

Supporting Information for World Wide Web Edition

NMR chemical shifts of plasminogen kringle 2 in presence of AMCHA ([K2]:[AMCHA] = 1:3), at pH* 5.1, 37°C.

Residue	ppm					
	$^{13}\text{C}^\alpha$	^{15}N	NH	H^α	$\text{H}^{\beta 2, \beta 3}$	others
Thr ¹	43.08			4.00	4.28	$\text{H}^{\gamma 2}$ 1.35
Ser ²	56.18			4.55	3.89	
Glu ²	54.53	122.2	8.60	4.37	2.19/2.04	H^γ 2.37
Glu ¹	53.06	122.2	8.49	4.82	2.24/1.79	H^γ 2.35
Cys ¹	51.58	114.1	7.88	5.00	2.94, 3.11	
Met ²	51.53	117.1	9.36	5.00	1.61, 1.85	H^γ 2.31/2.13, H^ϵ 2.13
His ³	52.46	123.5	9.59	4.92	3.17, 3.30	$\text{H}^{\delta 2}$ 8.17, $\text{H}^{\epsilon 1}$ 8.49
Gly ⁴	45.51	114.8	9.21	4.13/3.88		
Ser ⁵	55.67	121.3	8.97	4.71	3.99	
Gly ⁶	45.47	108.1	9.01	4.16/3.97		
Glu ⁷	58.28	122.6	9.47	4.25	2.10	H^γ 2.36
Asn ⁸	49.51	112.3	8.36	5.03	2.97, 2.83	$\text{N}^{\delta 2}$ 112.14, $\text{H}^{\delta 2 1}$ 7.63, $\text{H}^{\delta 2 2}$ 6.87
Tyr ⁹	57.60	120.8	7.55	4.46	3.15/3.08	H^δ 7.22, H^ϵ 6.81
Asp ¹⁰	49.93	128.9	8.633	4.61	2.43/2.36	
Gly ¹¹	42.44	104.2	4.57	4.10/3.74		
Lys ¹²	53.10	117.1	9.30	3.33	1.35, 1.65	H^γ 1.09/0.70, H^δ 1.57, H^ϵ 2.96
Ile ¹³	61.96	122.2	7.58	4.01	1.99	$\text{H}^{\gamma 1}$ 1.72/1.24, $\text{H}^{\gamma 2}$ 1.26, $\text{H}^{\delta 1}$ 1.02
Ser ¹⁴	55.34	121.8	8.77	5.16	3.54/4.45	
Lys ¹⁵	51.41	119.1	7.20	5.52	1.64/1.55	H^γ 1.41, H^ϵ 3.02
Thr ¹⁶	58.79	110.7	9.09	4.65	4.53	$\text{H}^{\gamma 1}$ 5.99, $\text{H}^{\gamma 2}$ 1.24
Met ¹⁷	56.46	117.2	9.25	4.16	2.14, 1.71	H^γ 2.59/2.35, H^ϵ 2.02

Ser ¹⁸	56.68	112.7	7.78	4.57	4.06/3.88	
Gly ¹⁹	42.85	109.9	8.15	4.30/3.52		
Leu ²⁰	51.81	119.8	7.15	4.35	1.20, 1.31	H ^γ 11.58, H ^{δ1/δ2} 0.90
Glu ²¹	54.22	121.6	8.66	4.50	2.07, 2.00	H ^γ 2.44
Cys ²²	52.78	124.6	8.50	4.84	3.24, 2.72	
Gln ²³	52.93	126.9	9.63	3.90	1.78, 1.25	H ^γ 2.47/2.25, N ^{ε2} 110.02, H ^{ε21} 6.19, H ^{ε22} 7.69
Ala ²⁴	50.21	128.1	8.71	4.08	1.35	
Trp ²⁵	57.35	122.5	7.71	4.26	2.97, 3.77	H ^{δ1} 7.13, N ^{ε1} 130.62, H ^{ε1} 11.42, H ^{ε3} 7.89, H ^{ε2} 7.47, H ^{ε3} 6.46, H ^{η2} 4.94
Asp ²⁶	51.81	112.2	8.66	4.67	2.89/2.71	
Ser ²⁷	54.41	113.8	8.01	4.75	3.98, 4.17	
Gln ²⁸	51.60	122.5	8.36	4.45	1.51, 2.66	H ^γ 2.28/2.15, N ^{ε2} 114.76, H ^{ε21} 7.77, H ^{ε22} 6.03
Ser ²⁹	52.46	112.2	7.74	4.52	3.54	
Pro ³⁰	61.72			4.54	1.23, 2.21	H ^γ 1.56/1.33, H ^δ 3.90/3.29
His ³¹	53.13	120.8	8.66	4.89	3.14/2.88	H ^{δ2} 8.56, H ^{ε1} 7.40
Ala ³²	49.30	128.1	8.73	4.55	1.48	
His ³³	53.81	120.6	9.28	4.81	3.06, 2.20	H ^{δ2} 6.84, H ^{ε1} 8.34
Gly ³⁴	42.47	105.8	8.81	4.54/3.70		
Tyr ³⁶			7.89	4.69	3.85/3.19	H ^δ 7.02, H ^ε 6.89
Ile ³⁷	56.10	116.1	6.99	4.61	1.80	H ^{γ1} 1.47/1.20, H ^{γ2} 1.04, H ^{δ1} 0.88
Pro ³⁸	64.65			4.21	2.14, 2.60	H ^γ 2.31/2.23, H ^δ 3.92
Ser ³⁹	58.16	108.2	8.08	4.15	3.94	
Lys ⁴⁰	54.34	120.0	7.90	4.19	1.79, 1.61	H ^γ 1.34/1.11, H ^ε 2.93

Phe ⁴¹	53.02	116.5	7.39	5.02	2.68, 3.04	H ^δ 7.36, H ^ε 7.50, H ^ζ 7.19
Pro ⁴²	62.99			4.48	2.31	H ^γ 2.04/1.95, H ^δ 3.58/3.30
Asn ⁴³	51.21	113.4	8.57	4.83	2.97	N ^{δ2} 112.12, H ^{δ21} 7.60, H ^{δ22} 7.02
Lys ⁴⁴	52.07	115.8	7.62	4.52	1.87/1.82	H ^γ 1.56/1.48 H ^δ 1.71, H ^ε 3.17/3.06
Asn ⁴⁵	51.61	115.0	8.01	4.33	3.11, 2.80	N ^{δ2} 112.91, H ^{δ21} 7.81, H ^{δ22} 6.87
Leu ⁴⁶	52.00	120.8	8.72	3.46	1.65, 0.49	H ^γ 1.04, H ^{δ1/δ2} -0.85/0.48
Lys ⁴⁷	52.55	123.5	6.99	4.36	1.79, 1.69	H ^γ 1.41/1.33, H ^ε 3.02
Lys ⁴⁸	54.14	117.8	8.72	3.75	0.83, 1.14	H ^γ 1.41/1.29, H ^δ 1.67, H ^ε 3.02
Asn ⁴⁹	48.83	122.9	7.60	4.67	2.46/1.92	N ^{δ2} 110.13, H ^{δ21} 7.71, H ^{δ22} 7.12
Tyr ⁵⁰	52.11	114.6	7.58	4.91	2.84, 3.34	H ^δ 6.92, H ^ε 6.81
Cys ⁵¹	57.55	118.7	9.11	4.50	3.40, 2.43	
Arg ⁵²	50.95	123.1	9.33	4.94	1.28, 1.50	H ^γ 1.94, H ^δ 3.71/3.09, H ^ε 7.89, N ^ε 88.29
Asn ⁵³	46.52	113.1	8.79	5.38	3.14, 1.89	N ^{δ2} 104.56, H ^{δ21} 6.81, H ^{δ22} 6.99
Pro ⁵⁴	61.16			4.55	1.65, 1.77	H ^γ 1.48/1.00 H ^δ 3.63/2.43
Asp ⁵⁵	50.83	120.4	8.92	4.80	3.08, 2.48	
Arg ⁵⁶	55.25	117.5	8.53	3.77	1.98/1.92	H ^γ 1.54, H ^δ 3.19, H ^ε 7.22, N ^ε 85.11
Glu ⁵⁷	52.59	120.7	9.26	4.16	2.24	H ^γ 2.59
Leu ⁵⁸	56.18	124.0	9.59	4.06	1.69, 1.77	H ^γ 1.87, H ^{δ1/δ2} 0.97/1.02
Arg ⁵⁹	51.37	108.8	7.46	4.92	2.18, 1.83	H ^γ 1.65, H ^δ 3.35, H ^ε 7.35, N ^ε 84.80
Pro ⁶¹	61.26			4.15	1.40, 1.78	H ^γ 2.03/1.63, H ^δ 4.07/3.22
Trp ⁶²	53.64	119.2	8.81	5.51	3.65, 3.40	H ^{δ1} 7.44, N ^{ε1} 129.39, H ^{ε1} 11.01, H ^{ε3} 6.92, H ^{ε2} 6.54, H ^{ε3} 4.90, H ^{η2} 6.00
Cys ⁶³	53.42	109.3	8.40	4.39	3.43, 2.91	
Phe ⁶⁴	57.19	120.1	8.06	5.42	2.39, 2.94	H ^δ 6.93, H ^ε 7.13, H ^ζ 7.58
Thr ⁶⁵	58.99	111.4	7.84	5.46	4.34	H ^{γ1} 6.12, H ^{γ2} 1.01
Thr ⁶⁶	60.29	104.6	8.15	4.05	4.56	H ^{γ2} 1.17

Asp ⁶⁷	49.07	125.2	8.95	4.97	2.63, 3.04
Pro ⁶⁸	62.52			3.95	1.93, 2.33 H ^γ 2.06/1.93, H ^δ 4.15/3.96
Asn ⁶⁹	51.26	113.4	8.93	4.85	2.75, 2.90 N ^{δ2} 114.49, H ^{δ21} 7.95, H ^{δ22} 6.98
Lys ⁷⁰	52.20	121.8	7.84	4.55	1.41, 1.76 H ^γ 1.10/1.02, H ^δ 1.54, H ^ε 2.84
Arg ⁷¹	58.25	128.1	8.76	2.18	1.97/1.77 H ^γ 1.52, H ^δ 3.57/3.38, H ^ε 8.94, N ^ε 85.88
Trp ⁷²	52.82	109.1	7.45	5.41	3.01, 2.58 H ^{δ1} 6.80, N ^{ε1} 128.99, H ^{ε1} 10.02, H ^{ε3} 6.97, H ^{ε2} 7.27, H ^{ε3} 6.43, H ^{η2} 6.84
Glu ⁷³	53.61	118.8	8.64	3.66	1.85/1.69 H ^γ 2.88/2.20
Leu ⁷⁴	53.65	119.9	7.50	4.56	1.83, 1.51 H ^γ 1.94, H ^{δ1/δ2} 0.96/1.20
Cys ⁷⁵	52.63	117.3	9.27	4.70	3.17, 2.93
Asp ⁷⁶	50.94	123.5	9.53	4.75	2.29, 2.77
Ile ⁷⁷	53.61	123.5	7.02	4.40	1.75 H ^{γ1} 1.10/0.72, H ^{γ2} 0.45, H ^{δ1} 0.37
Pro ⁷⁸	60.54			4.40	1.85, 2.32 H ^γ 2.12/2.01, H ^δ 3.79/3.58
Arg ⁷⁹	5.76	121.5	8.62	4.64	1.86/1.79 H ^γ 1.47, H ^δ 3.31, H ^ε 7.31, N ^ε 84.26
Cys ⁸⁰	52.39	122.8	8.71	4.59	1.97, 3.29
Thr ⁸¹	61.37	120.7	8.16	4.17	4.3 H ^{γ2} 1.22