Electronic Supplementary Material (ESI) for Molecular BioSystems.

Characterizing structure–function relationship reveals mode of action of a novel antimicrobial peptide, P1, from jumper ant *Myrmecia pilosula*

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Supporting Information

Methods

Circular dichroism (CD) spectroscopy of P1 in POPC and POPG LUVs

Far-UV CD experiments involved use of a Chirascan-Plus CD Spectrometer (Applied Photophysics Ltd., Leatherhead, UK). P1 was liquified in PBS buffer (137 mM NaCl, 2.7 mM KCl, 10 mM Na_2HPO_4, 1.8 mM KH_2PO_4, pH 7.4) to yield a 1.5 mM stock. CD samples for P1: POPC(G) = 1: 10 and 1: 20 (molar ratio) were prepared by diluting the P1 peptide stock (1.5 mM) into, POPC(G) LUVs (12 mM stock) with PBS buffer to reach the final concentrations (P1 = 60 μM) and molar ratios of interest. Far-UV CD spectra were recorded by using a 1-mm path length quartz cuvette at 25 °C with the observed wavelength range between 190 and 260 nm. All spectra were averaged over three scans and converted to mean residue ellipticity [θ].

Figures

Figure S1.

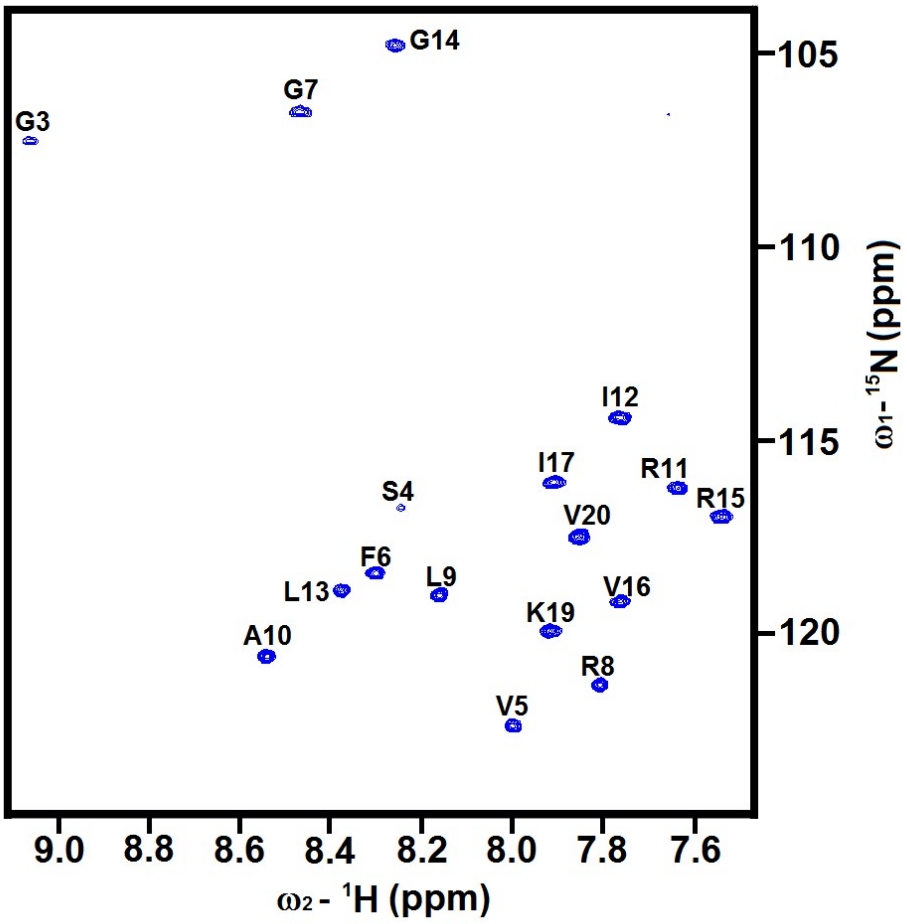

Figure S1. 2D ^{1}H, ^{15}N- HSQC spectra of naturally abundant P1 in DPC micelles at pH 5.0 and 310 K.

Figure S2.

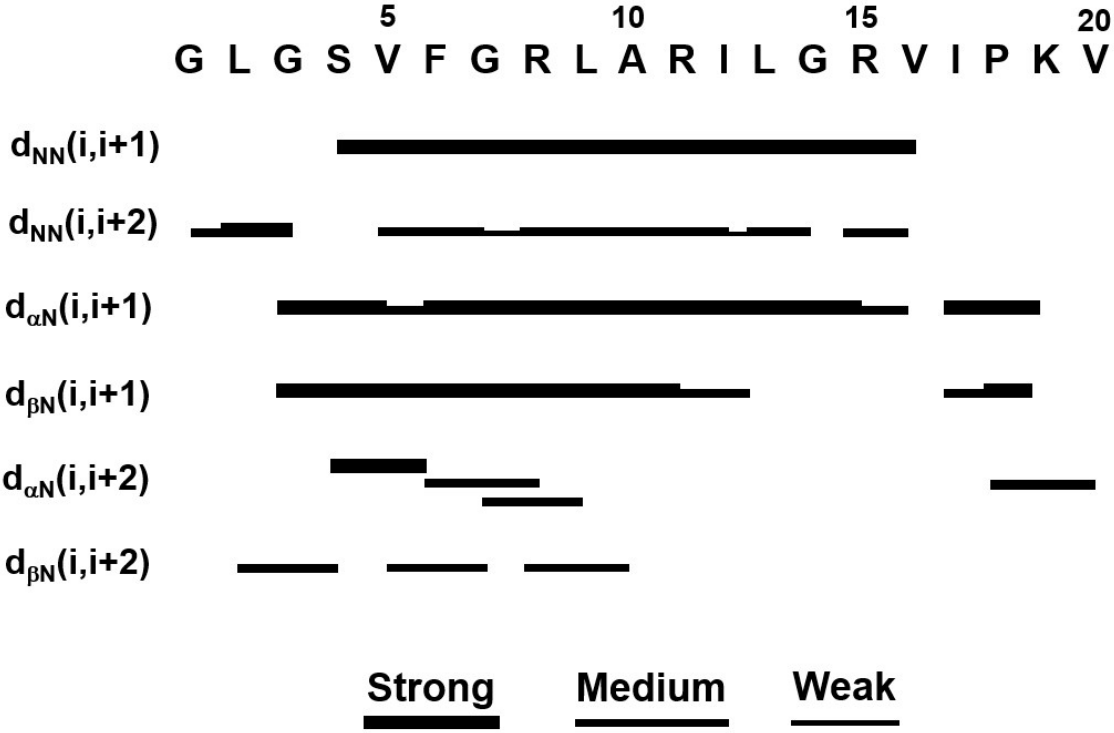

Figure S2. The NOE connectivity of P1 bound to DPC micelles. The thickness of the lines denotes strong (d < 2.5), medium (d 2.5–3.5), and weak (d 3.5–5.5) NOE intensities.

Figure S3.

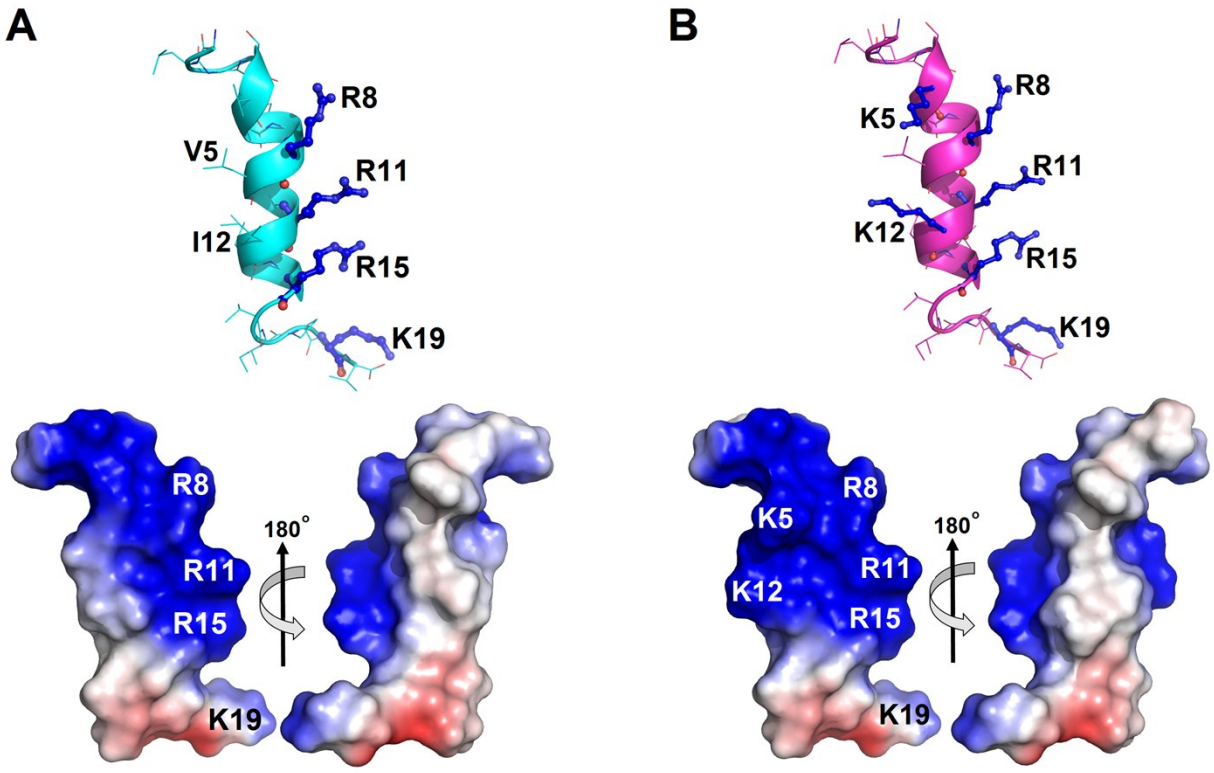

Figure S3. Structural comparison of P1 and its variant P2. (**A**) Ribbon representation of the DPC-bound solution structure of P1. Arginine and lysine residues are shown as ball-and-sticks in blue. **(B)** The modeled structure of P2 is built by Discovery Studio 3.5 (Accelrys Software, San Diego, CA, USA). The structure of P2 is presented in magenta ribbon with the arginine and lysine residues shown in ball-and-sticks in blue. In both **(A)** and **(B)**, the electrostatic surfaces are in blue (positive charge), red (negative charged), and white (neutral).