

**Online Supporting Information S1.** The benchmark dataset  $\mathbb{S} = \mathbb{S}^{\text{AMP}} \cup \mathbb{S}^{\text{non-AMP}}$ , where  $\mathbb{S}^{\text{AMP}}$  contains 878 AMP sequences while  $\mathbb{S}^{\text{non-AMP}}$  contains 2,405 non-AMP sequences. The AMP sequences are further classified into five subsets according to their attributes, i.e.,  $\mathbb{S}^{\text{AMP}} = \mathbb{S}_1^{\text{AMP}} \cup \mathbb{S}_2^{\text{AMP}} \cup \mathbb{S}_3^{\text{AMP}} \cup \mathbb{S}_4^{\text{AMP}} \cup \mathbb{S}_5^{\text{AMP}}$ , where  $\mathbb{S}_1^{\text{AMP}}$  contains 770 antibacterial peptides,  $\mathbb{S}_2^{\text{AMP}}$  140 anticancer/tumor peptides,  $\mathbb{S}_3^{\text{AMP}}$  366 antifungal peptides,  $\mathbb{S}_4^{\text{AMP}}$  86 anti-HIV peptides, and  $\mathbb{S}_5^{\text{AMP}}$  124 antiviral peptides. A sequence in  $\mathbb{S}^{\text{AMP}}$  may belong to more than one attributes. Of the 878 AMP sequences, 454 belong to one attribute, 296 to two attributes, 85 to three attributes, 30 to four attributes, and 13 to five attributes.

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## I. $\mathbb{S}^{\text{AMP}}$ : 878 AMP sequences

### (1) $\mathbb{S}_1^{\text{AMP}}$ : 770 antibacterial peptides

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#### (4) $S_4^{\text{AMP}}$ : 86 Anti-HIV peptides

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>AP00325  
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>AP00327  
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>AP00445  
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 >AP01273  
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## (5) $S_5^{\text{AMP}}$ : 124 Antiviral peptides

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 >AP00023  
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## II. $S^{\text{non-AMP}}$ : 2,405 non-AMP sequences

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