Supplementary Material

Investigation on Two Human Defensin Dimers: Structure Prediction and Refinement Using A Combined Simulation Strategy

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Tables

Docking result from ClusPro

TABLE S1: hBD-2 dimer and HD5 dimer Structures Prediction from Cluspro Docking, the Population, Score and RMSD

hBD-2 dimer	
cluster NO.	cluster1
member number	272
scores	-578.0
RMSD(Å)	11.035
HD-5 dimer	
cluster NO.	cluster1
member number	399
center scores	-585.8
RMSD (Å)	9.313

In the Cluspro docking, the cluster1 has the highest population and the lowest score of combined energy.

Figures

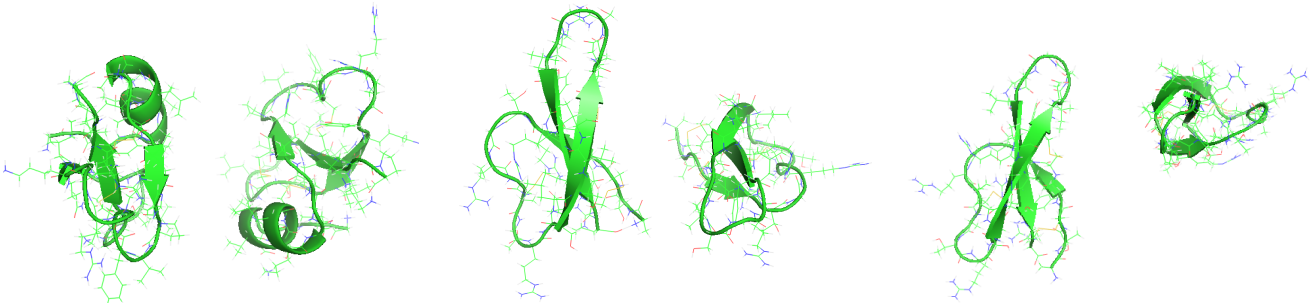

FIG. S1: Initial structures of hBD-2 molecules(Left) and HD5 molecules(Middle and Right) in the REX simulations.

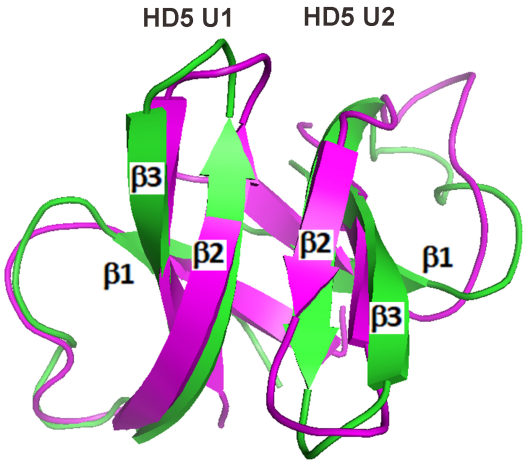

FIG. S2: The crystal structure of HD-5 dimer (shown in Green) in comparison with the REX predicted structure (HD5-dimer-2) (shown in Magenta), which started with the monomer structure of HD-5 with the PDB ID of 2LXZ.

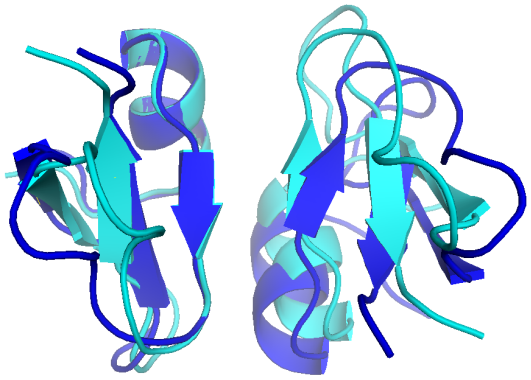

FIG. S3: The structure of hBD-2 dimer at 25 ns (in Blue) generated from the simulation initiated from the REX prediction, in comparison with the crystal structure (in Cyan).

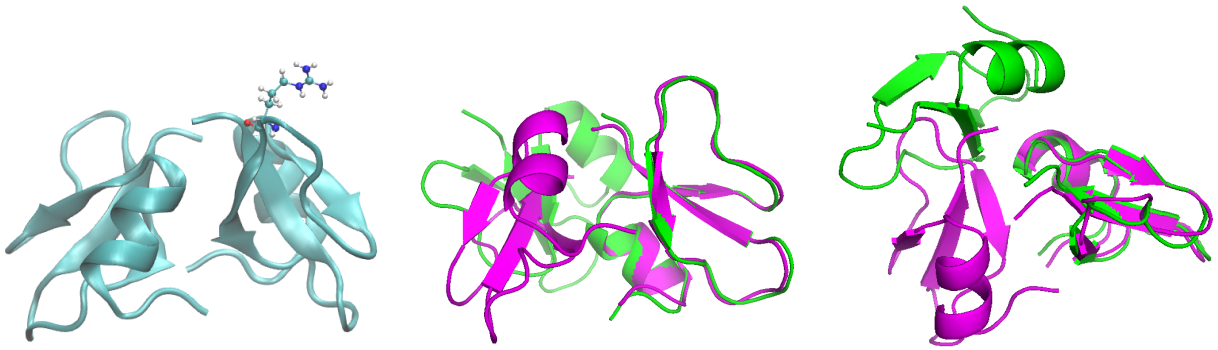

FIG. S4: Left). hBD-2 dimer structure at 125 ns extracted from the long-term simulation trajectory started from the REX predicted structure. The structure is in the opposite monoclinic form, with the dimer shown in New Cartoon with the reside Arg23 shown in CPK mode; Middle). Comparison of hBD-2 dimer structure at 125 ns (in Green) with the monoclinic form (in Magenta) of crystal structure in sideview and Right) in topview.

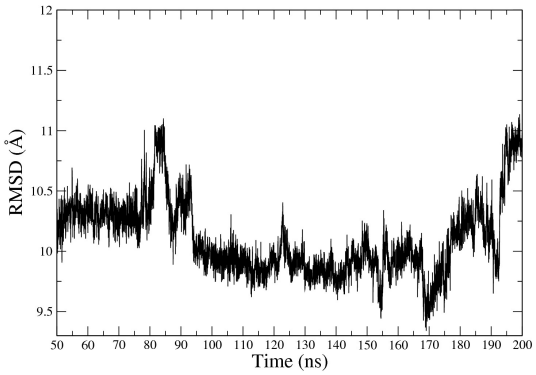

FIG. S5: RMSD of hBD-2 dimer in 50-200 ns during the microsecond-long simulation. The trajectories in the period were aligned on the hBD-2 monoclinic dimer form and the RMSD was calculated based on backbone CA atoms.

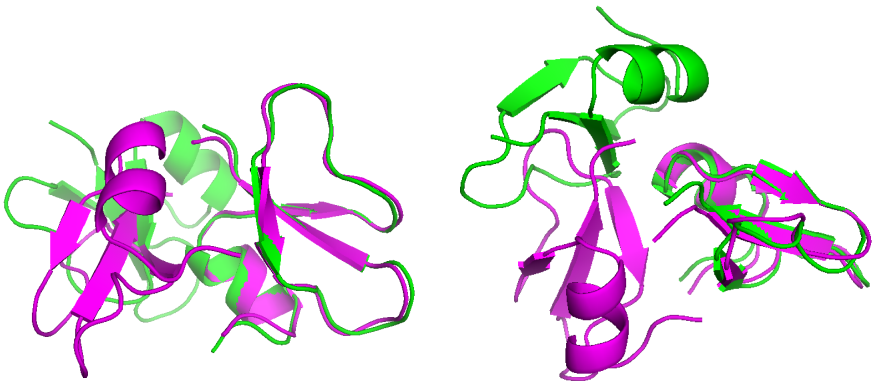

FIG. S6: Comparison of hBD-2 dimer structure at 125 ns (in Green) and at 200 ns (in Cyan) in the sideview (Left) and in the topview (Right) generated from REX initiated long-term simulations.

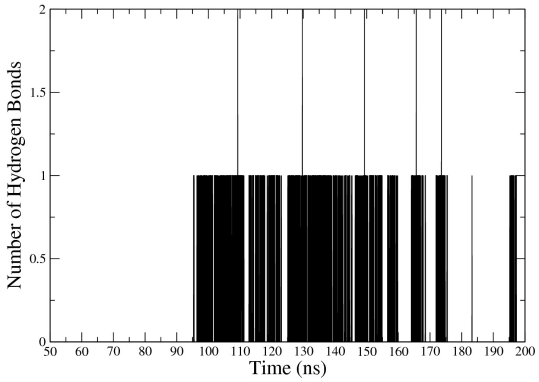

FIG. S7: Number of hydrogen bonds formed on the binding interface of hBD-2 dimer in the time range of 50 to 200 ns. The distance cutoff is 3.0 Å and the angle cutoff is 20 degrees in the hydrogen bonds calculations.

Movies

Movie S1. The movie shows the abrupt structure change of hBD-2 dimer during 50 to 200 ns time period corresponding to the abrupt increase of RMSD of hBD-2 dimer shown in Figure 3 (Left). The movie shows the Arg23 residue in CPK mode while the protein in Newcartoon. The movie was generated using VMD program.