

1 **Supplementary Materials**

2 **Table S1.** The systematic binding energies (ΔU values) regarding the systematic combinations between the four aromatic amino acids (Trp, Phe, Tyr and His) plus one non-aromatic amino acid (Ala) at the residues -1 and -4 of C3H1 peptide (unit: kcal/mol)

	Phe-4	Tyr-4	Trp-4	His-4	Ala-4
Trp-1	-12.5	-14.2	-13.7	-11.3	-9.1
Phe-1	-10.7	-11.4	-11.8	-10.2	-8.6
Tyr-1	-11.6	-12.3	-11.0	-10.7	-8.9
His-1	-10.2	-11.2	-10.6	-9.5	-8.4
Ala-1	-8.4	-8.7	-8.8	-8.5	-8.0