Supplementary material for Hoofnagle *et al*. (2001) *Proc. Natl. Acad. Sci. USA* **98** (3), 956–961. (10.1073/pnas.031562198)

Table 1. Amide hydrogen exchange rates[a]

Peptide	BE[b]	Amides	A[c]	B[c]	C[c]	k_1	k_2	k_3
2	30	30	20.9 (0.68)	4.1 (0.49)		10.19 (0.76)	0.347 (0.091)	
	30	30	20.9 (0.93)	4.1 (0.76)		10.03 (0.95)	0.582 (0.198)	
3[c]	23	11	6.0 (0.25)	**1.0**	**2.0**	8.46 (0.70)	0.144 (0.064)	0.0243 (0.0049)
	24	11	6.0 (0.25)	**2.0**	**1.0**	8.62 (0.70)	0.162 (0.033)	0.0307 (0.0106)
3/4[e]	20	13	6.0	**1.0**	**2.0**	8.46	0.192 (0.095)	0.0313 (0.0072)
	23	13	6.0	**2.0**	**1.0**	8.62	0.112 (0.037)	0.0464 (0.0275)
3/4-SY[e]	26	11	6.0 (0.26)		1.0	9.60 (0.83)		0.0243
	28	11	6.0 (0.29)		1.0	8.23 (0.74)		0.0307
4/5	37	5			3.0 (0.20)			0.0071 (0.0011)
	41	5			3.0 (0.17)			0.0091 (0.0015)
6[f]	20	23	7.5 (0.73)		2.5 (0.49)	2.50		0.0166
	22	23	7.7 (0.61)		2.3 (0.41)	2.50 (0.42)		0.0166 (0.0081)
7/8	25	16	2.4 (0.28)		3.6 (0.20)	1.82 (0.53)		0.0219 (0.0038)
	29	16	2.5 (0.26)		3.5 (0.18)	2.29 (0.53)		0.0166 (0.0024)
8	19	11	1.7 (0.17)		2.3 (0.13)	1.78 (0.45)		0.0210 (0.0036)
	18	11	1.9 (0.14)		2.1 (0.10)	1.85 (0.34)		0.0166 (0.0024)
L/8	17	12	1.9 (0.19)		2.1 (0.15)	1.59 (0.41)		0.0290 (0.0057)
	14	12	1.8 (0.17)		2.2 (0.13)	1.64 (0.37)		0.0171 (0.0027)
9	19	3	2.0 (0.12)			11.53 (1.53)		
	17	3	2.0 (0.07)			10.36 (1.27)		
9/10[g]	18	10	4.1 (0.69)	3.9 (0.65)	2.0 (0.22)	3.61 (0.86)	0.449 (0.124)	0.0147 (0.0052)
	17	10	4.1 (0.32)	3.8 (0.25)	2.2 (0.16)	3.61	0.449	0.0147
9/11[g]	19	12	3.9 (0.26)	3.9 (0.21)	2.2 (0.14)	3.62	0.449	0.0147
	19	12	3.9	3.9	2.2	3.66 (0.40)	0.673 (0.070)	0.0189 (0.0036)
9/12[g]	15	17	3.6 (0.38)	4.7 (0.31)	2.6 (0.20)	3.62	0.449	0.0147
	16	17	3.6	4.7	2.6	4.41 (0.79)	0.473 (0.066)	0.0179 (0.0047)
11/12[d]	14	6		**1.0**	**1.0**		0.277 (0.067)	0.0350 (0.0080)
	19	6			**2.0** (0.10)			0.0291 (0.0046)
12[d]	19	4		**1.0**	**1.0**		0.207 (0.021)	0.0293 (0.0027)
	22	4			**2.0** (0.07)			0.0345 (0.0036)
12/ME[h]	21	6	2.0	**1.0**	**1.0**	5.18 (0.88)	0.207	0.0293
	22	6	2.0 (0.15)		**2.0**	4.16 (0.58)		0.0345
13[i]	23	4	1.0		1.0	1.17 (0.25)		**0.0130** (0.0027)
	23	4	1.0		1.0	1.35 (0.27)		**0.0605** (0.0137)
13/14	23	20	4.4 (0.31)		2.6 (0.18)	4.86 (0.66)		0.0150 (0.0036)
	23	20	4.5 (0.34)		2.5 (0.19)	4.16 (0.61)		0.0160 (0.0036)
14	11	15	3.0 (0.30)		2.0 (0.26)	5.59 (1.04)		0.0093 (0.0038)
	10	15	3.1 (0.28)		1.9 (0.19)	5.48 (0.96)		0.0110 (0.0032)
LL/17	18	6	2.7 (0.22)		1.3 (0.11)	9.61 (1.72)		0.0630 (0.0150)
	21	6	2.9 (0.18)		1.1 (0.08)	8.26 (1.06)		0.0455 (0.0105)
L/17/L[j]	34	6	3.6		1.4 (0.20)	7.05 (1.44)		0.0312
	31	6	3.5 (0.19)		1.5 (0.12)	6.98 (1.03)		0.0312 (0.0074)
20/23	18	19	**7.3** (0.80)	**5.7** (0.60)		**10.82** (2.72)	**0.437** (0.095)	
	16	19	**10.1** (0.36)		**2.9** (0.18)	**8.28** (0.60)		**0.0791** (0.0156)
23	21	5	**1.8** (0.26)		**2.2** (0.26)	0.62 (0.20)		0.0255 (0.0065)

	30	5			**3.0** (0.12)			0.0350 (0.0044)
23/L[i]	14	6	**2.0**		**3.0**	1.20 (0.34)		0.0255 (0.0051)
	19	6			**4.0** (0.15)			0.0435 (0.0056)
24[k]	17	10	4.8 (0.55)		2.2 (0.27)	**10.85**		**0.0194**
	17	10	4.4 (0.53)		2.6 (0.39)	**3.30**		**0.0098**
24/25	25	14	5.2 (0.23)		1.8 (0.11)	**10.85** (1.05)		**0.0194** (0.0041)
	29	14	5.2 (0.25)		1.8 (0.21)	**3.30** (0.31)		**0.0098** (0.0033)
27[l]	26	25	9.4 (0.87)	5.6 (0.50)	**1.0**	4.50 (0.83)	0.049 (0.012)	0.0017
	28	25	9.7 (0.78)	5.3 (0.45)		3.84 (0.62)	0.049	
27/DL[l]	25	27	9.5 (0.84)	6.5 (0.47)	**1.0**	3.67 (0.68)	0.053 (0.010)	0.0057
	27	27	9.1 (0.55)	6.9 (0.33)		3.79 (0.48)	0.058 (0.008)	
27/28[l]	22	29	11.5 (0.73)	6.5 (0.35)	**1.0**	4.61 (0.59)	0.039 (0.006)	0.0069
	22	29	11.5 (0.62)	6.5 (0.33)		4.45 (0.46)	0.039	
29/30[m]	10	9	4.0 (0.32)	2.4	1.6	6.46 (0.94)	1.646	0.0253
	10	9	4.6 (0.29)	2.6	1.9	8.65 (1.03)	1.646	0.0253
30[l,n]	18	5	2.4 (0.28)	1.6 (0.20)		1.65	0.025	
	20	5	2.3 (0.32)	1.7 (0.23)	**1.0**	1.65 (0.55)	0.025 (0.007)	0.0019
31	28	21	8.3 (0.50)		5.7 (0.25)	8.57 (1.04)		0.0259 (0.0035)
	26	21	8.2 (0.55)		5.8 (0.26)	8.83 (1.21)		0.0282 (0.0037)
32	26	23	3.5 (0.45)	7.5 (0.29)		4.81 (1.24)	0.101 (0.010)	
	25	23	3.7 (0.47)	7.3 (0.31)		3.56 (0.96)	0.090 (0.001)	
33	18	12	6.2 (0.37)	3.8 (0.29)		13.81 (2.26)	0.647 (0.091)	
	18	12	6.3 (0.46)	3.7 (0.37)		9.87 (1.54)	0.546 (0.104)	
33/34	24	15	9.2 (0.48)	3.8 (0.35)		11.69 (1.49)	**0.439** (0.085)	
	25	15	9.2 (0.46)	3.8 (0.30)		9.15 (0.99)	**0.277** (0.060)	
33/34/L	23	16	10.3 (0.45)	3.7 (0.35)		14.10 (1.65)	**0.643** (0.114)	
	22	16	10.3 (0.38)	3.7 (0.27)		9.99 (0.82)	**0.368** (0.065)	
35[l]	28	11	3.2 (0.16)	1.4 (0.22)	2.5 (0.20)	7.60 (0.81)	0.178 (0.060)	**0.0139** (0.0029)
	29	11	3.0 (0.22)	1.5 (0.16)	2.5 (0.23)	7.26 (1.08)	0.112 (0.033)	**0.0064**
35/36[l]	16	22	8.4 (0.91)	5.9 (0.39)	1.8	14.13 (4.19)	0.078 (0.016)	**0.0139**
	17	22	8.9 (0.50)	5.4 (0.23)	1.8	8.74 (1.03)	0.066 (0.009)	**0.0019**
36	15	10	6.0 (0.45)	3.0 (0.25)		13.81 (2.74)	0.149 (0.035)	
	16	10	6.0 (0.18)	3.0 (0.09)		13.28 (1.10)	0.128 (0.013)	

[a] Listed are values of non-linear least squares fitted parameters for each peptide with standard errors in parentheses. Inactive ERK is listed above ppERK for each peptide. Numbers in bold indicate significant differences between ERK and ppERK samples. Where errors are not given, values were constrained as described below.

[b] Estimates of back-exchange calculated as in Resing, *et al* (16). For peptides 2, 4/5, L/17/L, 20/23, 31, 35/36, and 36, back-exchange values were chosen to agree with those calculated from primary structure effects using the program HXpep (see methods) (23).

[c] Values of A, B, and C are corrected for back-exchange and 100% D_2O as described in Methods.

[d] Values of B and C were fixed to integral values in order to obtain good fits to the other parameters.

[e] Peptides 3/4 and 3/4-SY were fit using parameters constrained to values in peptide 3 in order to enable comparison between overlapping peptides.

[f] Rate constants for peptide 6 in ERK were constrained to fitted values for ppERK.

[g] Fitted parameters from peptide 9/10 in inactive ERK were used to fit peptides 9/10 in ppERK, peptide 9/11, and peptide 9/12 in order to enable comparison between overlapping peptides. For peptides 9/11 and 9/12, values of A, B and C for ppERK were constrained values obtained in the fit to ERK.

[h] Values of B, C, k_2 and k_3 for ERK and ppERK were constrained to fitted values from peptide 12. The value of A in ERK was constrained to the value derived from the fit to 12/ME, ppERK.

[i] Values of A and C were fixed to integral values in order to obtain good fits to the other parameters.

[j] The parameters k_3 and A for the peptide in ERK were constrained to fitted values for ppERK.

[k] Rate constants for peptide 24 were constrained to values obtained for peptide 24/25.

[l] Late time points in peptide time courses were fit by linear least squares in order to obtain estimates of k_3 and C. Values of other parameters were then obtained from nonlinear least squares fitting to the same data set. In peptide 35, only k_3 was obtained by linear least squares.

[m] Values of parameters in peptide 29/30 were constrained to values in peptide 30. Not shown is a slow amide that exchanges with rate 0.0019 min^{-1}.

[n] For peptide 30, k_1 and k_2 in ERK were constrained to values obtained for ppERK.