

Supplementary Materials: Evaluation of a Novel Synthetic Peptide Derived from Cytolytic Mycotoxin Candidalysin

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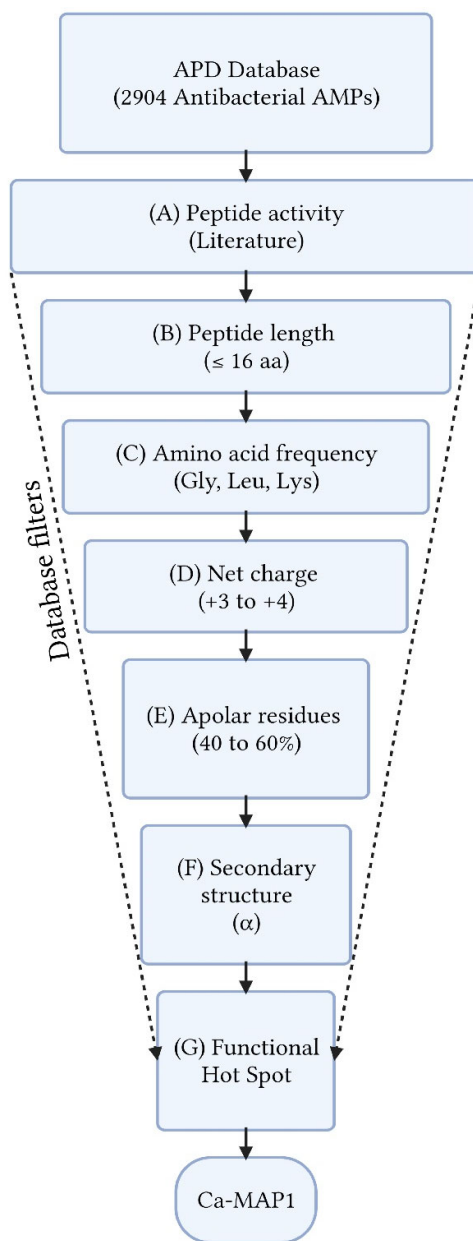


Figure S1. Database filtering technology schematic: (A) Candidalysin activity, (B) Determination of peptide length, (C) Amino acids frequency, (D) Net charge, (E) Hydrophobic content, (F) Structure type (F) Functional hot spot. The designed peptide is called Ca-MAP1.

Table S1. Strategy for the selection of peptide based on physical chemical parameters of candidalysin. Legend: <H> = Hydrophobicity in the Eisenberg scale; <μH> = Hydrophobic moment.

Sequence	Length	Net charge	Nonpolar residues (%)	<H>	<μH>
SIIGIIMGILGNIPQVIQIIMSIVKAFKGNKR	32	+4	56.25	0.679	0.408
SIIGIIMGILGNIPQV-----	16	0	62.50	0.926	0.526
-----IQIIMSIVKAFKGNKR	16	+4	50.00	0.432	0.409
-----QIIMSIVKAFKGNKR	15	+4	46.67	0.341	0.446
-----IIMSIVKAFKGNKR	14	+4	50.00	0.381	0.463
-----IMSIVKAFKGNKR	13	+4	46.15	0.272	0.439
-----MSIVKAFKGNKR	12	+4	41.67	0.144	0.350
-----SIVKAFKGNKR	11	+4	36.36	0.045	0.472
-----IVKAFKGNKR	10	+4	40.00	0.054	0.518
-----VKAFKGNKR	9	+4	33.33	-0.140	0.381
-----IQIIMSIVKAFKGNK-	15	+3	53.33	0.528	0.382
-----IQIIMSIVKAFKGN--	14	+2	57.14	0.636	0.464
-----IQIIMSIVKAFKG---	13	+2	61.54	0.732	0.521
-----IQIIMSIVKAFK----	12	+2	66.67	0.792	0.565
-----IQIIMSIVKAF-----	11	+1	72.73	0.955	0.607
-----IQIIMSIVKA-----	10	+1	70.00	0.871	0.491
-----MSIVKAFKG-----	9	+2	55.56	0.481	0.477
-----QIIMSIVKAFKGNK-	14	+3	50.00	0.437	0.410
-----IIMSIVKAFKGN--	12	+2	58.33	0.611	0.507
-----IMSIVKAFKG---	10	+2	60.00	0.613	0.593

Table S2. Antibioqram assay against Gram-negative and -positive bacteria. (+) resistant at the concentrations tested.

Microorganism	Amoxicilin	Imipenem	Eritromicin	Ampicilin
Gram-negative	>350.3 (μM)	>427.6 (μM)	>174.4 (μM)	>366.3 (μM)
<i>Acinetobacter baumannii</i> (clinical isolated)	+	+	+	+
<i>Escherichia coli</i> (clinical isolated)	+	+	+	+
<i>Escherichia coli</i> (KPC)	+	+	+	+
<i>Klebsiella pneumoniae</i> (ATCC)	+	+	+	+
<i>Klebsiella pneumoniae</i> (KPC)	+	+	+	+
<i>Pseudomonas aeruginosa</i> (ATCC)	+	+	+	+
Gram-positive				
<i>Staphylococcus aureus</i> (clinical isolated)	+	+	+	+