

**Supplemental Table** Observed vicinal ( $J_{\alpha\beta1}$  and  $J_{\alpha\beta2}$ ) and geminal ( $J_{\beta1\beta2}$ )  $^1\text{H}$ - $^1\text{H}$  coupling constants among  $\alpha$ - and  $\beta$ -protons of D-Phe and Asp residues in 1 mM achatin-I in methanol- $d_4$  solution.

Ionization State	$J$	D-Phe	Asp
( $\alpha$ -ND <sub>3</sub> <sup>+</sup> , $\alpha$ -CO <sub>2</sub> <sup>-</sup> , $\beta$ -CO <sub>2</sub> <sup>-</sup> )	$J_{\alpha\beta1}$	8.21 ± 0.02	5.48 ± 0.01
	$J_{\alpha\beta2}$	7.35 ± 0.03	4.97 ± 0.01
	$J_{\beta1\beta2}$	13.50 ± 0.02	16.10 ± 0.02