Supporting Information for World Wide Web Edition

NMR Solution Structure of the Glucagon Antagonist [desHis¹, desPhe⁶, Glu⁹]Glucagon Amide in the Presence of Perdeuterated Dodecylphosphocholine Micelles

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Table S1. ¹H Chemical Shifts of the Glucagon Antagonist, [desHis¹, desPhe⁶, Glu⁹]Glucagon Amide, Bound to Perdeuterated Dodecylphosphocholine Micelles at pH 6.0 and 37 °C

residue	Chemical shift ^a (ppm)						
	H ^N	H ^α	H ^β	H ^γ	H ^δ	H ^ε	Others
Ser ²		4.23	4.02, 4.06				
Gln ³	8.81	4.47	2.07, 2.18	2.43* ^b		6.84, 7.51	
Gly ⁴	8.51	4.08*					
Thr ⁵	8.16	4.40	4.28	1.25			
Thr ⁷	8.28	4.31	4.26	1.25			
Ser ⁸	8.29	4.48	3.88, 3.97				
Glu ⁹	8.64	4.22	1.97*	2.30*			
Tyr ¹⁰	7.98	4.58	2.98, 3.21		7.10*	6.83*	
Ser ¹¹	7.96	4.09	3.94, 3.99				
Lys ¹²	7.80	4.09	1.63, 1.72	0.98, 1.13	1.55*	2.85*	
Tyr ¹³	7.54	4.43	2.97, 3.19		7.20*	6.87*	
Leu ¹⁴	7.68	4.27	1.68, 1.81	1.93	0.92, 0.98		
Asp ¹⁵	7.68	4.83	2.84, 2.97				
Ser ¹⁶	7.84	4.43	4.07, 4.25				
Arg ¹⁷	8.75	4.13	1.96*	1.75*	3.28*	7.33	
Arg ¹⁸	8.35	4.19	1.95*	1.84*	3.21, 3.27	7.68	H ^η 6.99*
Ala ¹⁹	7.89	4.17	1.61				
Gln ²⁰	8.25	4.03	2.25*	2.47, 2.56		6.76, 7.42	
Asp ²¹	8.61	4.51	2.86, 3.13				

^a The chemical shifts were referenced to the internal H₂O resonance as 4.63 ppm.

^b Asterisks indicate degenerate ¹H chemical shifts.

Table S1 (Continued)

residue	Chemical shift ^a (ppm)						
	H ^N	H ^α	H ^β	H ^γ	H ^δ	H ^ε	Others
Phe ²²	8.20	4.49	3.40*		7.23		
Val ²³	8.35	3.51	2.29	1.05, 1.25			
Gln ²⁴	8.26	4.02	2.25*	2.47, 2.59		6.83, 7.43	
Trp ²⁵	7.98	4.29	3.35, 3.63		7.36	10.47	H ^{ζ2} 7.49
						7.29	H ^{ζ3} 6.89
							H ^{η2} 7.08
Leu ²⁶	8.30	3.34	1.46, 1.61	1.57	0.77*		
Met ²⁷	8.06	4.18	2.11*	2.55 2.75			
Asn ²⁸	7.69	4.00	2.75, 2.88		6.87, 7.61		
Thr ²⁹	7.71	3.99	3.86	0.99			
NH ₂	6.96, 7.33						