

Supplementary MaterialChemical shifts of [*D*-Y¹³]MVIIA in aqueous solution (pH 3.5, T 293 K)

Residue	NH	H α	H β	other
C1		4.73	3.09, 3.33	
K2	9.12	4.57	1.87	H γ 1.46, 1.55; H δ 1.73; H ϵ 3.04
G3	8.87	3.80, 4.15		
K4	8.22	3.75	1.70, 1.78	H γ 1.34; H δ 1.50; H ϵ 2.99
G5	9.06	3.58, 4.34		
A6	7.71	4.35	1.46	
K7	8.26	4.74	1.73, 1.79	H γ 1.43, H δ 1.65; H ϵ 3.02
C8	8.16	4.9	2.93, 2.22	
S9	8.89	4.66	3.80, 3.90	
R10	8.15	4.4	1.63, 1.84	H γ 1.57; H δ 3.21
L11	8.42	4.07	1.65	H γ 1.58; H δ 0.92, 0.99
M12	8	4.6	1.26	H γ 2.0, 2.15
Y13	8.49	4.73	2.77, 3.41	H δ 7.17; H ϵ 6.85
D14	8.26	4.85	2.72, 2.83	
C15	8.43	4.95	2.57, 3.30	
C16	9.75	4.46	2.90, 3.28	
T17	8.31	4.56	4.06	H γ 1.13
G18	8.56	3.84, 4.12		
S19	8.32	4.94	3.74, 3.80	
C20	8.93	4.69	2.94, 3.01	
R21	8.57	4.63	1.82, 1.85	H γ 1.55, 1.66; H δ 3.21
S22	9.35	4.03	3.89, 4.13	
G23	8.25	3.82, 4.15		
K24	7.74	5.36	1.61, 1.69	H γ 1.29, 1.37; H δ 1.55; H ϵ 3.0
C25	8.83	4.87	3.09, 3.27	NH ₂ 8.55, 7.44