Supporting Information

A Two-State Model Describes the Temperature-Dependent Conformational Equilibrium in the Alanine-Rich Domains in Elastin

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Figure S1. Representative ¹³CO-Ala lineshape simulations of (Ala)_n with n = 6-16. Bixon-Scheraga-Lifson's approach ^{S1} was used with the statistical weights, w, v, u, and σ of 1.0, 0.03, 1.0, and 1.7, respectively. Ullman's method ^{S2} is used to generate the ¹³CO NMR lineshape for each (Ala)_n peptide from the sum of the Gaussian lines that are (each) positioned at the resonance frequencies marked by the vertical lines. The vertical lines correspond to the predicted chemical shifts for each of the alanines in (Ala)_n. For the simulation, the highest probability for α -helix is assigned to the ¹³CO resonance of 180.0 ppm, whereas the lowest probability (i.e., coil) is set to 175.0 ppm.

Table S1. Sequences of the alanine-containing hydrophobic (HP) and crosslinking (CL) domains of rat tropoelastin ^{s3}. Alanines (A) are indicated in bold, and all tandem alanines are underlined (<u>AA</u>, <u>AAA</u>, etc.). Asterisks (*) indicate HP domains with tandem alanines.

Domain type	EX	Sequence
HP	2	GVPGAVPGGVPGGLPGGVPGGVYYP
	3	GAGIGGGLGGG
	4A	GAGLLGAFGA
	5	GPGGLGGAGPGA
	7	GAGLGGIGGVPGGVGGVPGAVGGVPGAVGGIGGIGGLGVST
	9	GVGLPGVYPGGVLPGT
	11	GGGGGAFSGIP
	13	GGYGLPYTNGKLPY
	14	GVAGAGGKAGYPTGT
	16	GAGGGGVLPGVGGGGIPGGAGAIPGIGGIT
	18*	G <u>AA</u> GGLVPGGPGVRVPG A GIPGVGIPGVGGIPGVGGIPGVGGPGIGGPGIVGGP
	20	GARGGVGIPTYGVGAGGFPGYGVGAGAGLG
	22	GAGGAGTLGGLVPGAVPGALPGAVPGALPGAVPGALPGAVPGVPGTGGVP
	24	GLGPGVGGVPGGVGVGGLPGGVGPGGVTGIGTGPGTGLVPGDLG
	26*	G <u>AAA</u> GLGAGVPGLGVGAGVPGFGAGAGGFGAGAGVPGFGAGA
	28*	GAAGGLGGPGGLGGPGGLGGPGGLGGPGGLGGVPGGVA
	30	GLGGAGGLGAGGLGAGGLGAGGLGAGGLGAGGVIPGAVGLG
	32*	G <u>AA</u> GLGGVLGARPFPGG
	33*	GV <u>AA</u> RPGFGLSPIYP
	34	GGGAGGLGVG
CL	4	ALGPGGKPPKP
	6	GGVLVPGGG A G <u>AAAA</u> YK <u>AAA</u> KA
	8	GAVVPQLGAGVGAGGKPGKVP
	10	GARFPGVGVLPGVPTGTGVKAKVP
	12	GVGPFGGQQPGVPLGYPIK A PKLP
	15	GVGSQ <u>AA</u> V <u>AAA</u> K <u>AA</u> KY
	17	GAGTP AAAAAA K AAA K AA KY
	19	GAVSP <u>AAAA</u> K <u>AAA</u> KY
	21	GASQ <u>AAAAAAAA</u> K <u>AA</u> KY
	23	GTP <u>AAAAAAAA</u> K <u>AAA</u> KAGQY
	25	G A GTP <u>AAA</u> KS <u>AA</u> K <u>AAA</u> KAQY
	27	VPGSL <u>AA</u> SK <u>AA</u> KY
	29	G AP<u>AAAAAA</u>K<u>AAA</u>QY
	31	GVSP <u>AAAA</u> K <u>AA</u> KY
	35	GKPPKPYGG A LG A LGYQ
	36	GGGCFGKSCGRKRK

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