

## SUPPLEMENTARY MATERIAL

<sup>1</sup>H assignments for pentapeptide 2 in D<sub>2</sub>O, pH 5.2

<u>Residue</u>	<u>Atom</u>	<u>Chemical Shift (p.p.m.)</u>
DPro-1	C <sup>α</sup> H	4.32
	C <sup>β</sup> H <sub>2</sub>	2.17, 1.96
	C <sup>γ</sup> H <sub>2</sub>	2.15, 1.97
	C <sup>δ</sup> H <sub>2</sub>	2.68, 3.55
Ala-2	NH	8.90
	C <sup>α</sup> H	4.21
	C <sup>β</sup> H <sub>3</sub>	1.40
Lys-3	NH	7.79
	C <sup>α</sup> H	4.50
	C <sup>β</sup> H <sub>2</sub>	1.96, 1.80
	C <sup>γ</sup> H <sub>2</sub>	1.40, 1.31
	C <sup>δ</sup> H <sub>2</sub>	1.67
	N <sup>ε</sup> H <sub>3</sub>	2.94
Lys-4	NH	7.93
	C <sup>α</sup> H	3.98
	C <sup>β</sup> H <sub>2</sub>	1.85
	C <sup>γ</sup> H <sub>2</sub>	1.45, 1.40
	C <sup>δ</sup> H <sub>2</sub>	1.66
	N <sup>ε</sup> H <sub>3</sub>	2.94
Arg-5	NH	7.73
	C <sup>α</sup> H	4.54
	C <sup>β</sup> H <sub>2</sub>	1.77, 1.51
	C <sup>γ</sup> H <sub>2</sub>	1.62
	C <sup>δ</sup> H <sub>2</sub>	3.19
	N <sup>ε</sup> H	7.20

Dihedral Angles (in degrees) for the backbone of the NMR structure of pentapeptide 2

<u>Residue</u>	<u>Angle</u>	<u>Average value</u> <u>± SD</u>
DPro-1	φ	83.36 ± 3.3
	ψ	-109.2 ± 2.4
	ω	-170.7 ± 1.1
Ala-2	φ	-41.4 ± 3.8
	ψ	-68.0 ± 1.8
	ω	180.0 ± 0.0
Lys-3	φ	-119.7 ± 0.3
	ψ	-102.9 ± 4.0
	ω	180.0 ± 0.0
Lys-4	φ	-42.0 ± 2.2
	ψ	-58.3 ± 2.3
	ω	180 ± 0.0
Arg-5	φ	83.36 ± 3.3
	ψ	-109.2 ± 2.4
	ω	-170.7 ± 1.1