Supplementary Information

Solution NMR and racemic crystallography provide insights into a novel structural class of cyclic plant peptides

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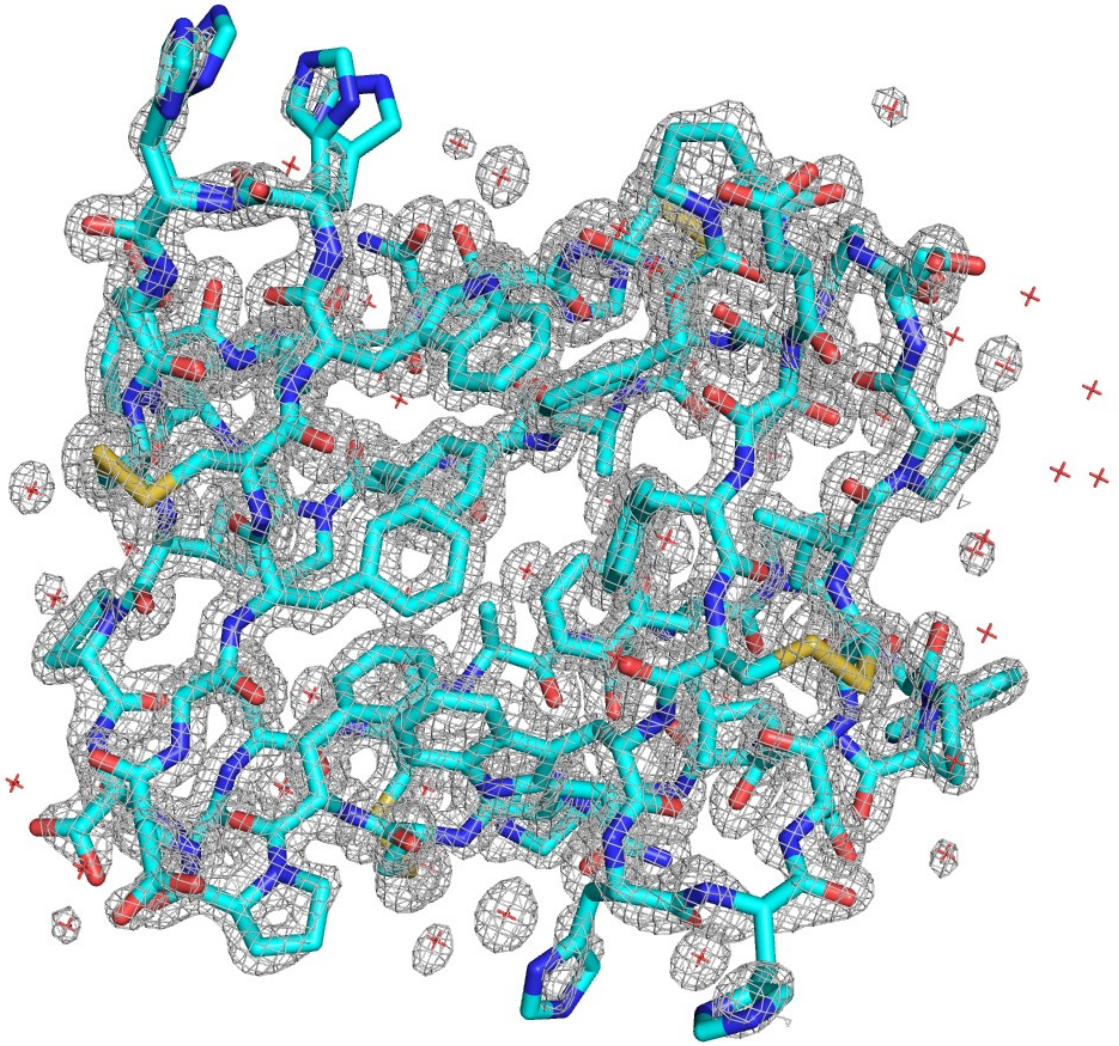
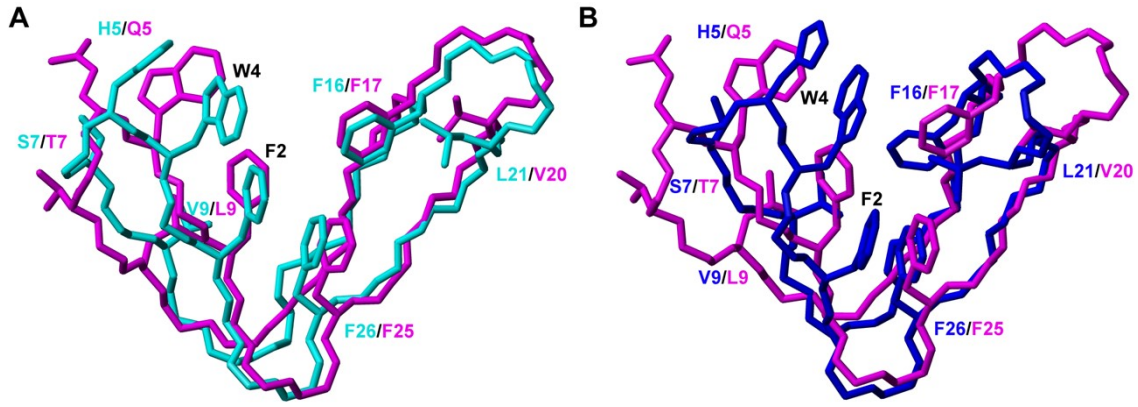


Supplementary Figure 1: Validation of L-PDP-23 dimer electron density map. The L-PDP-23 crystal structure is an excellent fit within a composite omit map (generated using PHENIX),[1] except for His5 and His6 in each monomer.



Supplementary Figure 2: Overlay of the 3D structures of PDP-23 in both monomeric and dimeric forms with PDP-24. (A) Overlay of one molecule of the symmetrical homodimeric form of PDP-23 (cyan) with PDP-24 (magenta). (B) Overlay of the monomeric form of PDP-23 (blue) with PDP-24 (magenta). Labels are supplied for orientation and are given in colour when there is a difference in residue between the two peptides. PDP-24 adopts a structure more akin to the structure of dimeric PDP-23 than monomeric PDP-23 but yet does not adopt a homodimer in aqueous solution.

Supplementary Table 1: Minimum inhibitory concentrations of PDP-23 and -24 against common microbes

Peptides	MIC (μM)		
	E. coli	*S. aureus*	*C. albicans*
PDP-23	>80	>80	>80
PDP-24	>80	>80	>80
LL-37 (Positive control)	0.625	1.25	2.5

Supplementary Table 2: Insecticidal assay dosages, insect weights, N values and % healthy specimens 24 h post injection

Peptide	Average dose (μg/kg)	Average weight (g)	*N*	% Healthy
PDP-23				
	3897.1	2.57	5	100
	382.8	2.61	5	100
	37.0	2.71	5	100
	4.0	2.48	5	100
	0.4	2.41	5	100
α-1 (no HYP)				
	203.9	2.45	3*	0
	109.1	2.29	5	0
	23.1	2.17	5	20
	4.9	2.03	5	100
	0.8	2.56	5	100
	0.2	2.23	5	100
Control (H_2O)				
	0.0		5	100

*Two animals were excluded from the assay due to failed injections.

References:

1. D. Liebschner, P. V. Afonine, M. L. Baker, G. Bunkóczi, V. B. Chen, T. I. Croll, B. Hintze, L. W. Hung, S. Jain, A. J. McCoy, N. W. Moriarty, R. D. Oeffner, B. K. Poon, M. G. Prisant, R. J. Read, J. S. Richardson, D. C. Richardson, M. D. Sammito, O. V. Sobolev, D. H. Stockwell, T. C. Terwilliger, A. G. Urzhumtsev, L. L. Videau, C. J. Williams and P. D. Adams, *Acta Crystallogr. D* 2019, **75**, 861-877.