

Table S1. Minimum inhibitory concentration (MIC) of TcPaSK against *S. aureus*. Experiments were performed in triplicate.

TcPaSK concentration ($\mu\text{g/mL}$)	128	64	32	16	8	4	2	1	0.5	0.25
	-	-	-	+	+	+	+	+	+	+

(+) visible growth appearance.

(-) no visible growth appearance.

Table S2. Hemolytic activity of TcPaSK peptide against human red blood cells at different concentrations. Percentage of haemolysis were calculated as described in Material and Methods using the control hemolytic peptide Melittin. Values are mean \pm SE of three independent experiments.

Concentration (μM)	2.35	4.7	9.4	18.75	37.5	75
TcPaSK (% hemolysis)	7.28 ± 0.1	10.00 ± 0.7	11.44 ± 2.0	12.7 ± 0.9	14.0 ± 2.4	16.0 ± 3.4

Model-Template Alignment				QMEAN
TcPaSK	KVNHAACA AHCLLKRKRGGYCNKRRICVCRN	31		
2LLD	-VKHSAACA AHCLLRGNRGGYCNGRAICVCRN	40		-0.63
TcPaSK	KVNHAACA AHCLLKRKRGGYCNKRRICVCRN	31		
2NZ3	.TCDLASIFNVNHALCAAHCLIRRYRGGYCNKAVCVCRN	40		-0.97
TcPaSK	KVNHAACA AHCLLKRKRGGYCNKRRICVCRN	31		
1ICA	.TCDLLSGTGINHSACA AHCLLRGNRGGYCNKGVICVCRN	40		-2.05
TcPaSK	KVNHAACA AHCLLKRKRGGYCNKRRICVCRN	31		
1L4V	.TCDLLSGTGINHSACA AHCLLRGNRGGYCNKAVCVCRN	40		-2.71

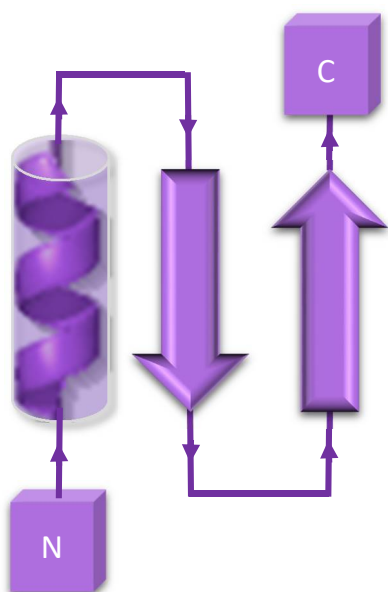
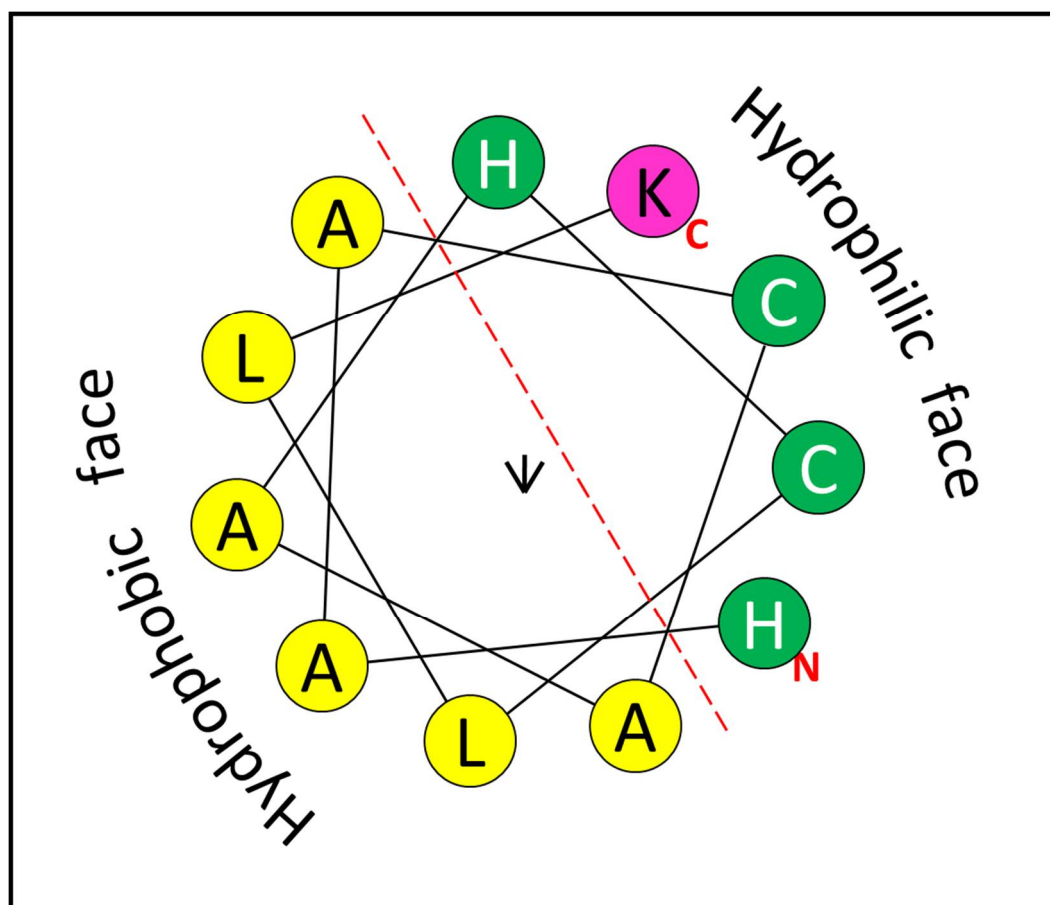


Figure S1. (A) Quality assessment of TcPaSK peptide structure prediction based on the composite scoring function QMEAN (Swiss Model platform <https://swissmodel.expasy.org/qmean/>) which estimates the likelihood that a given model is of comparable quality to experimental structures [30]. **(B)** Topology diagram of TcPaSK peptide derived from the model-template based structural alignment of the four top hits in the PDB data bank. Diagram shows how the alpha-helix (cylinder with a spiral ribbon inside) is located relative to the beta strands (represented by the large arrows) that forms and antiparallel beta-sheet. Small arrows indicate the directionality of the protein chain, from the N- to the C-terminus.



- Polar amino-acids
- Non-polar amino-acids
- Positively charged amino-acids

Figure S2. Helical wheel projection of the predicted α -helix region of TcPaSK peptide. Amino acids in yellow color are hydrophobic (nonpolar), amino acids in green color are polar (hydrophilic) and amino acids in magenta color are positively charged. Red line denotes the spatial separation of the hydrophobic and hydrophilic faces of the amphipathic α -helix. The letters N and C in the projections indicate the N- and C-terminals, respectively. Arrow represents the hydrophobic moment and indicate the direction of summed vectors of hydrophobicity estimated using HELIQUEST software (<https://heliquet.ipmc.cnrs.fr/>).