

Formation of nanostructures by self-assembly of an elastin peptide

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Supplementary Material

Table SI: Assignments of proton resonances of peptide *EX30N* in H₂O/D₂O (80/20, v/v) at 298 K

residue ^a	Chemical shift of proton resonance (ppm)				- $\Delta\delta/\Delta T$ (ppb/K)
	NH	H α	H β	others	
Gly ¹		3.836			
Leu ²	8.563	4.412	1.596	H γ 1.569 H δ 0.903/0.866	7.1
Val ³	8.300	4.111	2.049	H γ 0.967/0.942	6.7
Gly ⁴	8.492	3.939			7.0
Ala ⁵	8.175	4.285	1.384		6.2
Ala ⁶	8.335	4.294	1.386		6.2
Gly ⁷	8.267	3.928			5.7
Leu ⁸	8.123	4.356	1.655	H γ 1.607 H δ 0.912/0.860	6.4
Gly ⁹	8.481	3.940			6.8
Gly ¹⁰	8.221	3.946			5.1
Leu ¹¹	8.149	4.350	1.628	H γ 1.586 H δ 0.905/0.859	5.8
Gly ¹²	8.431	3.951			5.5
Val ¹³	8.005	4.141	2.114	H γ 0.935/ 0.914	7.3
Gly ¹⁴	8.568	3.968			5.2
Gly ¹⁵	8.229	3.948			4.7
Leu ¹⁶	8.161	4.395	1.635	H γ 1.590 H δ 0.902/0.857	6.1
Gly ¹⁷	8.173	3.846			6.3

Table SII: Assignments of proton resonances of peptide *EX30N* in TFE-d₃/H₂O (80/20, v/v) at 298 K

residue ^a	Chemical shift of proton resonance (ppm)				- $\Delta\delta/\Delta T$ (ppb/K)
	NH	H α	H β	others	
Gly ¹		HA3 3.809			
Leu ²	8.171	4.419	QB 1.680	H γ 1.650 H δ 0.968/0.919	6.1
Val ³	7.680	4.117	2.089	H γ 0.977	5.0
Gly ⁴	8.046	4.019/3 3.841			5.5
Ala ⁵	7.819	4.326	QB 1.426		5.8
Ala ⁶	7.896	4.301	1.435		5.5
Gly ⁷	7.978	4.003/ 3.931			4.3
Leu ⁸	7.788	4.398	1.740/1.693	H γ 1.674 H δ 0.961/0.915	4.8
Gly ⁹	8.123	3.976/3 3.93			5.0
Gly ¹⁰	7.976	QA 3.966			4.3
Leu ¹¹	7.770	4.405	QB 1.732	H γ 1.672 H δ 0.963/0.914	4.3
Gly ¹²	8.116	4.006/3.947			4.6
Val ¹³	7.628	4.169	2.150	H γ 0.976	4.5
Gly ¹⁴	8.157	3.990/3.945			6.2
Gly ¹⁵	7.932	3.973			4.1
Leu ¹⁶	7.726	4.478	QB 1.673	H δ 0.949/0.908	4.4
Gly ¹⁷	7.632	3.884/3.768			5.1

Table SIII. NOE ratio analysis results for the residues of *EX30N* peptide in H₂O/D₂O (80/20, v/v) at 298 K.

	$\frac{\alpha N(i,i+1)}{NN(i,i+1)}$
G ¹	
L ²	0.71
V ³	5.0
G ⁴	-
A ⁵	-
A ⁶	-
G ⁷	11
L ⁸	3.30
G ⁹	-
G ¹⁰	-
L ¹¹	3.60
G ¹²	2.13
V ¹³	1.99
G ¹⁴	-
G ¹⁵	-
L ¹⁶	-
G ¹⁷	-