## SUPPLEMENTARY FIGURE AND TABLES



**Supplementary Figure S1: NC1(XIX) domain of collagen XIX makes disulfide bond in solution. (A)** MALDI-ToF MS analysis showing that P36 peptide in solution at T0 presented no disulfide bond. **(B)** MALDI-ToF MS analysis at 1 h demonstrating that the P36 peptide of collagen XIX made a disulfide bond in its NC1(XIX) domain over the time. **(C)** MALDI-ToF MS analysis showing that in the presence of dithiothreitol (DTT), the disulfide bond disappeared

Peptides	Starting structure	Sequence of typeI turn above threshold	
P19	Elongated	SHAH ; HAHQ ; QRTG	
	Itasser prediction	NPED ; LYPV ; VSHA ; QRTG	
	Pepfold prediction	NPED ; PVSH ; VSHA ; AHQR ; RTGG	
F4 without disulfide bridge	Elongated	SHAH	
	Itasser prediction	NPED ; VSHA ; SHAH ; HAHQ	
	Pepfold prediction	NPED ; SHAH	
F4 with disulfide bridge	From Elongated start	NPED ; PEDC	
	Pepfold prediction	NPED ; DCLY ; PVSH ; VSHA ; SHAH ; HAHQ ; AHQR	

## Supplementary Table S1: β-turn analysis of the trajectories

## Supplementary Table S2: Sequences of the peptides used in the study

Names	Peptide sequences	Substitutions
P19	<sup>1124</sup> NPEDCLYPVSHAHQRTGGN <sup>1142</sup>	
P36	<sup>1107</sup> SPGAPGPQGPPGPSGRCNPEDCLYPVSHAHQRTGGN <sup>1142</sup>	
P36G <sup>1122</sup>	<sup>1107</sup> SPGAPGPQGPPGPSG <u>G</u> CNPEDCLYPVSHAHQRTGGN <sup>1142</sup>	$\operatorname{Arg}^{1122} \rightarrow \operatorname{Gly}$
P36W <sup>1121</sup>	<sup>1107</sup> SPGAPGPQGPPGPS <u>W</u> RCNPEDCLYPVSHAHQRTGGN <sup>1142</sup>	$Gly^{1121} \rightarrow Trp$
P36W <sup>1120</sup>	<sup>1107</sup> SPGAPGPQGPPGP <u>W</u> GRCNPEDCLYPVSHAHQRTGGN <sup>1142</sup>	$\mathrm{Ser}^{1120} \rightarrow \mathrm{Trp}$
P36W <sup>1123</sup>	<sup>1107</sup> SPGAPGPQGPPGPSGR <b>W</b> NPEDCLYPVSHAHQRTGGN <sup>1142</sup>	$Cys^{1123} \rightarrow Trp$
P36W <sup>1124</sup>	<sup>1107</sup> SPGAPGPQGPPGPSGRC <u>W</u> PEDCLYPVSHAHQRTGGN <sup>1142</sup>	$Asp^{1124} \rightarrow Trp$