

Article

Inhibition of ACE2–S Protein Interaction by a Short Functional Peptide with a Boomerang Structure

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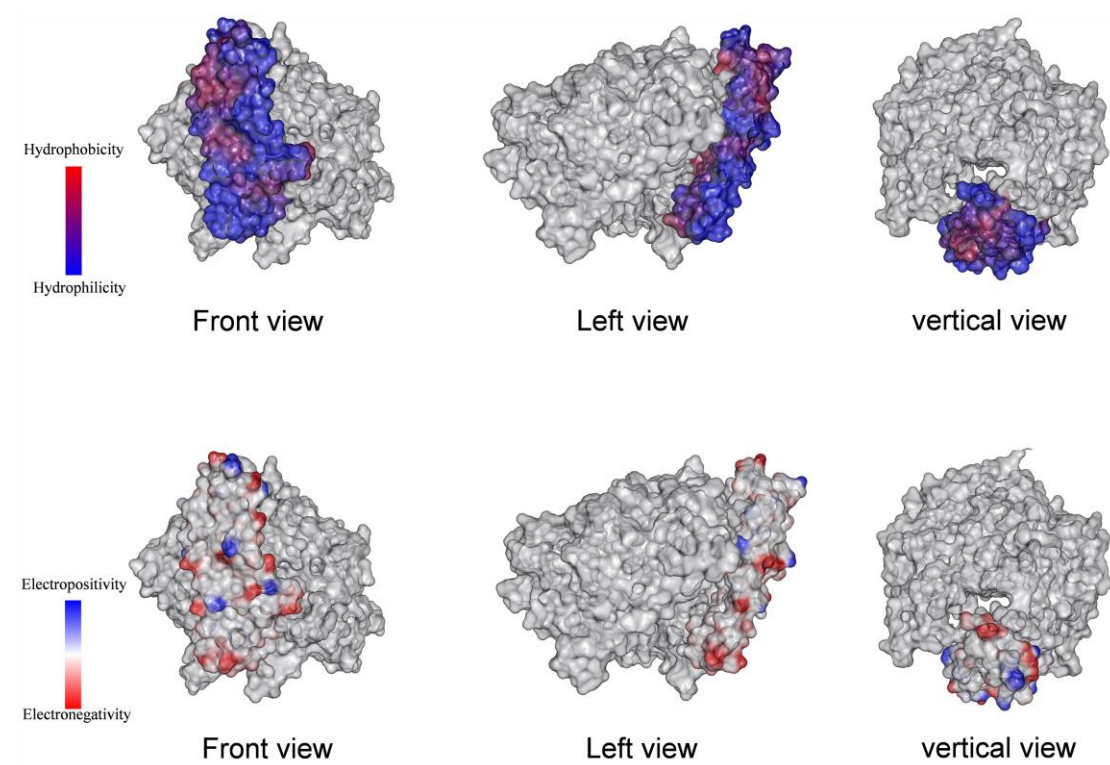


Figure S1. Topographic analysis of ACE2 LBD.

Table S1. Docking results for candidate peptides binding to ACE2 LBD.

	Sequence	E _{Binding} energy (Kcal/mol)
Control sequence	YRLFRR	-3.21
Peptide	RCPNG	-5.01
	RYPFL	-5.11
	KEPEQ	-5.22
	REPEQ	-5.32
	KRPEL	-5.36
	RLPAG	-5.50
	RLPRK	-5.56
	KYPPY	-5.58
	RYPWK	-5.59
	RGPAK	-5.60
	KYPFY	-5.62
	KAPWK	-5.67
	KYPQY	-5.75
	KYPMY	-5.93
	KYPAY	-6.91

The chemical formula of K5

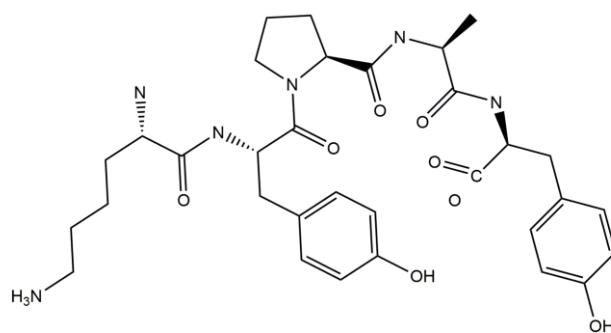


Figure S2. The chemical formula of K5.

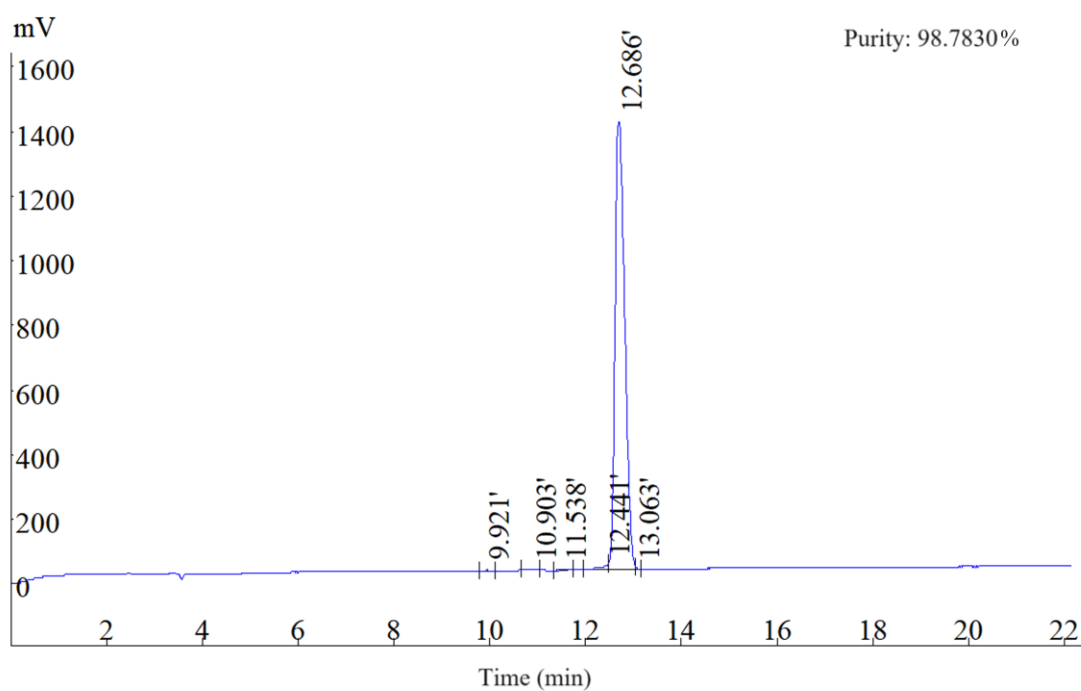


Figure S3. The HPLC analysis of K5. Elution gradient: from 11% acetonitrile to 36% acetonitrile

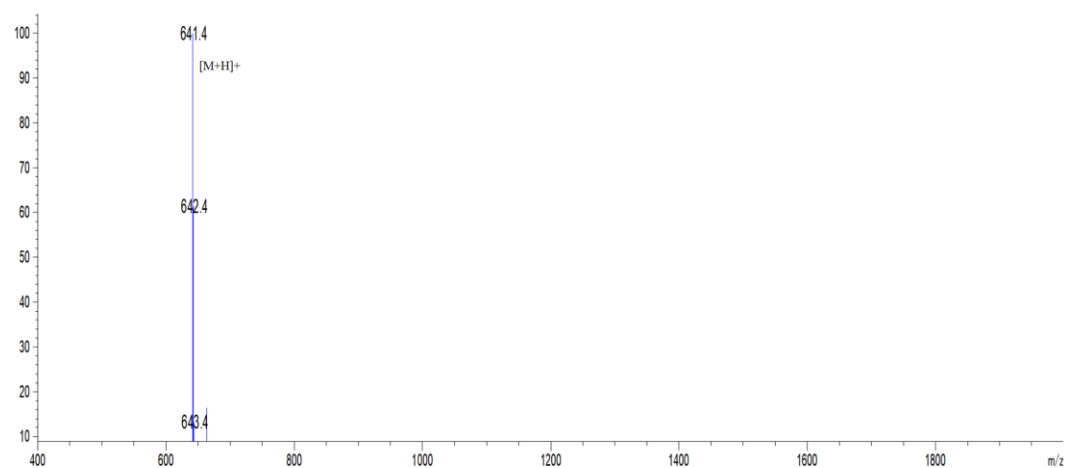


Figure S4. The mass spectrometer analysis of K5.

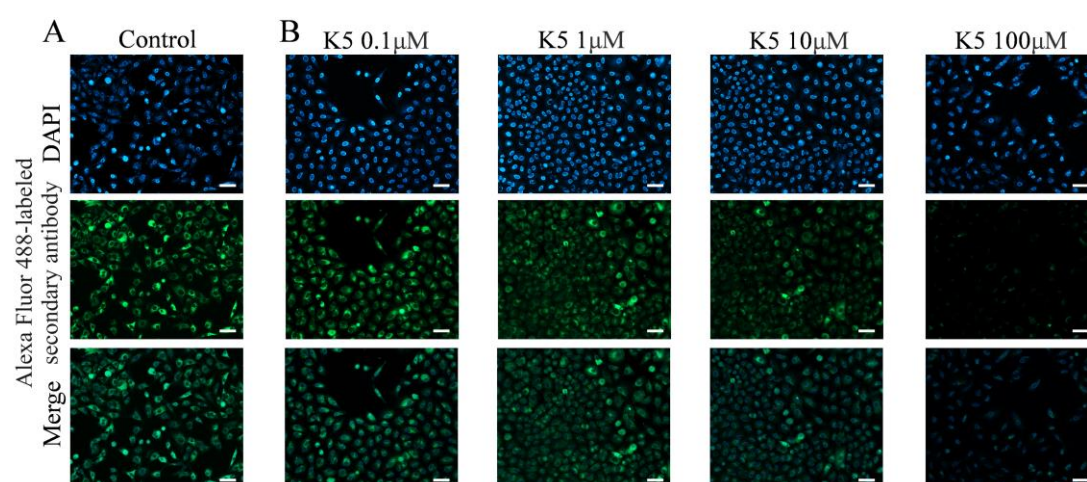


Figure S5. The cellular adsorption of K5 by A549 cells. (A) The fluorescence microscope images of control group for 1 hour and their distribution. (B) Visualization of SARS-CoV-2 S protein-ACE2 attachment blocking by K5. Bar = 50 μ m.

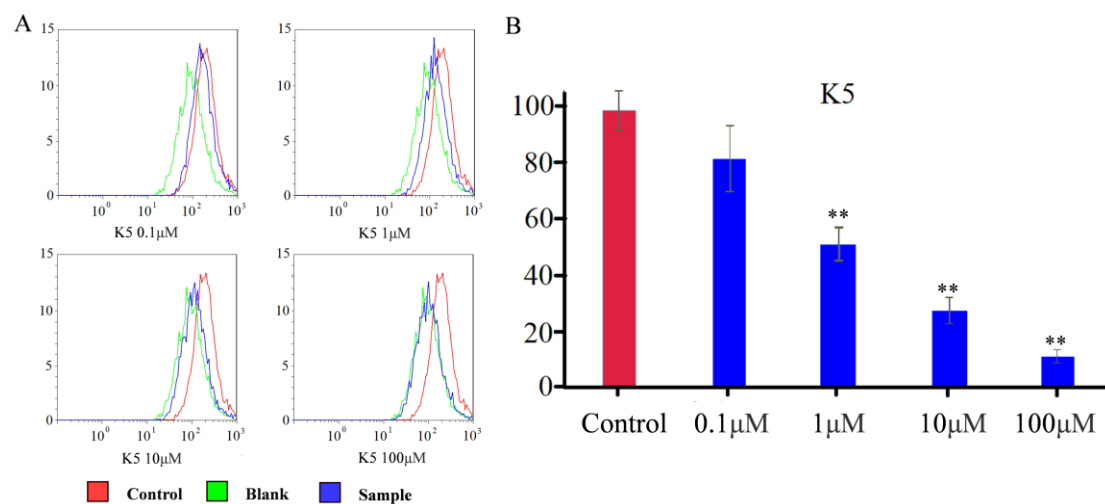


Figure S6. The flow cytometry analysis of inhibitory effect of K5 on S protein-ACE2 interaction. (A) FACS analysis of effect of K5 on SARS-CoV-2 S protein-A549 cell attachment. (B) MFI analysis of effect of K5 on SARS-CoV-2 S protein-A549 cell attachment.

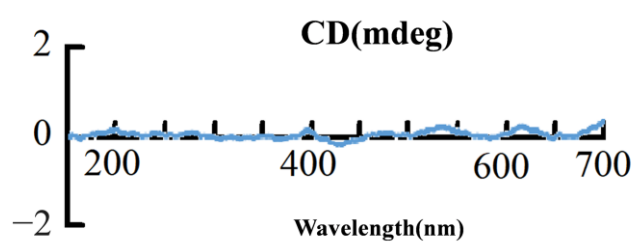


Figure S7. Circular dichroic analysis of K5.

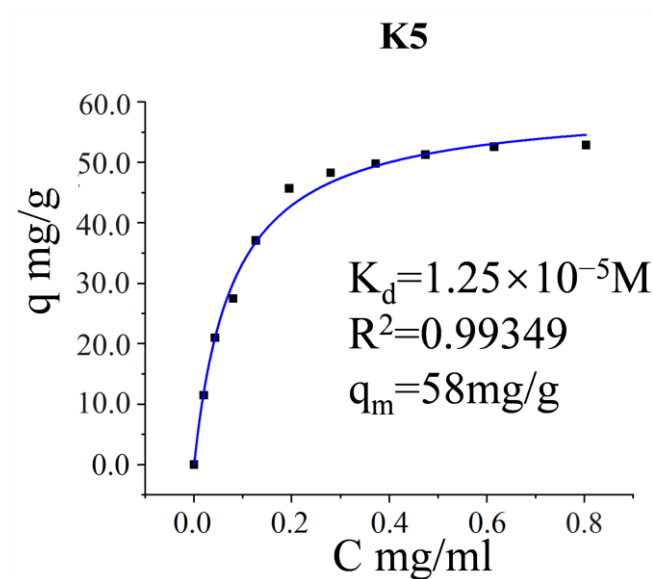


Figure S8. Adsorption kinetics analysis of K5.