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-\( \alpha \) 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-\( \alpha \) 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.