marine drugs

MDPI

Supplementary Materials

A Synthetic Derivative of Antimicrobial Peptide Holothuroidin 2 from Mediterranean Sea Cucumber (*Holothuria tubulosa)* in the Control of *Listeria monocytogenes*

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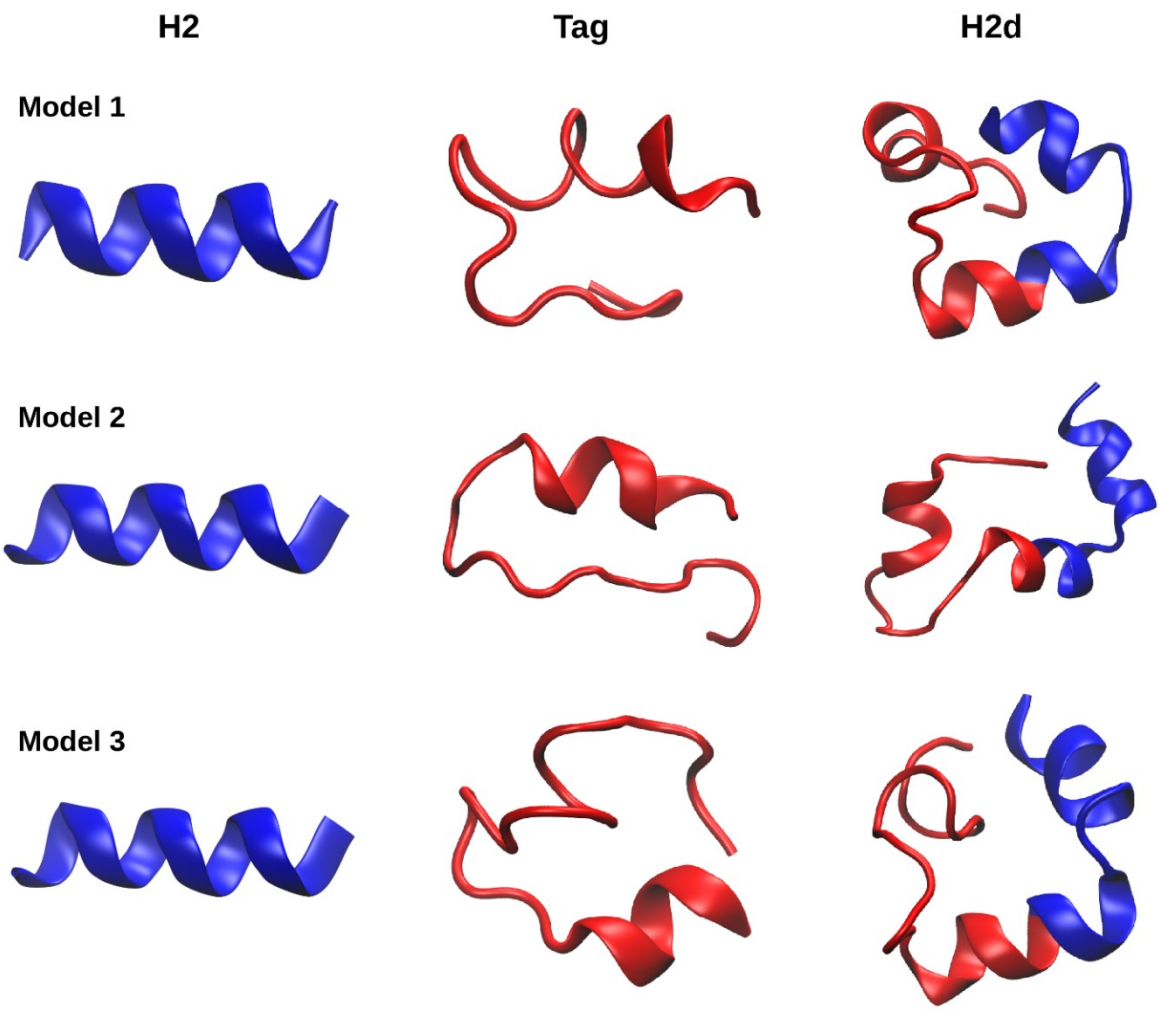

Figure S1. Structures of the best three models predicted by PEP-FOLD3 software for H2, Tag and H2d peptides.

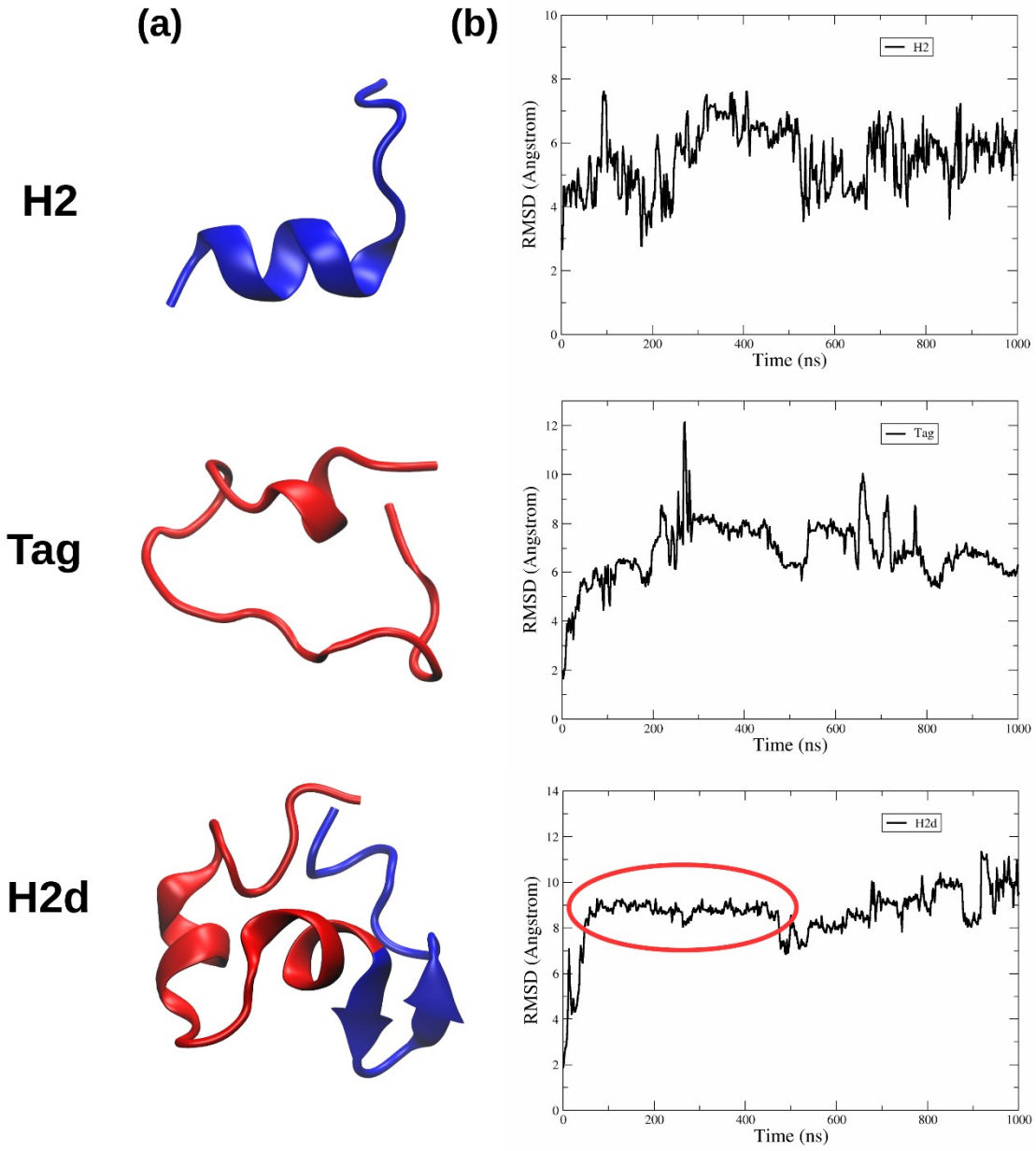

Figure S2. (**a**) The most representative cluster extracted from the Molecular Dynamics (MD) trajectories. (**b**) Root Mean Square Deviation (RMSD) of the MD simulations. H2 and Tag peptides are more flexible, while H2d adopts a stable tertiary structure for about 500 ns (highlighted in red).