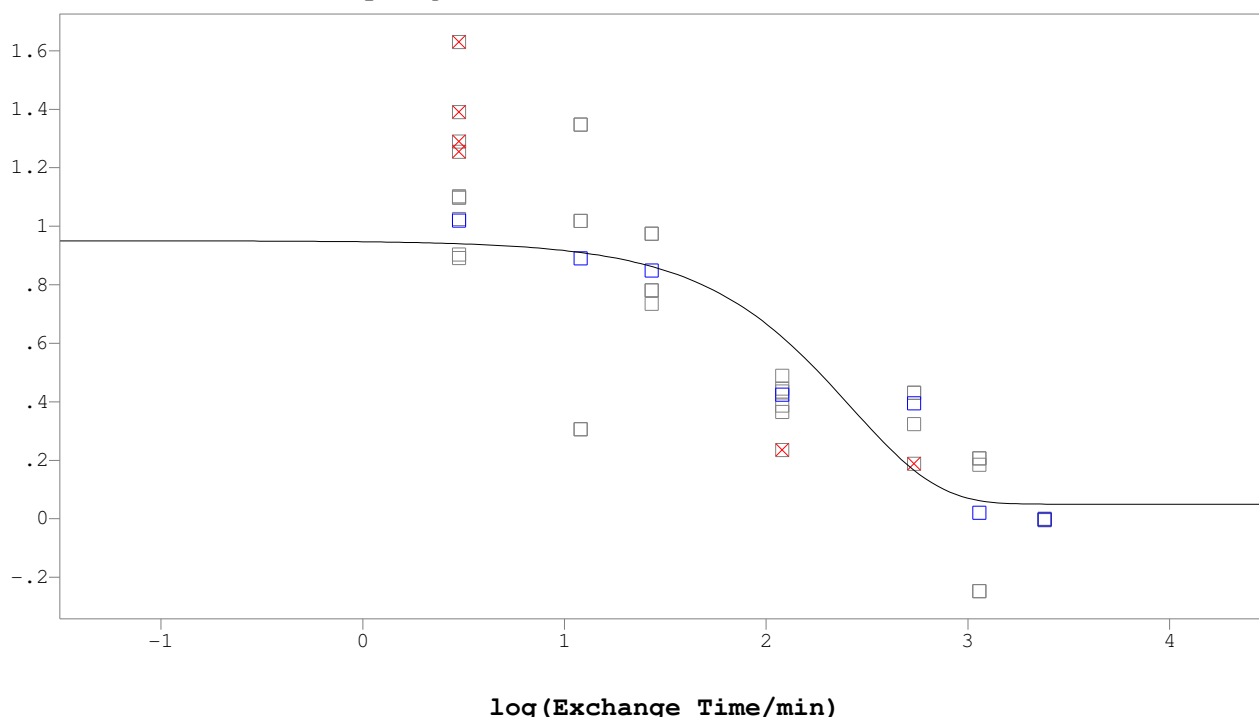
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: .95
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	1.0203	1.0989	1.0989	(1.2905)	(1.3904)	0.8924	1.1026
		0.9038	(1.2552)	1.0253	(1.6304)		
12	0.8912	0.3068	0.3068	1.0185	1.0185	1.3481	1.3481
27	0.8497	0.7809	0.7809	0.9752	0.9752	0.7360	
56	56	D numbers lacking					
120	0.4250	(0.2352)	0.4357	0.3653	0.4896	0.3879	0.4459
240	240	D numbers lacking					
540	0.3953	0.4309	0.4309	0.3239	(0.1883)		
1140	0.0211	0.1856	-0.2469	-0.2469	0.2067	0.2067	
2400	-0.0018	0.0000	0.0000	-0.0036	-0.0036		

Fitted rate constant (RC): $\log(\text{RC} \cdot \text{min}) = -2.4215 \pm 0.3506$

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBP1u wt

Peptide sequence: KKKISPWILAVLTLQIQS <L> ISCWAFKKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 19)

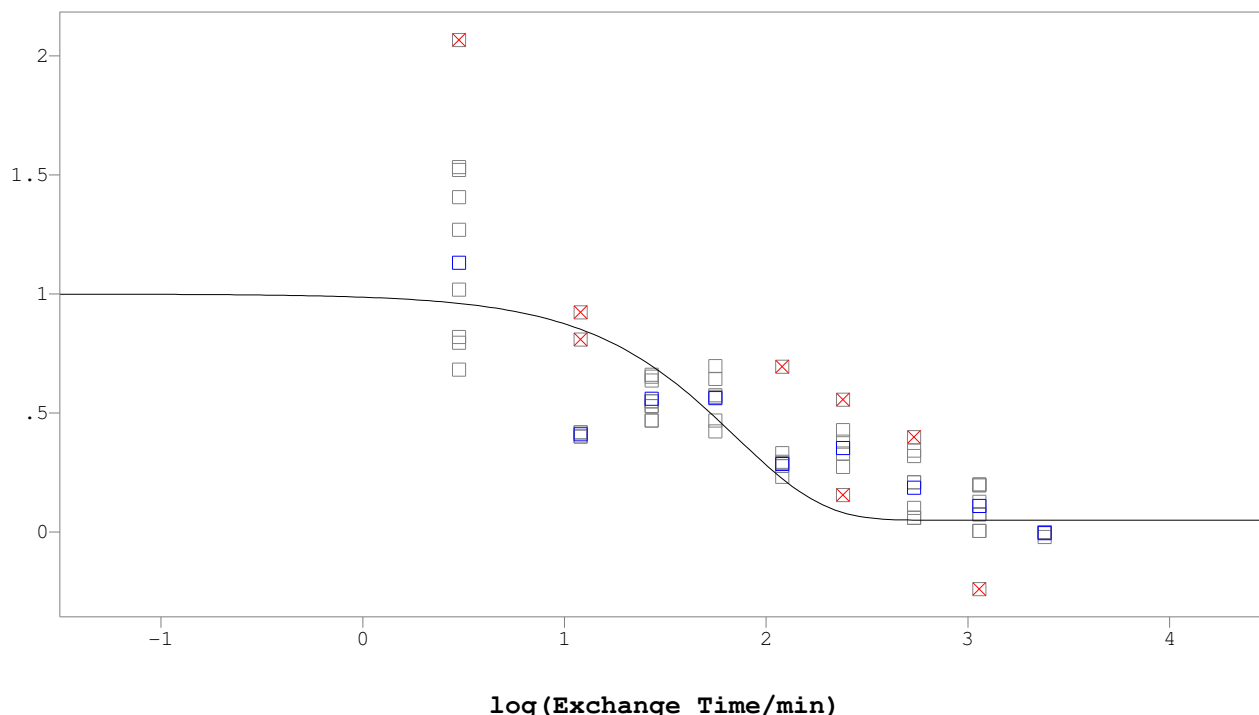
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: 1
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	1.1312	1.5218	1.2701	0.7956	(2.0670)	1.0184	0.8194
		1.4075	0.6830	1.5330			
12	0.4111	0.4025	0.4025	0.4196	0.4196	(0.8091)	(0.9233)
27	0.5609	0.5494	0.5494	0.6615	0.4691	0.4691	0.6366
		0.5296	0.5296	0.6534			
56	0.5631	0.5751	0.6976	0.4239	0.6441	0.4696	0.5682
120	0.2860	0.2332	0.3319	0.2784	0.2907	(0.6951)	0.2954
240	0.3534	0.3800	0.2739	0.4291	(0.1561)	0.3306	(0.5567)
540	0.1864	0.1024	0.3422	0.2096	0.2096	(0.3996)	0.0608
		0.0608	0.3193				
1140	0.1110	0.0056	0.0056	0.1284	0.2004	0.2004	(-0.2391)
		0.0756	0.0756	0.1959			
2400	-0.0039	0.0000	0.0000	0.0000	0.0000	-0.0193	

Fitted rate constant (RC): $\log(\text{RC} \cdot \text{min}) = -1.8508 \pm 0.3219$

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBP1u wt

Peptide sequence: KKKISPWILAVLTLQIQSL <I> SCWAFKKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 20)

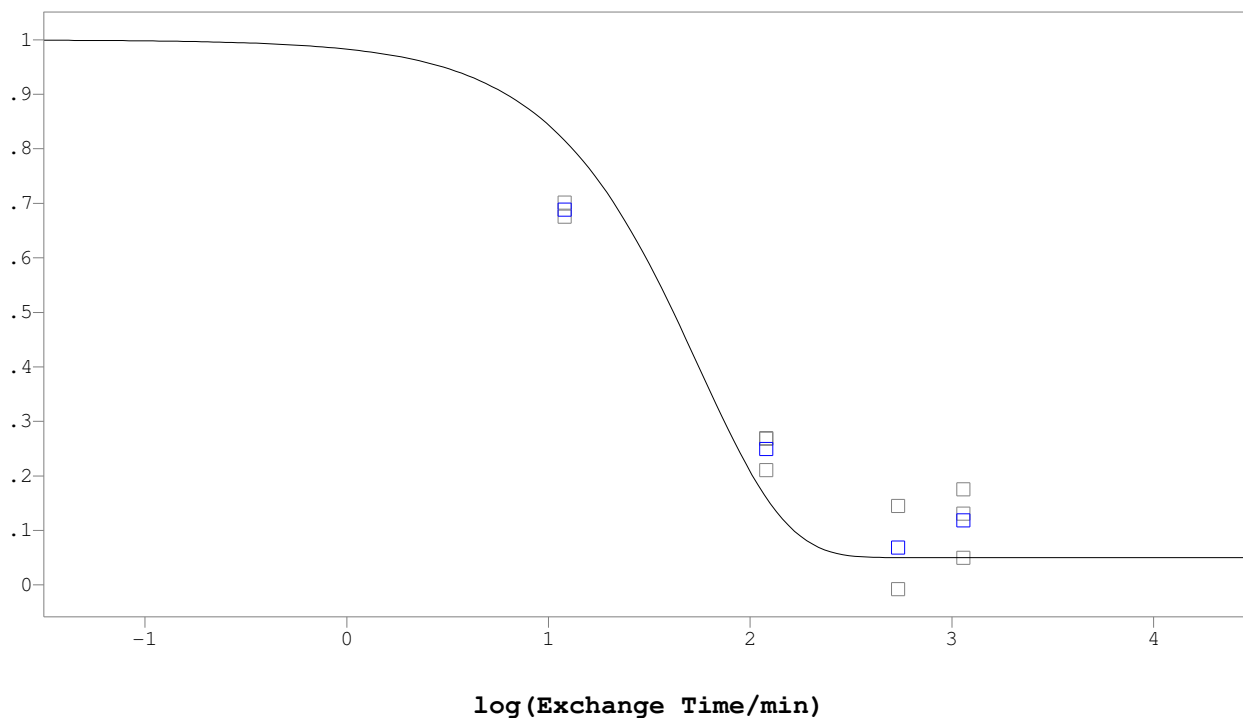
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: 1
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)
3	3	D numbers lacking
12	0.6888	0.7015 0.6760
27	27	D numbers lacking
56	56	D numbers lacking
120	0.2496	0.2695 0.2686 0.2106
240	240	D numbers lacking
540	0.0688	-0.0076 0.1452
1140	0.1188	0.1759 0.1307 0.0498
2400	2400	D numbers lacking

Fitted rate constant (RC): $\log(\text{RC} \cdot \text{min}) = -1.7465 \pm 0.3247$

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBP1u wt

Peptide sequence: KKKISPWILAVLTLQIQSLI <S> CWAFKKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 21)

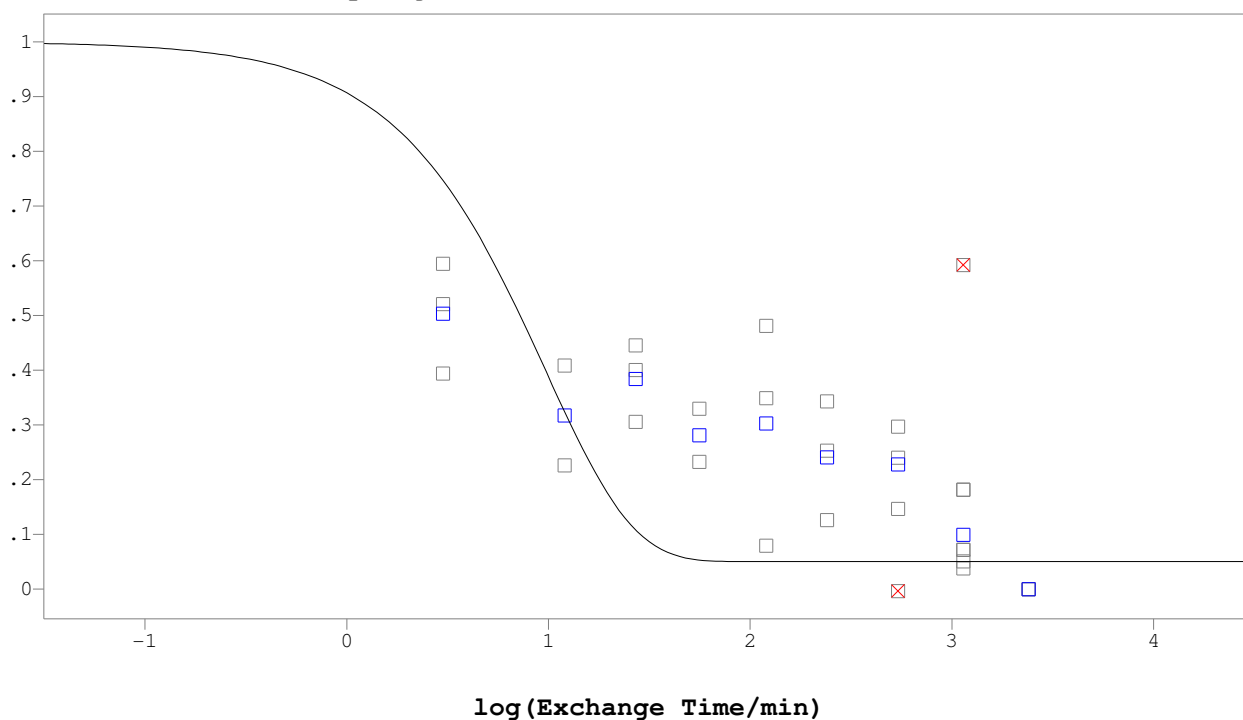
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: 1
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)	
3	0.5033	0.5212	0.3939 0.5947
12	0.3172	0.2260	0.4083
27	0.3840	0.4005	0.4456 0.3058
56	0.2814	0.2328	0.3299
120	0.3030	0.3487	0.0792 0.4810
240	0.2408	0.2528	0.1260 0.3434
540	0.2279	0.1464 (-0.0037)	0.2971 0.2400
1140	0.0992	0.1815	0.1815 0.0507 0.0718 0.0718 (0.5921)
		0.0379	
2400	0.0000	0.0000	0.0000

Fitted rate constant (RC): $\log(\text{RC} \cdot \text{min}) = -0.9858 \pm 0.5881$

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBP1u wt

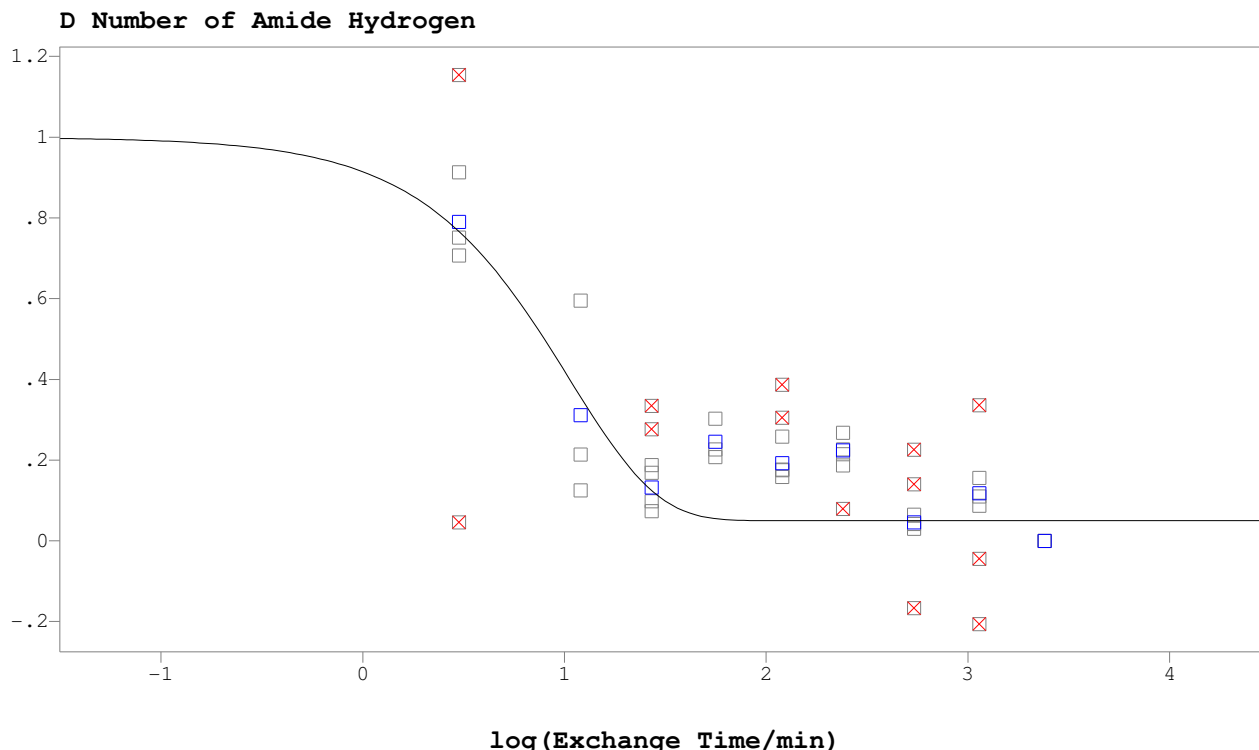
Peptide sequence: KKKISPWILAVLTLQIQLIS <C> WAFKKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 22)

Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: 1
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)				
3	0.7907	(1.1545)	0.7075	0.7513	0.9132	(0.0462)
12	0.3115	0.5956	0.2138	0.1249		
27	0.1324	(0.3342)	0.0983	(0.2764)	0.0741	0.1880 0.1689
56	0.2457	0.3027	0.2077	0.2266		
120	0.1924	(0.3867)	0.1753	(0.3051)	0.1588	0.2585 0.1767
240	0.2244	0.1872	0.2683	(0.0796)	0.2147	0.2270
540	0.0458	(0.2259)	0.0654	(-0.1662)	0.0418	0.0302 (0.1403)
1140	0.1180	(0.3365)	0.0872	(-0.2061)	0.1564	(-0.0442) 0.1102
2400	0.0000	0.0000	0.0000			

Fitted rate constant (RC): $\log(\text{RC} \cdot \text{min}) = -1.0272 \pm 0.1164$

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBP1u wt

Peptide sequence: KKKISPWILAVLTLQIQSLISC <W> AFKKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 23)

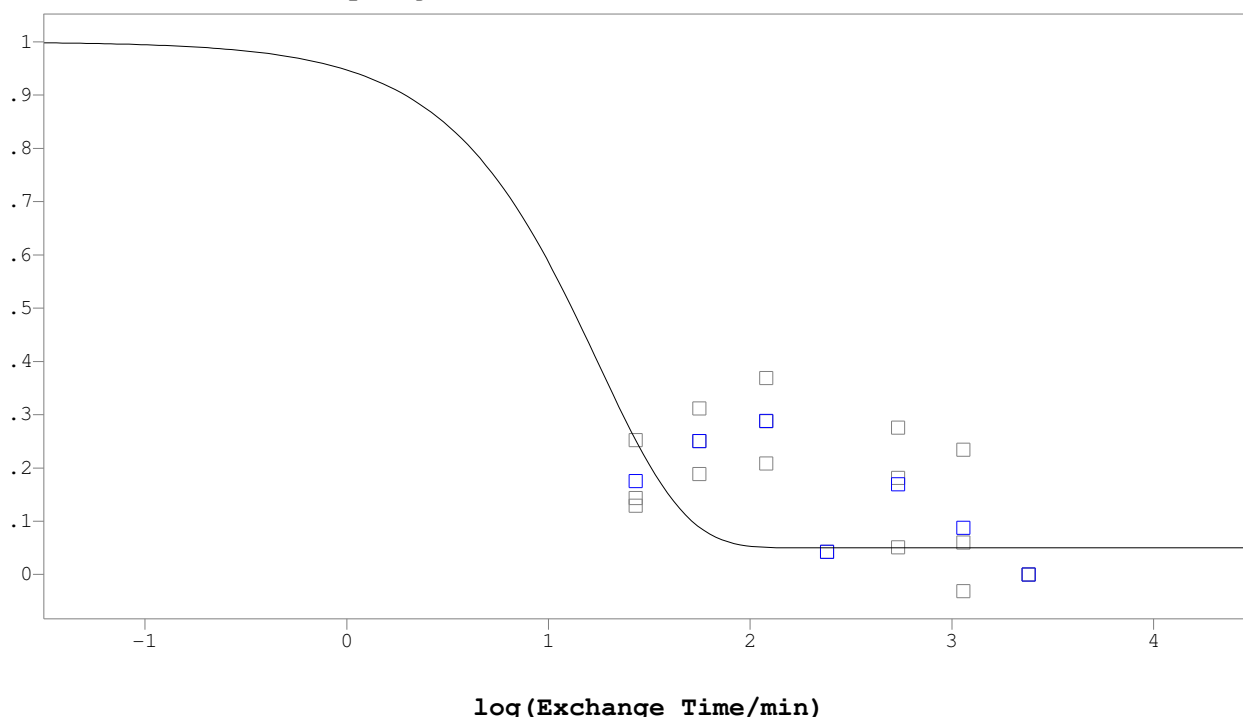
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: 1
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)		
3	3	D numbers lacking		
12	12	D numbers lacking		
27	0.1755	0.2527	0.1296	0.1440
56	0.2507	0.3122	0.2508	0.1888
120	0.2886	0.2880	0.3692	0.2084
240	0.0429	0.0428		
540	0.1697	0.2759	0.0512	0.1817
1140	0.0879	0.2344	-0.0310	0.0603
2400	0.0000	0.0000	0.0000	

Fitted rate constant (RC): $\log(\text{RC} \cdot \text{min}) = -1.2435 \pm 0.1241$

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBP1u wt

Peptide sequence: KKKISPWILAVLTLQIQLISCW <A> FKKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 24)

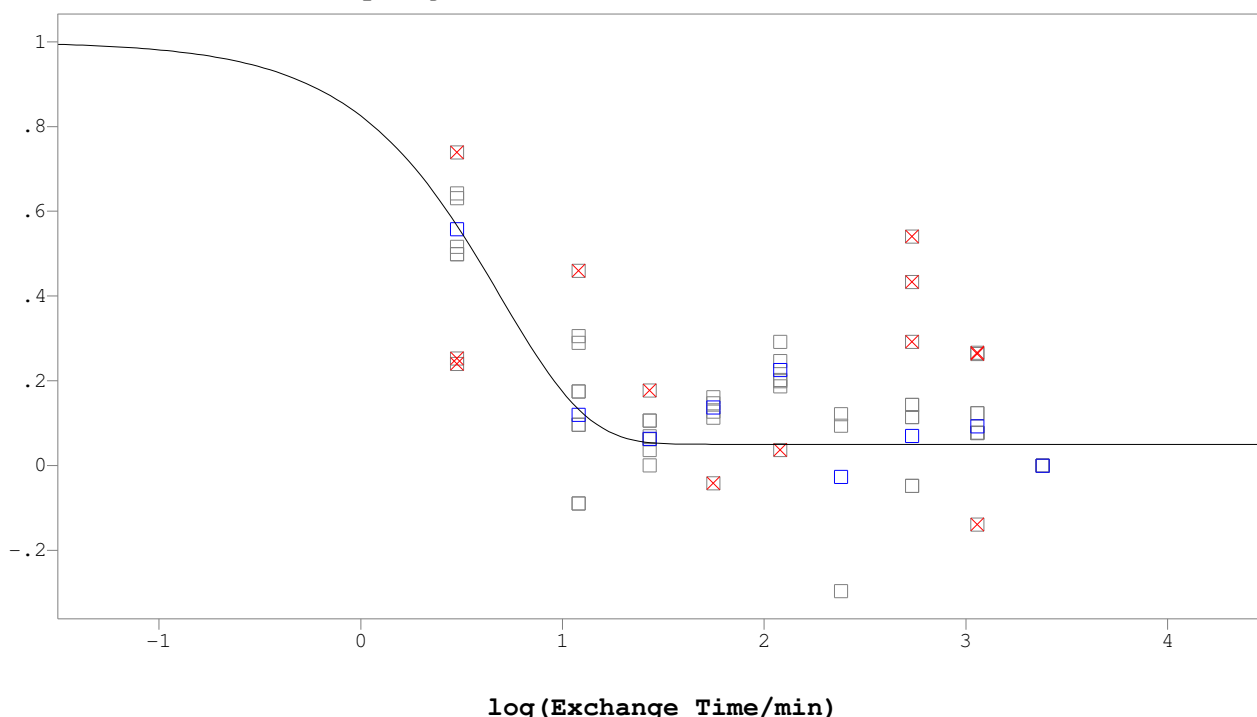
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: 1
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)		D Number (s)			
3	0.5577	(0.2398)	(0.2529)	0.5164	0.6311	0.6423	(0.7391)
		0.4991	0.4991				
12	0.1197	0.3053	0.1748	0.1748	(0.4597)	0.0962	0.0962
		0.2895	-0.0896	-0.0896			
27	0.0634	0.0003	0.0624	0.0624	0.0370	0.1061	0.1061
		(0.1770)	0.0690				
56	0.1373	(-0.0415)	0.1274	0.1128	0.1616	0.1472	
120	0.2253	(0.0371)	0.1990	0.2917	0.1867	0.2468	0.2020
240	-0.0270	0.0940	-0.2964	0.1214			
540	0.0701	(0.2920)	0.1434	0.1434	(0.5408)	0.1146	0.1146
		(0.4334)	-0.0478	-0.0478			
1140	0.0927	(-0.1388)	0.0769	0.0769	(0.2635)	0.0777	0.0777
		(0.2663)	0.1234	0.1234			
2400	0.0000	0.0000	0.0000	0.0000	0.0000		

Fitted rate constant (RC): log(RC*min) = -.6917 +/- .0836

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBP1u wt

Peptide sequence: KKKISPWILAVLTLQIQLISCWA <F> KKK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 25)

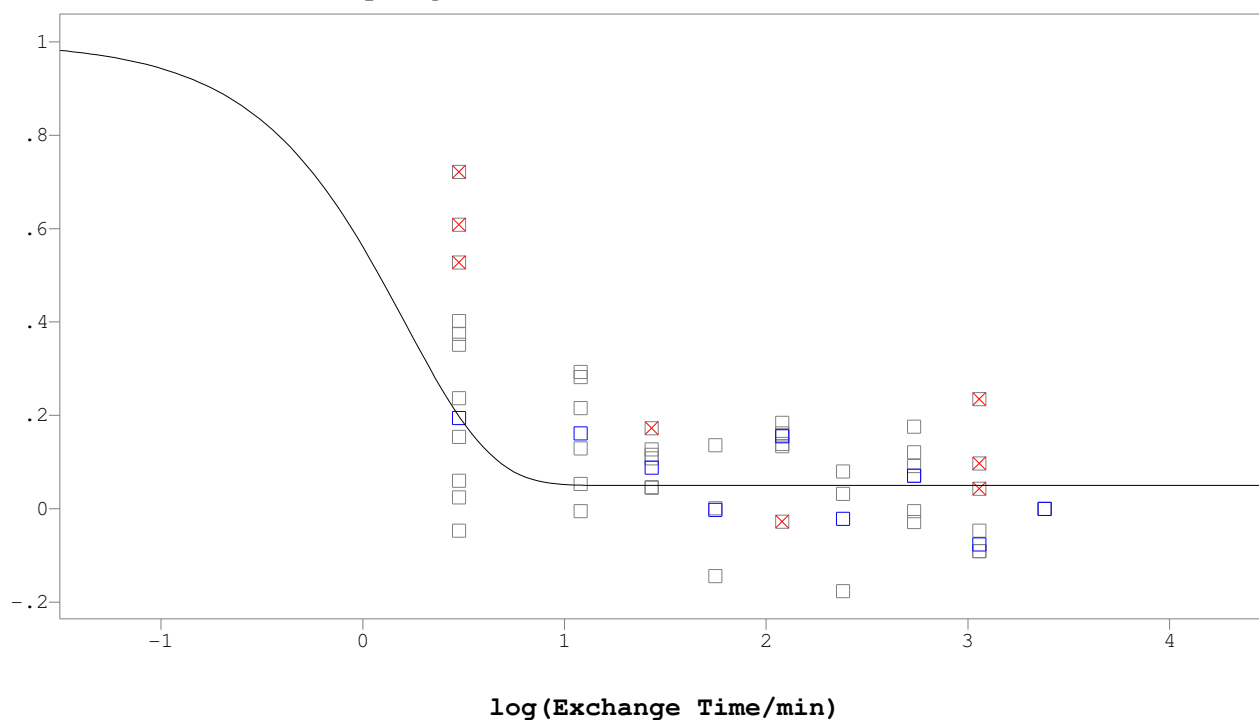
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: 1
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	0.1949	0.0249	(0.5277)	(0.6085)	0.3517	0.2371	0.3747
		0.4024	-0.0461	0.1540	0.0603	(0.7216)	
12	0.1617	0.2935	0.0535	0.2825	0.1297	0.2157	-0.0048
27	0.0889	0.1160	0.0455	(0.1725)	0.1274	0.1084	0.0468
56	-0.0019	0.0014	-0.1437	0.1366			
120	0.1554	(-0.0274)	0.1615	0.1341	0.1841	0.1575	0.1394
240	-0.0212	0.0321	-0.1760	0.0802			
540	0.0713	0.1764	0.1211	0.0709	0.0918	-0.0046	-0.0277
1140	-0.0758	-0.0464	(0.0430)	(0.2349)	-0.0904	-0.0904	(0.0974)
2400	0.0000	0.0000	0.0000				

Fitted rate constant (RC): $\log(\text{RC} \cdot \text{min}) = -0.2081 \pm 0.1471$

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBP1u wt

Peptide sequence: KKKISPWILAVLTLQIQLISCWAF <K> KK
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 26)

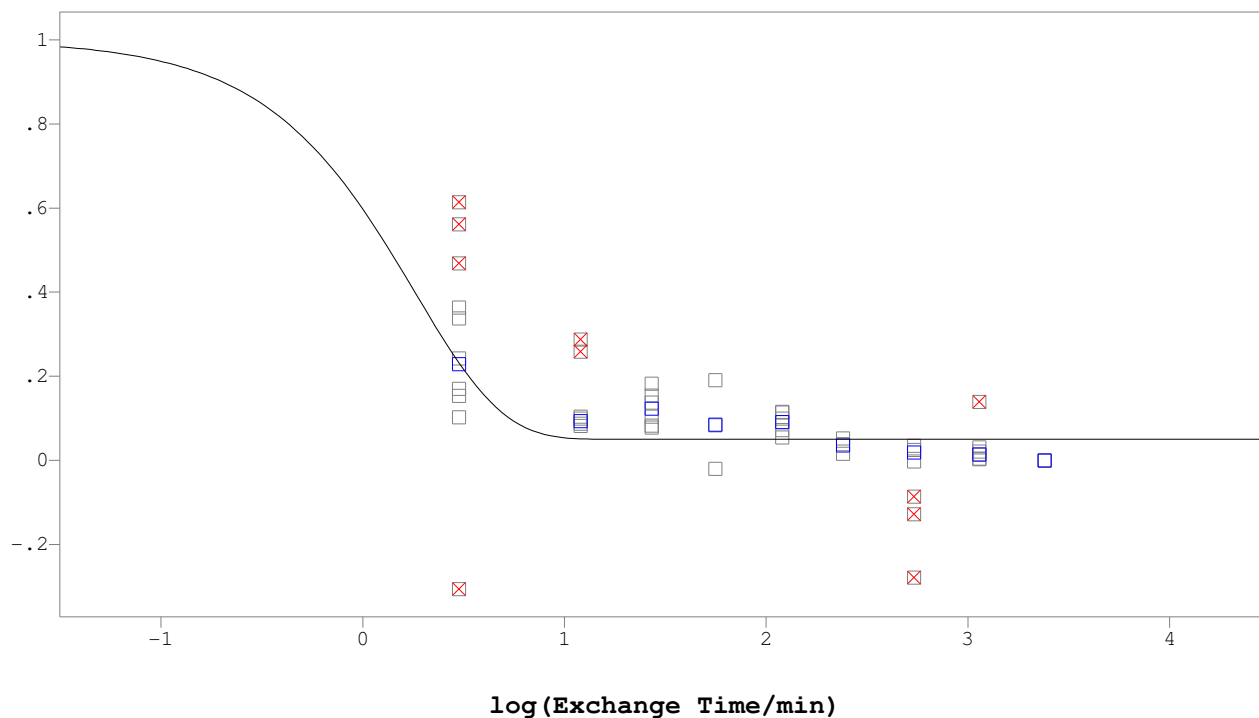
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: 1
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	0.2287	(0.4687)	(0.6143)	0.3639	0.1029	0.3382	0.2429
		0.1534	(-0.3059)	0.1705	(0.5616)		
12	0.0935	(0.2877)	0.0998	(0.2585)	0.0875	0.1042	0.0822
27	0.1236	0.1378	0.1548	0.1829	0.1045	0.0785	0.0830
56	0.0851	0.1910	-0.0195	0.0839			
120	0.0912	0.0545	0.1140	0.1160	0.0719	0.0994	0.0912
240	0.0357	0.0157	0.0522	0.0391			
540	0.0192	(-0.0857)	0.0351	(-0.1277)	-0.0026	(-0.2781)	0.0249
1140	0.0148	0.0315	0.0045	(0.1395)	0.0136	0.0027	0.0212
2400	0.0000	0.0000	0.0000				

Fitted rate constant (RC): $\log(\text{RC} \cdot \text{min}) = -0.2592 \pm 0.0666$

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBP1u wt

Peptide sequence: KKKISPWILAVLTLQIQLISCWAFK <K> K
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 27)

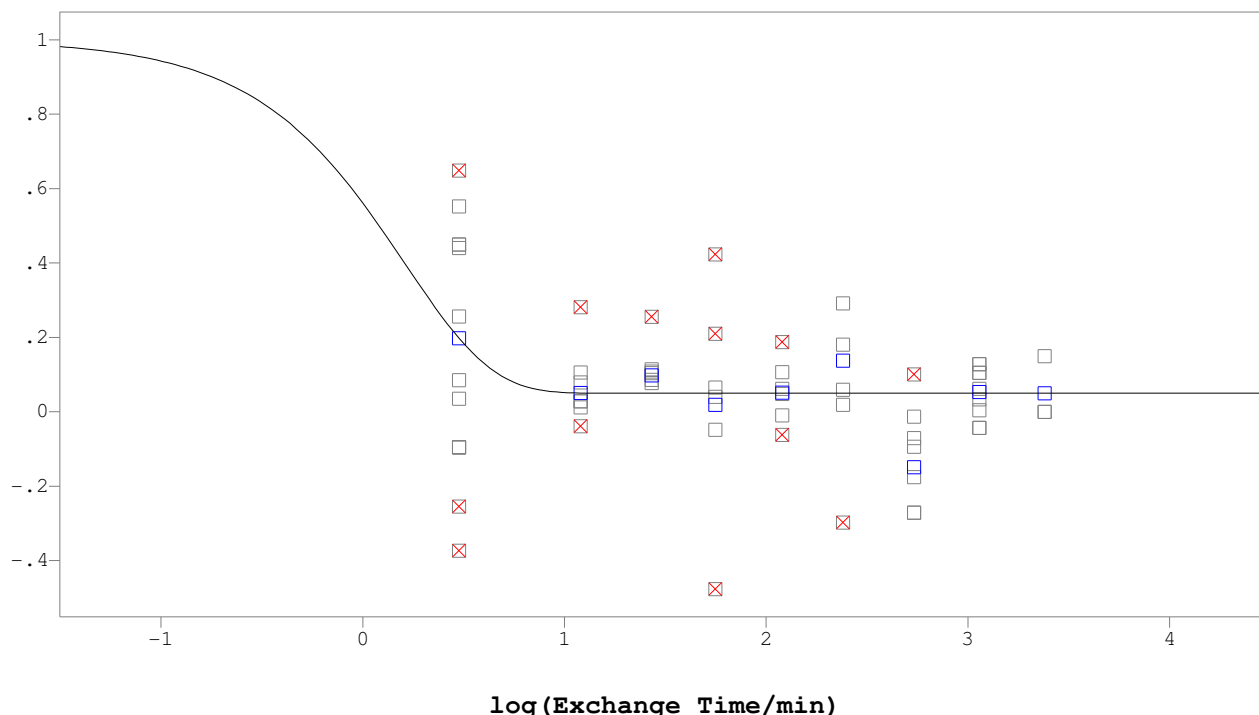
Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: 1
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	0.1985	-0.0944	-0.0944	0.2568	-0.0961	0.4498	0.4498
		(-0.2542)	0.0355	0.0850	0.5522	(-0.3729)	(0.6484)
		0.4405					
12	0.0507	(0.2817)	0.1058	0.0283	0.0283	(-0.0384)	0.0120
		0.0791					
27	0.0983	0.1147	(0.2556)	0.1082	0.0864	0.0778	0.1043
56	0.0191	(0.4233)	(-0.4764)	(0.2098)	0.0402	0.0653	-0.0482
120	0.0519	(0.1879)	-0.0093	0.1066	(-0.0620)	0.0482	0.0621
240	0.1377	0.0595	0.1805	0.2919	0.0187	(-0.2975)	
540	-0.1489	-0.1756	-0.0129	-0.0931	-0.0705	-0.2707	-0.2707
		(0.1012)					
1140	0.0534	-0.0431	-0.0431	0.0049	0.1049	0.1049	0.0623
		0.1281	0.1281	0.0338			
2400	0.0500	0.0000	0.1499	0.0000			

Fitted rate constant (RC): log(RC*min) = -.2081 +/- .1471

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers

D Number of Amide Hydrogen



hdx_etd_kin-File: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\...
 ...wild_type_B.hdx_etd_kin

Peptide name: XBP1u wt

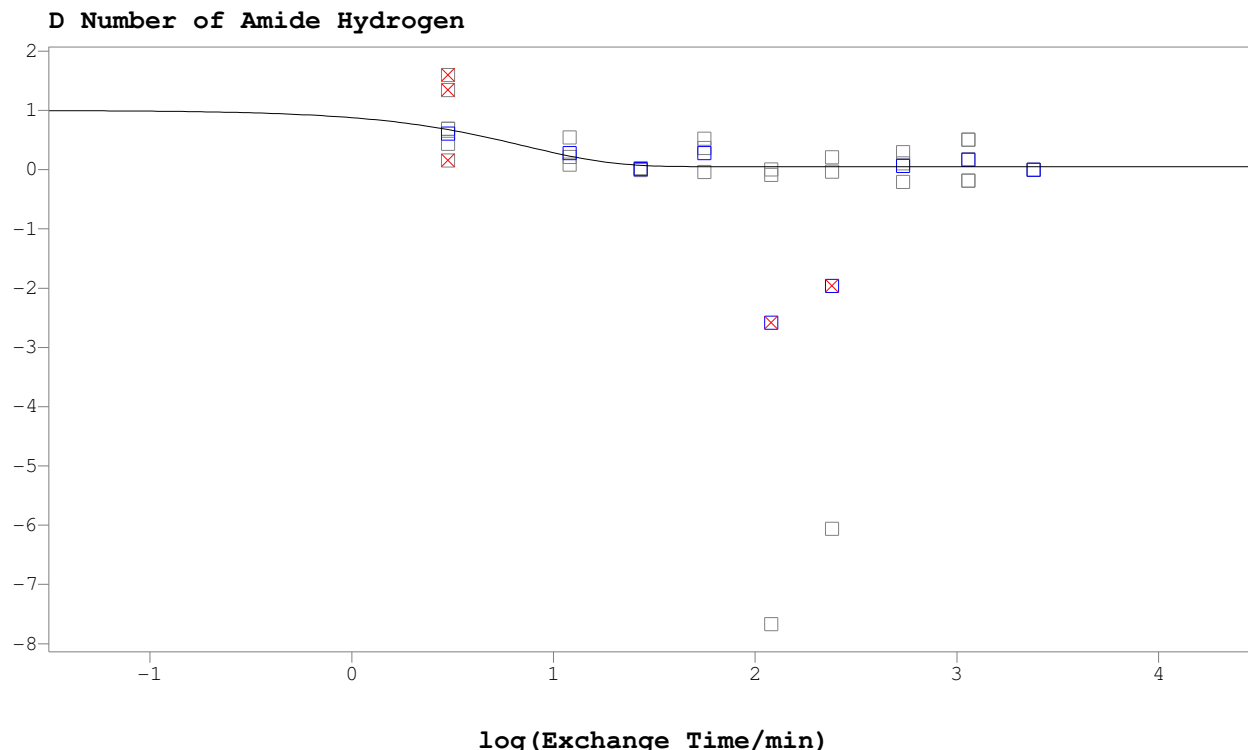
Peptide sequence: KKKISPWILAVLTLQIQLISCWAFKK <K>
 (Amino acid of amide hydrogen enclosed by parentheses, number of amino acid: 28)

Automated outlier determination: medium sensitivity
 Asymptotic D number: .05
 Starting D number: 1
 Numbers in parentheses: Not used for calculation of mean or for curve fitting

Exchange Time [min]	Mean D Number	D Number (s)					
3	0.6090	(0.1591)	0.6936	0.6936	0.4398	(1.3454)	(1.6009)
12	0.2835	0.5447	0.2181	0.0875			
27	0.0095	-0.0038	0.0276	0.0049			
56	0.2847	0.5247	0.3674	-0.0382			
120	(-2.5820)	-7.6686	0.0071	-0.0844			
240	(-1.9592)	-6.0587	0.2145	-0.0332			
540	0.0662	-0.2060	0.1084	0.2964			
1140	0.1668	-0.1796	-0.1796	0.1802	0.5063	0.5063	
2400	0.0000	0.0000	0.0000				

Fitted rate constant (RC): $\log(\text{RC} \cdot \text{min}) = -0.8568 \pm 0.1392$

Grey/blue square: Individual D number / mean D number
 Red cross: Not used individual D Number / mean D number
 Black curve: Fitted time course of D numbers



Path of file: C:\massmap\web_site_etc\homepage_versionen\pdf-files\reports\hdx\kinetics\lis_etc\...
 ...wild_type_kex.txt

SPHERE Report of backbone amide proton exchange rates:

HISpka ASPpka GLUpka NH3pka COOHpka
 6.750000 4.500000 4.500000 8.020001 3.720000
 Rate basis form poly-DL-Ala

Temp =20.00C, pH = 5.00, Exchange in H2O

(N-term. blocked?) n, (C-term. blocked?) n;
 Activation Eas (kcal/mol) are: acid: 15.00, base: 2.60, water: 13.00;

AA pair	kex (sec-1)	Time Const. (min.)	HalfLife (min.)	kexmin (sec-1)	T.C.max (m *in.)	H.L.max min.	pHmin
2 KK	0.523E+01	0.319E-02	0.221E-02	0.119E-02	0.141E+02	0.974E+01	0.87
3 KK	0.126E+00	0.132E+00	0.915E-01	0.962E-03	0.173E+02	0.120E+02	2.33
4 KI	0.261E-01	0.638E+00	0.442E+00	0.583E-03	0.286E+02	0.198E+02	2.50
5 IS	0.145E+00	0.115E+00	0.797E-01	0.892E-03	0.187E+02	0.130E+02	2.21
6 SP							
7 PW	0.239E-01	0.699E+00	0.484E+00	0.735E-03	0.227E+02	0.157E+02	2.83
8 WI	0.155E-01	0.107E+01	0.743E+00	0.525E-03	0.318E+02	0.220E+02	2.54
9 IL	0.166E-01	0.100E+01	0.695E+00	0.555E-03	0.300E+02	0.208E+02	2.62
10 LA	0.650E-01	0.257E+00	0.178E+00	0.131E-02	0.127E+02	0.882E+01	2.84
11 AV	0.213E-01	0.782E+00	0.542E+00	0.670E-03	0.249E+02	0.172E+02	2.78
12 VL	0.204E-01	0.819E+00	0.567E+00	0.630E-03	0.265E+02	0.183E+02	2.72
13 LT	0.553E-01	0.301E+00	0.209E+00	0.750E-03	0.222E+02	0.154E+02	2.48
14 TL	0.440E-01	0.378E+00	0.262E+00	0.676E-03	0.247E+02	0.171E+02	2.47
15 LQ	0.745E-01	0.224E+00	0.155E+00	0.974E-03	0.171E+02	0.119E+02	2.57
16 QI	0.313E-01	0.532E+00	0.369E+00	0.603E-03	0.277E+02	0.192E+02	2.47
17 IQ	0.712E-01	0.234E+00	0.162E+00	0.738E-03	0.226E+02	0.156E+02	2.35
18 QS	0.389E+00	0.428E-01	0.297E-01	0.154E-02	0.108E+02	0.750E+01	2.16
19 SL	0.553E-01	0.301E+00	0.209E+00	0.735E-03	0.227E+02	0.157E+02	2.46
20 LI	0.124E-01	0.134E+01	0.929E+00	0.554E-03	0.301E+02	0.209E+02	2.75
21 IS	0.145E+00	0.115E+00	0.797E-01	0.892E-03	0.187E+02	0.130E+02	2.21
22 SC	0.741E+00	0.225E-01	0.156E-01	0.137E-02	0.121E+02	0.841E+01	1.81
23 CW	0.118E+00	0.141E+00	0.980E-01	0.870E-03	0.191E+02	0.133E+02	2.28
24 WA	0.817E-01	0.204E+00	0.141E+00	0.112E-02	0.149E+02	0.103E+02	2.63
25 AF	0.606E-01	0.275E+00	0.190E+00	0.968E-03	0.172E+02	0.119E+02	2.66
26 FK	0.110E+00	0.151E+00	0.105E+00	0.850E-03	0.196E+02	0.136E+02	2.29
27 KK	0.126E+00	0.132E+00	0.915E-01	0.962E-03	0.173E+02	0.120E+02	2.33
28 KK	0.288E-02	0.580E+01	0.402E+01	0.636E-03	0.262E+02	0.182E+02	3.65

1. LYS LYS LYS ILE SER PRO TRP ILE LEU ALA
 11. VAL LEU THR LEU GLN ILE GLN SER LEU ILE
 21. SER CYS TRP ALA PHE LYS LYS LYS

The molecular weight is: 3275.90
 The pkw is: 14.17
 The molar absorbtivity at 280 nm is: 11550 per cm per mol.
 The rotational correlation time is about: 1.3532 ns