Supplementary materials

Table S1: Information of the theory and experimental mass for the synthesized peptides.

Peptide	Mass theory (m)	Experimental, $[M+H]^+$ (m/z)
DKPRR	670.8	671.5
DKPPR	611.7	612.5
DKPPR-NH_2	610.7	661.0
TKPRR	656.8	657.5
TKPPR	597.7	598.4
TKPRR-NH_2	655.8	656.5
CDKPRR	773.9	773.5
APQPRPL	777.9	778.6
CPQPRPL	810.0	810.6

Table 2: Chemical shifts of ^{1}H NMR for the synthesized peptides.

			DKPRR			
	NH	α-H	β-H	γ-H	δ-H	Others
Asp	8.10	4.06	2.51, 2.76			
Lys	8.82	4.36	1.68		1.65	ε-CH_2 = 2.78; γ-CH_2 = 1.56
Pro		4.51	1.84, 2.49		3.08, 3.10	
Arg	8.37	4.11	1.70		2.76	
Arg	8.40	4.13	1.73		2.78	
			DKPPR			
	NH	α-H	β-H	γ-H	δ-H	Others
Asp		4.12	2.54, 2.58			
Lys	8.23	4.12	1.70			ε-NH_3^+ = 8.00; ε-CH_2 =

						3.09; δ-CH_2 = 1.60
Pro		4.55	1.70, 1.90		3.55, 3.65	
Pro		4.48	1.68, 1.89		3.52, 3.55	
Arg	8.76	4.44	1.51, 1.60			ε-NH = 8.58; δ-CH_2 = 3.52
DKPPR-amide						
	NH	α-H	β-H	γ-H	δ-H	Others
Asp	8.60	4.11	2.63, 2.73			
Lys	8.63	4.47	1.64			ε-NH_3^+ = 7.69; ε-CH_2 = 2.73; δ-CH_2 = 1.62; γ-CH_2 = 1.38
Pro		4.29	1.89, 2.01		3.53, 3.64	
Pro		4.56	1.89, 2.15		3.53, 3.64	
Arg	8.18	4.14	1.46, 1,64			ε-NH = 7.71; δ-CH_2 = 3.10
TKPRR						
	NH	α-H	β-H	γ-H	δ-H	Others
Thr		3.81	3.68			γ-CH_3 = 1.14
Lys	8.63	4.54	1.72			ε -CH_2 = 2.76; γ-CH_2 = 1.42; δ-CH_2 = 1.57
Pro		4.32	1.72, 2.12		3.68	
Arg	8.36	4.05	1.57, 1.72			δ-CH_2 = 3.08
Arg	8.52	4.32	1.57, 1.72			δ-CH_2 = 3.08
TKPPR						
	NH	α-H	β-H	γ-H	δ-H	Others
Thr	8.10	3.60	3.58			γ-CH_3 = 1.14
Lys	8.61	4.56	1.60			ε-NH_3^+ = 7.77; ε-CH_2 = 2.74; δ-CH_2 = 1.53; γ-CH_2 = 1.40
Pro		4.56	1.89, 2.20		3.58, 3.60	

Pro		4.34	1.89, 2.10		3.11, 3.58	
Arg	8.00	4.34	1.53, 1.89			ε-NH = 7.60; δ-CH_2 = 3.09
TKPRR-NH_2						
	NH	α-H	β-H	γ-H	δ-H	Others
Thr		3.80	3.30			γ-CH_3 = 1.10
Lys	8.63	4.51	1.68, 2.76			ε-NH_3^+ = 8.47; ε-CH_2 = 3.30; δ-CH_2 = 1.63; γ-CH_2 = 1.42
Pro		4.36	1.91, 2.08		3.64	
Arg	7.96	4.13	1.55, 1.68			ε-NH = 7.63; δ-CH_2 = 3.09; γ-CH_2 = 1.53
Arg	7.89	4.13	1.55, 1.68			ε-NH = 7.60; δ-CH_2 = 3.09; γ-CH_2 = 1.53

Table 2: Chemical shifts of ^{1}H NMR for the synthesized peptides.

CDKPRR						
	NH	α-H	β-H	γ-H	δ-H	Others
Cys		4.08	2.89, 3.33			
Asp	8.83	4.57	2.67, 2.72			
Lys	8.18	4.45	1.74			ε-NH_3^+ = 7.84; ε-CH_2 = 2.27; δ-CH_2 = 1.54; γ-CH_2 = 1.38
Pro		4.36	1.84, 2.05		3.52, 3.60	
Arg	8.13	4.17	1.75, 1.83			ε-NH = 7.84; δ-CH_2 = 3.09
Arg	8.10	4.26	1.54, 1.84			ε-NH = 7.84; δ-CH_2 = 3.10
APQPRPL						
	NH	α-H	β-H	γ-H	δ-H	Others

Ala	8.07	4.17	1.33			
Pro		4.17	1.34, 1.50			
Gln	8.12	4.35	1.91	2.43		
Pro		4.17	1.34, 1.50			
Arg		4.46	1.70		3.37	ε-NH = 7.46; γ-CH_2 = 1.67
Pro		4.17	1.34, 1.50			
Leu	8.10	4.15	1.67	1.53		δ-CH_3 = 0.83

CPQPRPL

	NH	α-H	β-H	γ-H	δ-H	Others
Cys	7.52	4.46	3.08, 3.25			
Pro		4.36	2.11		3.75	γ-CH_2 = 1.87
Gln	8.23	4.38	1.53, 1.91	2.14		
Pro		4.36	2.11		3.75	γ-CH_2 = 1.87
Arg	8.10	4.44	1.53, 1.81			ε-NH = 7.52; δ-CH_2 = 3.10; γ-CH_2 = 1.51
Pro		4.36	2.11		3.75	γ-CH_2 = 1.87
Leu	8.10	4.10	1.70	1.53		δ-CH_3 = 0.91

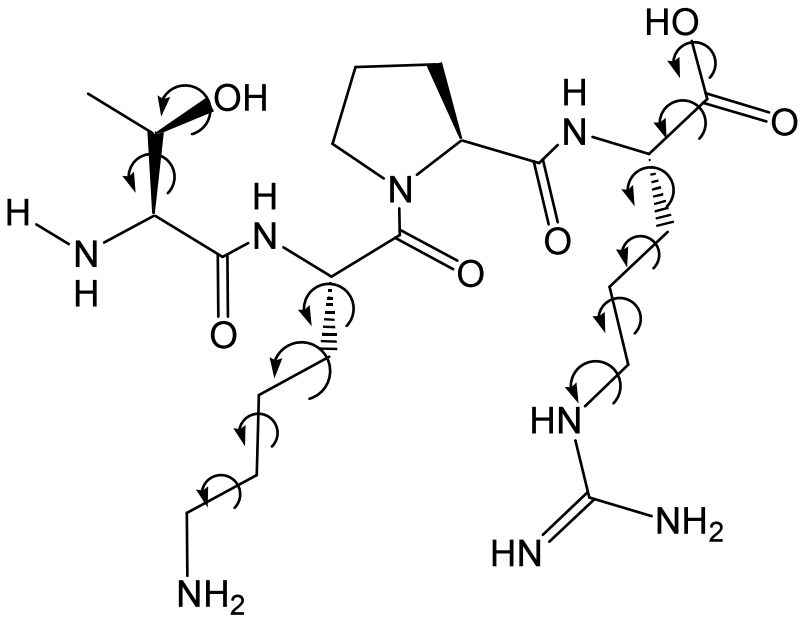

Figure S1: The rotatable bonds assigned to tuftsin in the docking study.