Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information for "Potential Blockade of the human Voltage-dependent Anion Channel by MoS_2 Nanoflakes: A Molecular Dynamics Simulation Study"

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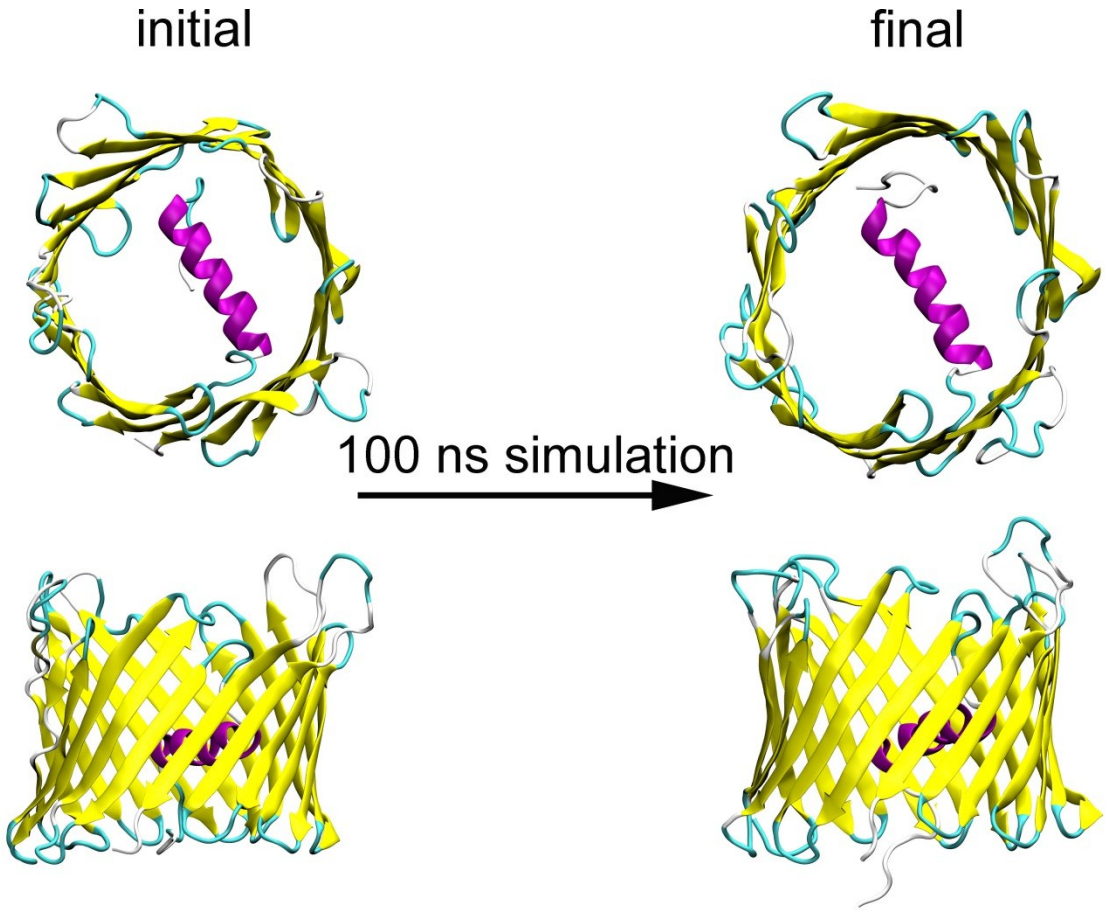

Figure S1. The initial and final configurations of hVDAC1 in control simulation. Yellow and purple ribbons represent the β-sheet and α-helix.

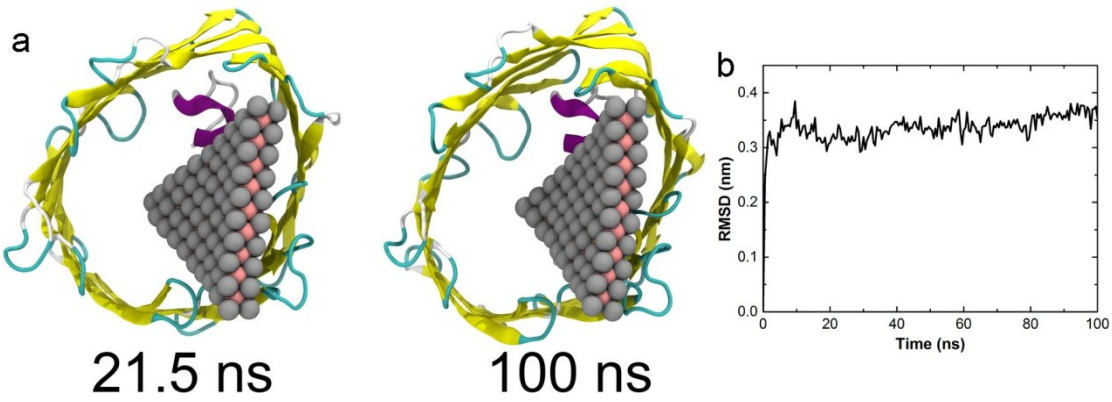

Figure S2. (a) Binding conformations corresponding to figure 3 at 21.5 ns and 100 ns. (b) Root mean square deviation evolution of C-α atoms of protein.

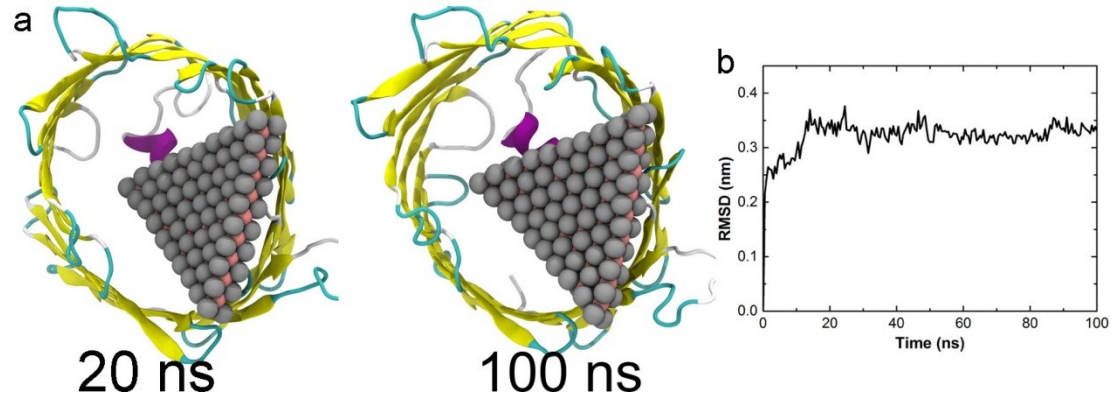

Figure S3. (a) Binding conformations corresponding to figure 5 at 20 ns and 100 ns. (b) Root mean square deviation evolution of C-α atoms of protein.

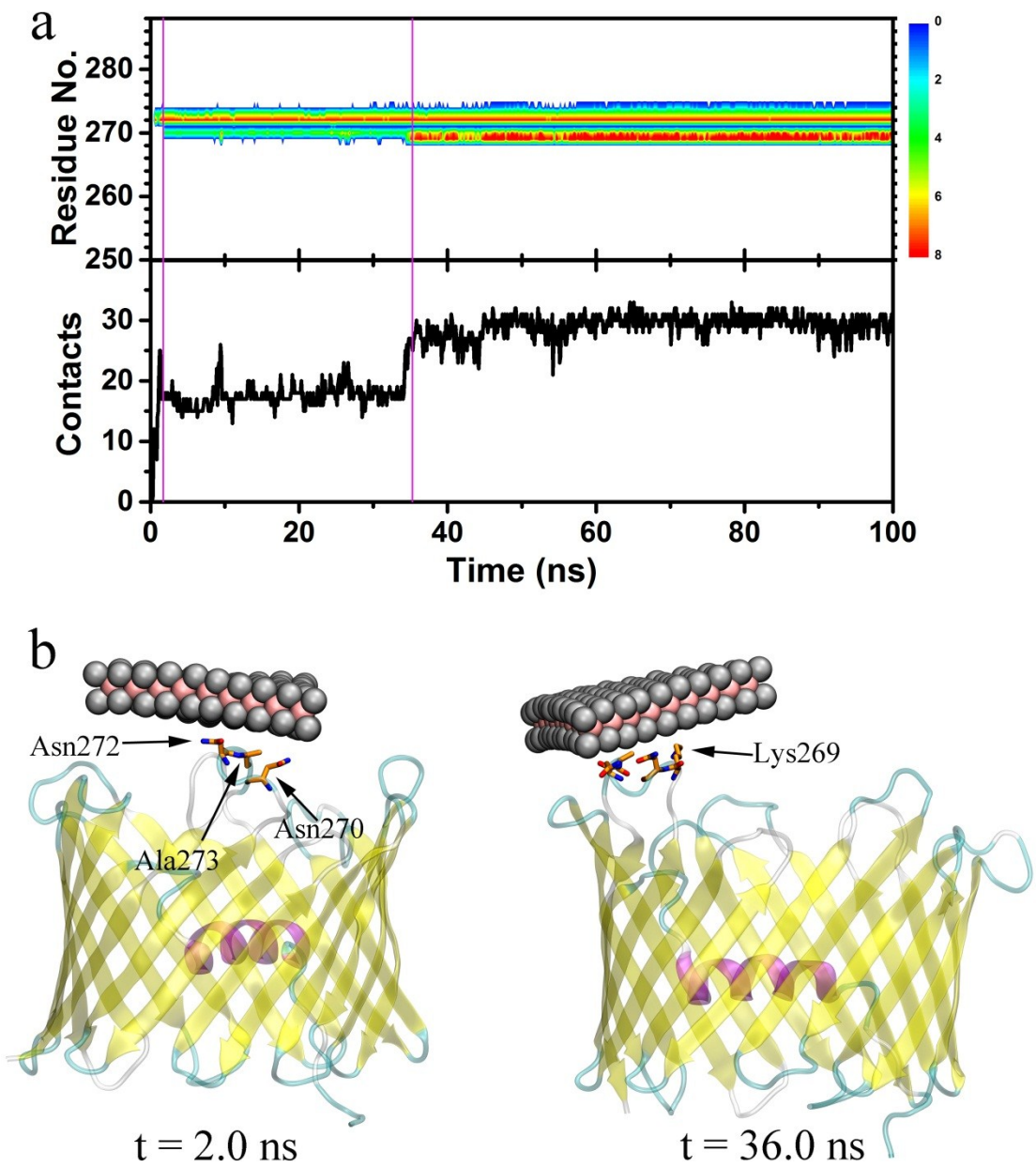

Figure S4. (a) Time evolutions of residue-dependent atom contact number (top) and total atom contact number (bottom) of run 1 trajectory from sys-2. The magenta lines represent key time points of protein-nanoflake interaction. (b) The binding conformations of MoS_2 nanoflake to hVDAC1 at two key time points corresponding to (a). The key residues that contacting MoS_2 nanoflake are shown with sticks and are also labeled. Other settings are as in Fig. 2.

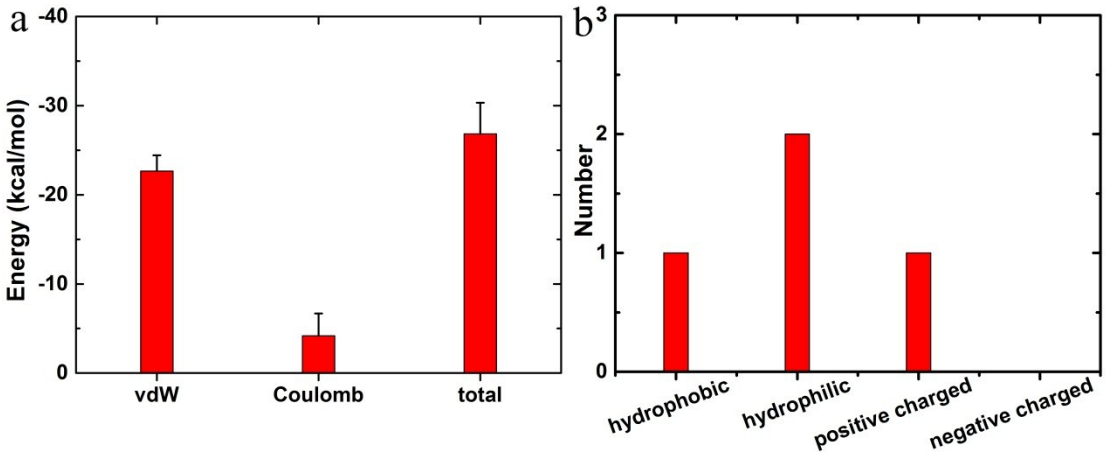

Figure S5. (a) Interaction energies (including vdW and Coulomb energies) between hVDAC1 and MoS_2 nanoflake computing from last 25 ns of run 1 in sys-2 simulation. (b) The contact residue number (including hydrophobic, hydrophilic, positive charged and negative charged residue types) of run 1 in sys-2 simulation.