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Supporting Information

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Supporting Information

for

A Combined Solid-state NMR and MD Characterization of the Stability and Dynamics of the HET-s(218-289) Prion in its Amyloid Conformation

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Table S1. ^{13}C and ^1H chemical shifts^[a] of flexible parts of HET-s(218-289) in ppm.

Res.	CO	C α	C β	C γ (1)	C γ 2	C δ (1)	C δ 2	C ϵ (1)	H α	H β	H γ (1)	H γ 2	H δ (1)	H δ 2	H ϵ (1)
A	177.9	52.9 (53.2)	19.4 (19.0)	-	-	-	-	-	4.43	1.50	-	-	-	-	-
E	178.8	56.6 (57.4)	30.8 (30.0)	36.6	-	184.0	-	-	3.71	2.08	2.36	-	-	-	-
H	175.2	56.5 (56.5)	31.3 (30.2)	134.9	-	-	120.6	138.6	4.59	3.07	-	-	-	6.91	7.75
K	176.3	56.5 (57.0)	33.3 (32.8)	24.9	-	29.4	-	42.4	-	1.93	1.49	-	1.76	-	3.08
L	-	-	42.9 (42.3)	27.2	-	25.1	23.9	-	-	1.76	-	-	1.00	0.95	-

M	-	-	36.5 (33.0)	32.2	-	-	-	17.3	-	1.99	2.59	-	-	-	2.15
Q	-	-	29.9 (29.2)	34.1	-	180.6	-	-	-	2.16	2.44	-	-	-	-
R	-	-	31.1 (30.7)	27.3	-	43.7	-	-	-	1.96	1.73	-	3.29	-	-
S	174.9	58.7 (58.7)	64.3 (63.8)	-	-	-	-	-	-	3.96	-	-	-	-	-
D1	176.2	54.6 (54.7)	41.5 (40.9)	180.2	-	-	-	-	4.71	2.76	-	-	-	-	-
D2	-	-	39.7 (40.9)	180.4	-	-	-	-	-	2.77	-	-	-	-	-
G1	174.0	45.6 (45.4)	-	-	-	-	-	-	4.04	-	-	-	-	-	-
G2	175.4	44.7 (45.4)	-	-	-	-	-	-	3.65	-	-	-	-	-	-
I1	176.4	61.5 (61.6)	39.0 (38.6)	27.5	17.9	13.3	-	-	4.28	1.98	1.28	0.99	0.93	-	-
I2	-	-	-	27.5	-	14.1	-	-	-	-	-	-	-	-	-
T1	174.8	62.1 (62.2)	70.0 (69.7)	-	21.9	-	-	-	-	4.33	-	1.29	-	-	-
T2	-	-	69.3 (69.7)	-	22.5	-	-	-	-	4.31	-	1.41	-	-	-
V1	-	62.6 (62.5)	33.0 (32.7)	21.4	20.8	-	-	-	4.25	2.19	1.02	1.04	-	-	-
V2	-	63.9 (62.5)	32.1 (32.7)	20.9	19.6	-	-	-	-	-	-	1.09	-	-	-

[a] In case of multiple sets of the same amino-acid type the sets with highest intensity are listed first. The chemical shifts are referenced to DSS(internal). Values in brackets refer to random-coil values (Biological Magnetic Resonance Data Bank 02-05-2009)