SUPPLEMENTARY DATA

Effect of proline analogues on the conformation of elastin peptides

Antonietta Pepe,*[a] Maria Antonietta Crudele[a] and Brigida Bochicchio*[a]

Department of Science, University of Basilicata, Potenza, Italy. Fax: +39 0971205678; Tel: +39 0971205486-5481; E-mail: antonietta.pepe@unibas.it; brigida.bochicchio@unibas.it

Table S1: Assignments of proton resonances of peptide E7P in H_2O/D_2O (90/10, v/v) at 25°C

	Chemical shift of proton resonance (ppm)				
residue[a]	NH	Hα	Hβ	others	-Δδ/ΔT (ppb/K)
V[1]	-	3.85	2.24	1.05	-
G[2]	8.69	4.09/4.00			6.3
V[3]	8.25	4.46	2.08	0.98/0.95	9.1
P[4]	-	4.42	2.32/2.08	γ δ3.90/3.71	-
G[5]	8.46	3.99			7.6
V[6]	7.96	4.19	2.11	0.95	6.8
G[7]	8.48	4.00			7.5

Table S2: Assignments of proton resonances of peptide E7H in H_2O/D_2O (90/10, v/v) at 25°C

	Chemical shift of proton resonance (ppm)				
residue[a]	NH	Hα	Hβ	others	-Δδ/ΔT (ppb/K)
V[1]	-	3.85	2.22	1.04	-
G[2]	8.68	4.06/4.00			6.1
V[3]	8.29	4.43	2.05	0.99/0.97	9.1
Hyp[4]	-	4.62	2.34/2.08	γ 4.54 δ 3.93/3.84	-
G[5]	8.61	3.97			7.7
V[6]	7.96	4.20	2.11	0.93	6.5
G[7]	8.46	3.98			7.4

Table S3: Assignments of proton resonances of peptide E7M in H_2O/D_2O (90/10, v/v) at 25°C

	Chemical shift of proton resonance (ppm)				
residue[a]	NH	Hα	Hβ	others	-Δδ/ΔT (ppb/K)
V[1]	-	3.85	2.24	1.05	-
G[2]	8.69	4.09/4.00			6.3
V[3]	8.25	4.46	2.08	0.98/0.95	9.1
P[4]	-	4.42	2.32/2.08	γ δ3.90/3.71	-
G[5]	8.46	3.99			7.6
V[6]	7.96	4.19	2.11	0.95	6.8
G[7]	8.48	3.99			7.5

Table S4: Assignments of proton resonances of peptide E7P in TFE-$_{d3}$/H_2O (80/20, v/v) at 25°C

	Chemical shift of proton resonance (ppm)				-Δδ/ΔT (ppb/K)
residue[a]	NH	Hα	Hβ	others	
V[1]	-	3.79	2.24	1.07	-
G[2]	8.19	4.17/3.87			5.9
V[3]	7.72	4.50	2.05	1.00/0.97	8.3
P[4]	-	4.35		γ δ 3.89/3.70	-
G[5]	8.02	4.16/3.73			8.9
V[6]	7.64	4.22	2.10	0.97/0.92	**4.6**
G[7]	8.00	4.00			7.5

Table S5: Assignments of proton resonances of peptide E7H in TFE-$_{d3}$/H_2O (80/20, v/v) at 25°C

	Chemical shift of proton resonance (ppm)				-Δδ/ΔT (ppb/K)
residue[a]	NH	Hα	Hβ	others	
V[1]	-	3.80	2.2	1.06	-
G[2]	8.26	4.20/3.70			6.6
V[3]	7.90	4.40	2.02	0.97	9.6
P[4]	-	4.53	2.34/2.16	γ 4.61 δ 4.05/3.81	-
G[5]	8.24	4.26/3.85			8.9
V[6]	7.72	4.24	2.09	0.98/0.92	**5.1**
G[7]	8.01	4.05/3.96			8

Table S6: Assignments of proton resonances of peptide E7M in TFE-$_{d3}$/H_2O (80/20, v/v) at 25°C

	Chemical shift of proton resonance (ppm)				-Δδ/ΔT (ppb/K)
residue[a]	NH	Hα	Hβ	others	
V[1]	-	3.79	2.24	1.07	-
G[2]	8.19	4.21/3.88			5.5
V[3]	7.84	4.42	2.06	1.01	8.5
Mop[4]	-	4.42	2.45/2.09	γ 4.16 δ4.14/3.79 CH_3O 3.38	-
G[5]	8.22	4.23/3.72			8.2
V[6]	7.70	4.23	2.13	1.00/0.95	**4.3**
G[7]	8.01	4.06/3.99			7.3

MAGLTAAAPR[10] PGVLLLLLSI[20] LHPSRP|GVP[30] GAIPGGVPGG[40] VFYP|GAGLGA[50] LGG|GALGPGG[60]
Exon 2 ***Exon 3*** ***Exon 4***

KPLKPV|PGGL[70] AGAGLGA|GLG[80] AFPAVTFPGA[90] LVPGGVADAA[100] AAYKAAKA|GA[110] GLGG***VPGVG***G[120]
Exon 5 ***Exon 6*** ***Exon 7***

LGVSA|GAVVP[130] QPGAGVKPGK[140] ***VP|GVG***LPGVY[150] PGGVLPGA|RF[160] PGVGVLPGVP[170] TGAGVKPKAP[180]|
Exon 8 ***Exon 9*** ***Exon 10***

GVGGAFAGIP[190]| GVGPFGGPQP[200] GVPLGYPIKA[210] PKLP|GGYGLP[220] YTTGKLPY|GY[230] GPGGVAGAAG[240]
Exon 11 ***Exon 12*** ***Exon 13*** ***Exon 14***

KAGYPTGT|GV[250] GPQAAAAAAA[260] KAAAKF|GAGA[270] AGVLPGVGGA[280] GVPGVPGAIP[290] GIGGIA|GVGT[300]
Exon 15 ***Exon 16***

PAAAAAAAAA[310] AKAAKY|GAAA[320] GLVPGGPGFG[330] PGVVGVPGAG[340] ***VPGVG***VPGAG[350] IPVVPGAGIP[360]
Exon 17 ***Exon 18***

GAAVP|GVVSP[370] EAAAKAAAKA[380] AKY|GARPGVG[390] VGGIPTYGVG[400] AGGFPGFGVG[410] VGGIPGVAGV[420]
Exon 19 ***Exon 20***

PGVGG***VPGVG***[430] G***VPGVG***IS|PE[440] AQAAAAAAKAA[450] KY|GAAGAGVL[460] GGLVPGPQAA[470] VPGVP|GTGGV[480]
Exon 21 ***Exon 22***

PGVGTPAAAA[490] AKAAAKAAQF[500] |GL***VPGVG***VAP[510] GVGVAPGVGV[520] APGVGLAPGV[530] GVAPGVGVAP[540]
Exon 23 ***Exon 24***

GVGVAPGI|GP[550] GGVAAAAKSA[560] AKVAAKAQL|R[570] AAAGLGAGIP[580] GLGVGVGVPG[590] LGVGAGVPGL[600]
Exon 25 ***Exon 26***

GVGAGVPGFG[610] A|GADEGVRRS[620] LSPELREGDP[630] SSSQHLPSTP[640] SSPRV|PGALA[650] AAKAAKY|GAA[660]
Exon 26A ***Exon 27***

VPGVLGGLGA[670] LGGVGIPGGV[680] V|GAGPAAAAA[690] AAKAAAKAAQ[700] F|GLVGAAGLG[710] GLGVGGLG***VP***[720]
Exon 28 ***Exon 29*** ***Exon 30***

GVGGLG|GIPP[730] AAAAKAAKY|G[740] AAGLGGVLGG[750] AGQFPLG|GVA[760] ARPGFGLSPI[780] FP|GGACLGKA
Exon 31 ***Exon 32*** ***Exon 33*** ***Exon 36***

CGRKRK

Figure S1: Human tropoelastin protein sequence (Swiss Prot. Accession number P15502).
-VPGVG- sequences are underlined.

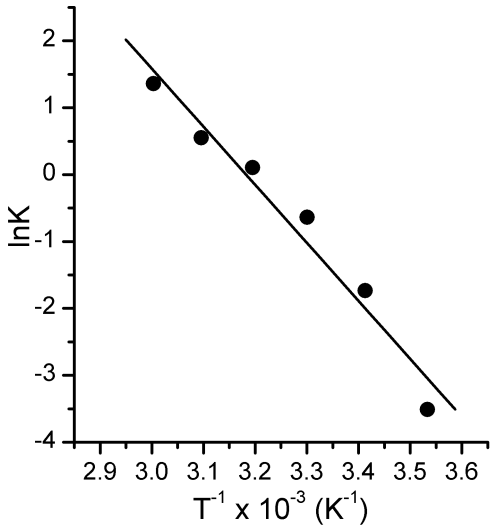

Figure S2: a) CD spectra of E7P peptide recorded at variable temperatures from 0 to 70°C, with a 10° C increment. b) Van't Hoff plot constructed from CD data at 198 nm of E7P recorded in water at different temperatures. The data were fitted to a two state model. By sing the fitted endpoints of the transition, a linear Van't Hoff plot is obtained, which allowed the calculation of the enthalpy change ΔH°, the entropy change ΔS°, and the transition temperature Tm of the conformational transition from the slope, the intercept and the ΔH°/ΔS° values, respectively. The linear correlation coefficient is r = -0.98.

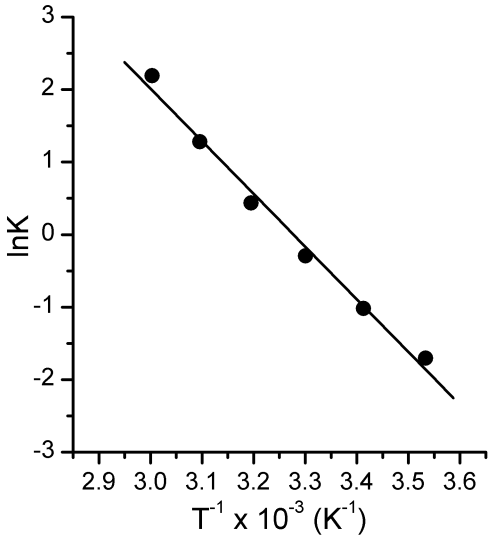

Figure S3: a) CD spectra of E7H peptide recorded at variable temperatures from 0 to 70°C, with a 10° C increment. b) Van't Hoff plot constructed from CD data at 198 nm of E7H recorded in water at different temperatures. The data were fitted to a two state model. By sing the fitted endpoints of the transition, a linear Van't Hoff plot is obtained, which allowed the calculation of the enthalpy change ΔH°, the entropy change ΔS°, and the transition temperature Tm of the conformational transition from the slope, the intercept and the ΔH°/ΔS° values, respectively. The linear correlation coefficient is r = -0.99.

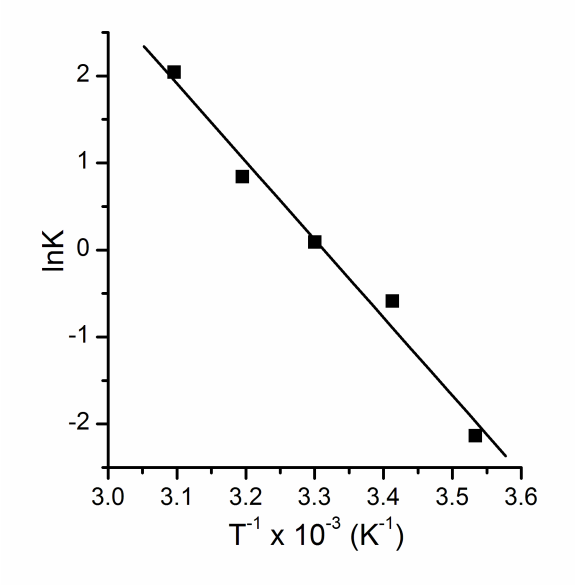

Figure S4: a) CD spectra of E7M peptide recorded at variable temperatures from 0 to 70°C, with a 10° C increment. b) Van't Hoff plot constructed from CD data at 198 nm of E7M recorded in water at different temperatures. The data were fitted to a two state model. By sing the fitted endpoints of the transition, a linear Van't Hoff plot is obtained, which allowed the calculation of the enthalpy change ΔH°, the entropy change ΔS°, and the transition temperature Tm of the conformational transition from the slope, the intercept and the ΔH°/ΔS° values, respectively. The linear correlation coefficient is r = -0.99.