

**Cell Selective Pore Forming Antimicrobial Peptides of the Prodomain of Human Furin:  
A Conserved Aromatic/Cationic Sequence Mapping, Membrane Disruption and  
Atomic-resolution Structure and Dynamics**

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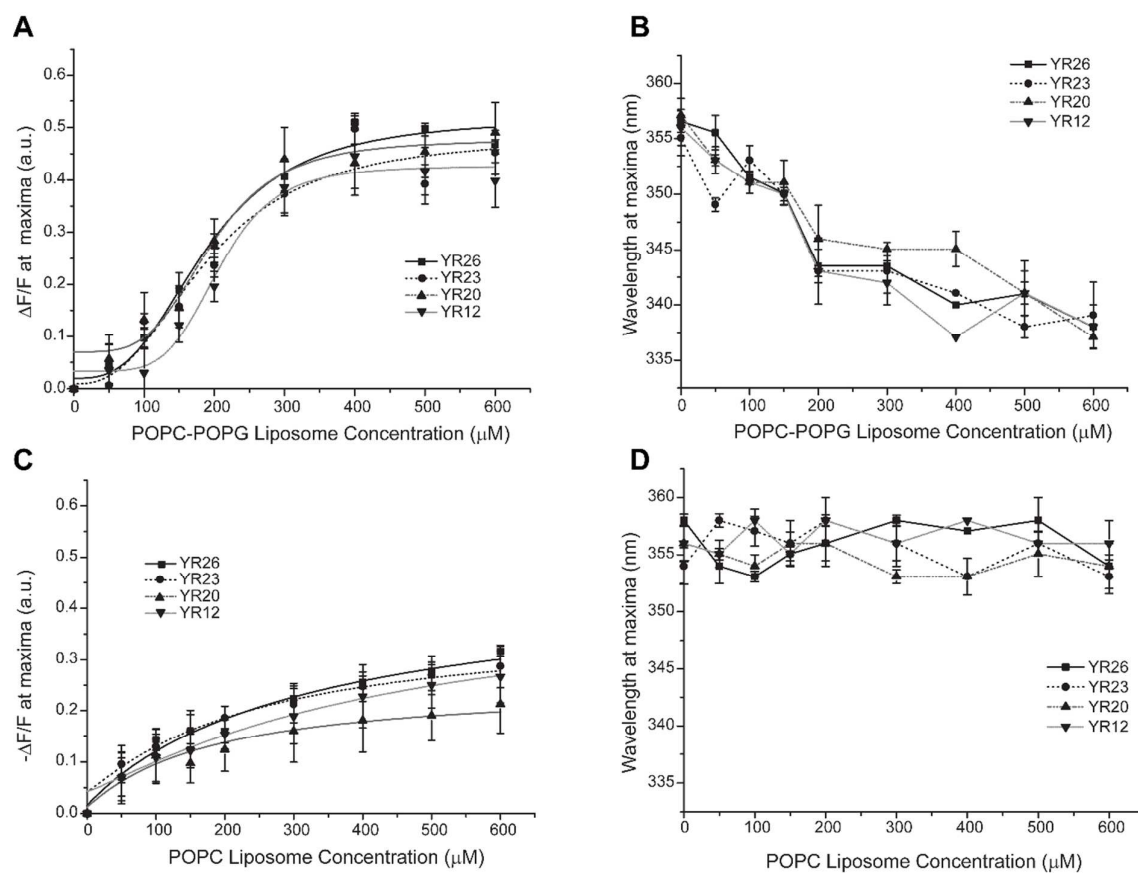
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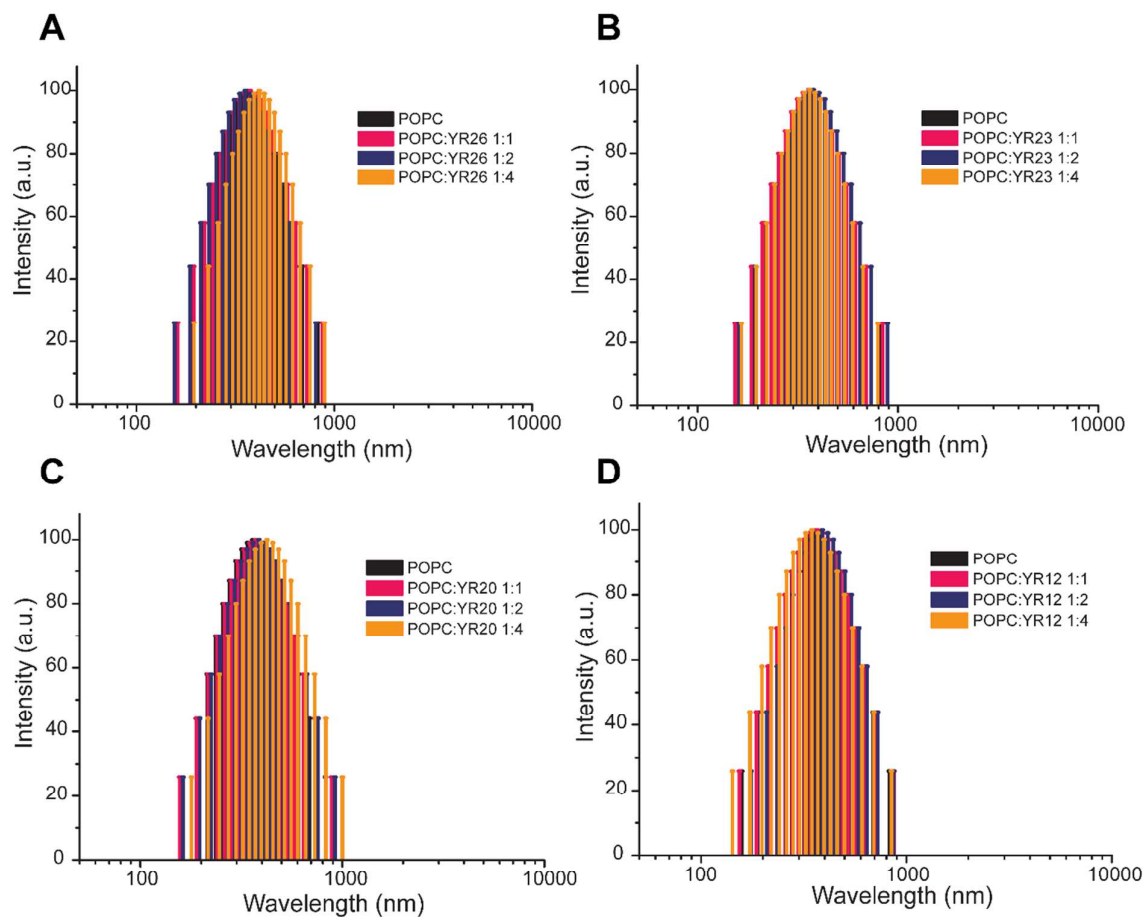
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**Supplementary Figure S1:** Intrinsic Trp fluorescence experiments of YR26, YR23, YR20 and YR12 peptides as a function of concentrations of liposomes. (A) Changes in fluorescence intensity at the emission maxima and (B) Changes in emission wavelength ( $\lambda_{\text{max}}$ ) induced by negatively charged POPC-POPG liposomes. (C) Changes in fluorescence intensity at the emission maxima and (B) Changes in emission wavelength ( $\lambda_{\text{max}}$ ) induced by zwitterionic POPC liposomes.



**Supplementary Figure S2:** Bar diagrams show particle size distribution of POPC vesicles, estimated from DLS experiments, in free solutions and at different molar ratios of peptides (A) YR26, (B) YR23, (C) YR20 and (D) YR12.

**Supplementary Table S1:** Particle size analysis (nm) of zwitterionic POPC liposomes. There is no significant change in the mean diameter of zwitterionic POPC liposomes even in presence of high peptide concentrations. This suggests that the tested peptides are highly selective and do not interact with these mammalian cell mimicking liposomes. The mean diameter of free POPC liposome was observed to be 370.8 nm.

Peptides	POPC: Peptide		
	1:1	1:2	1:4
YR26	379.2	351.3	406
YR23	362.5	374.3	352.4
YR20	375.8	382.9	412
YR12	368.9	385.7	337.1

**Supplementary Table S2:** Particle size analysis (nm) of POPC-POPG liposomes. Particle size distribution of POPC-POPG liposomes in presence of increasing concentrations of prodomain peptides. The mean diameter of free POPC-POPG liposome was observed to be 192.3 nm.

Peptides	POPC-POPG: Peptide		
	1:1	1:2	1:4
YR26	488.1	1193.5	2311.2
YR23	521.5	938.4	1515.9
YR20	420.2	658.6	1063.9
YR12	198.2	227.4	430.8

**Supplementary Table S3:** A summary of structural statistics of YR26 in presence of anionic SDS micelles.

	<b>YR26 in presence of SDS</b>
<b>Distance constraints</b>	
Sequential [ $ i-j =1$ ]	87
Medium range [ $1 <  i-j  < 4$ ]	19
Long range [ $ i-j  \geq 4$ ]	1
Total	191
<b>Dihedral-angle constraints</b>	40
<b>Deviation from mean structure (Å)</b>	
All backbone atoms	0.27
All heavy atoms	1.20
<b>Ramachandran plot for the mean structure (%residues)</b>	
Most favoured region	76.2
Additional allowed region	23.8
Generously allowed region	0
Disallowed region	0