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**Supporting Material**

# Interactions Between a Voltage Sensor and a Toxin via Multi-Scale Simulations

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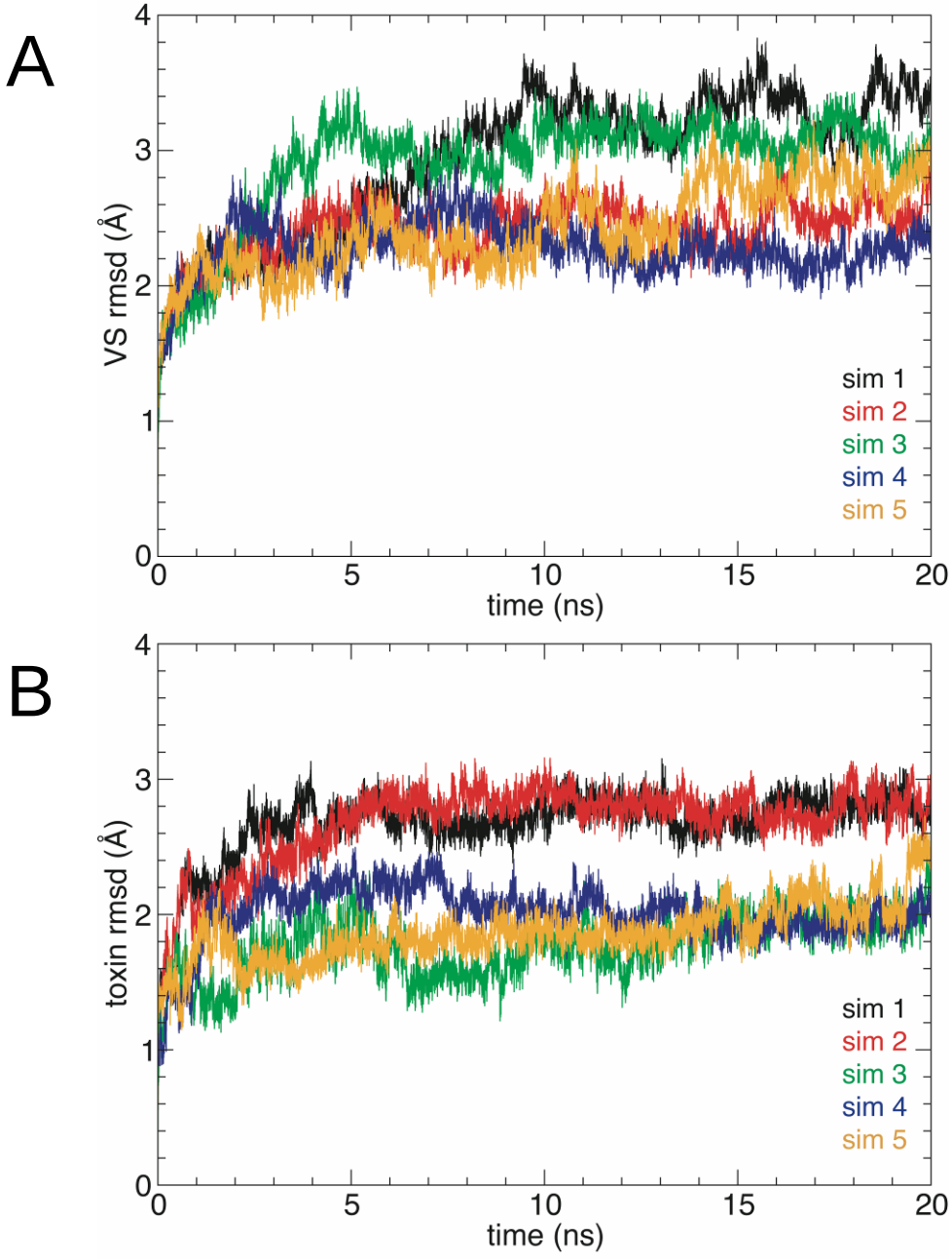
*Supplementary Information of 'Interactions Between a Voltage Sensor and a Toxin via Multi-Scale Simulations' by Chze Ling Wee, David Gavaghan, and Mark S. P. Sansom*

*Atomistic Simulations of the Toxin/Sensor Complex*



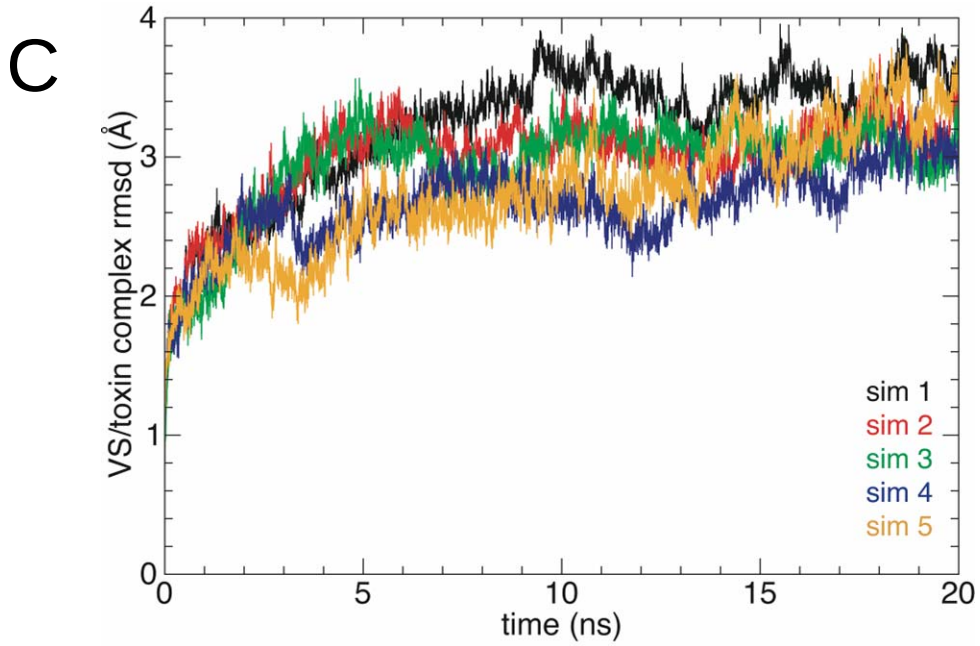



*Fig. S1:* Root-mean-squared-deviation (RMSD) of the Cαatoms of (A) VS, (B) toxin, and (C) VS/toxin complex in the AT simulations (after a Cα least-squared-fit to the initial (i.e. 0 ns) structure).

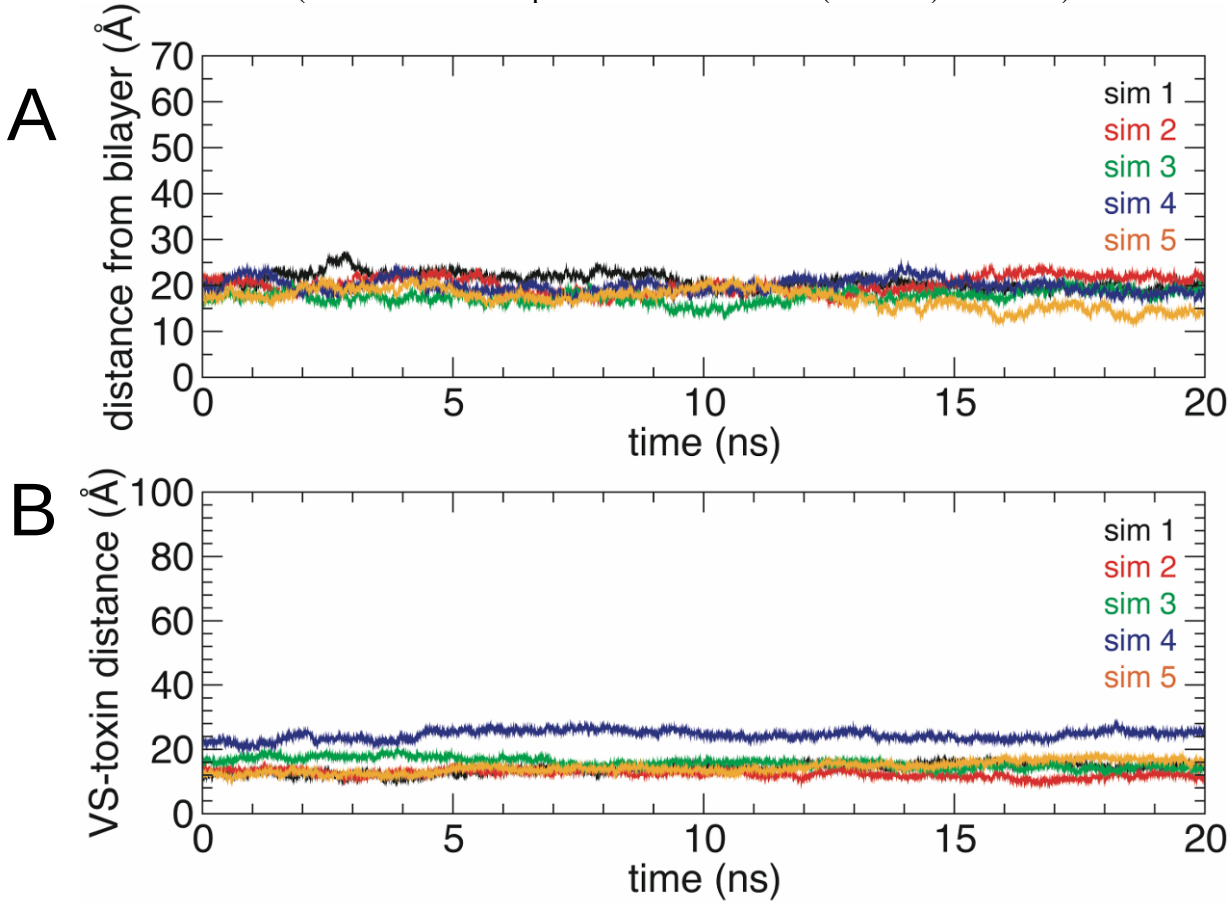


*Fig. S2:* (A) Distance between the COMs of VSTx1 and the POPC bilayer projected along the bilayer normal in the AT simulations. (B) Distance between the COMs of VSTx1 and VS projected along the plane of the membrane surface in the AT simulations.

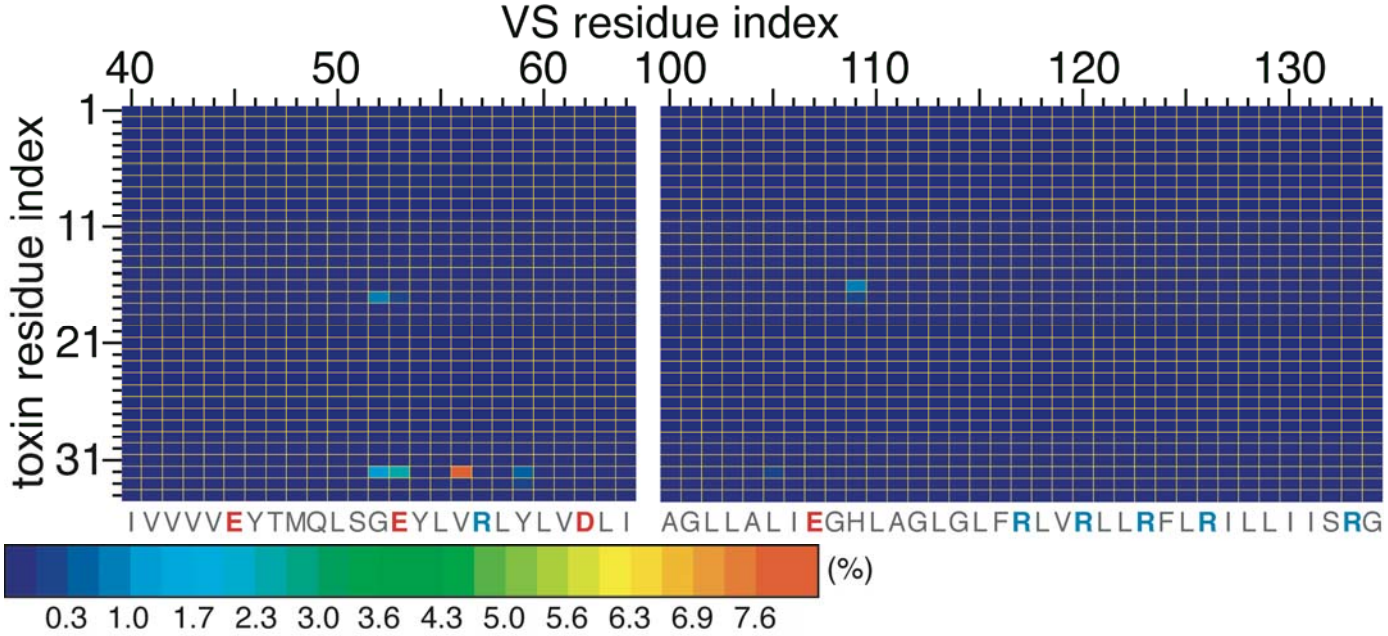
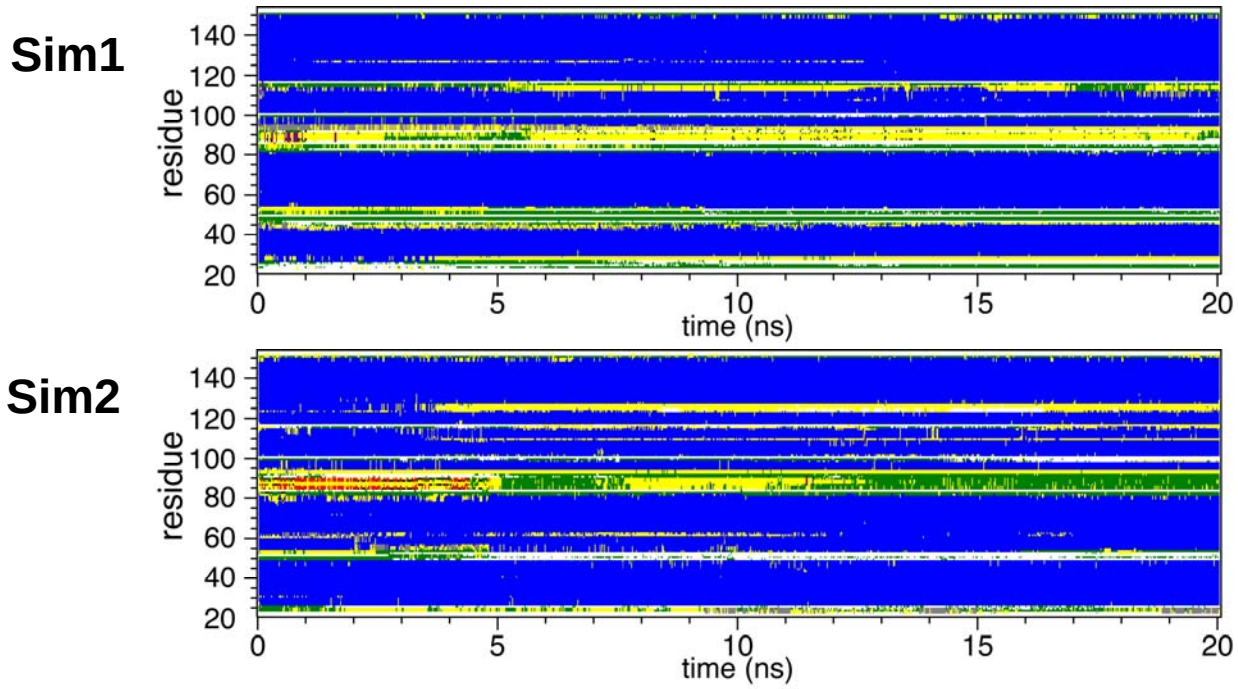



*Fig. S3:* Analyses of the VS/toxin interface in AT Simulation 4. Frequency of contacts (expressed as a percentage) between VS and toxin residues over 10 to 20 ns. A distance cut-off of 3.5 Å was used to define a contact. Basic and acidic residues are labelled in blue and red respectively.



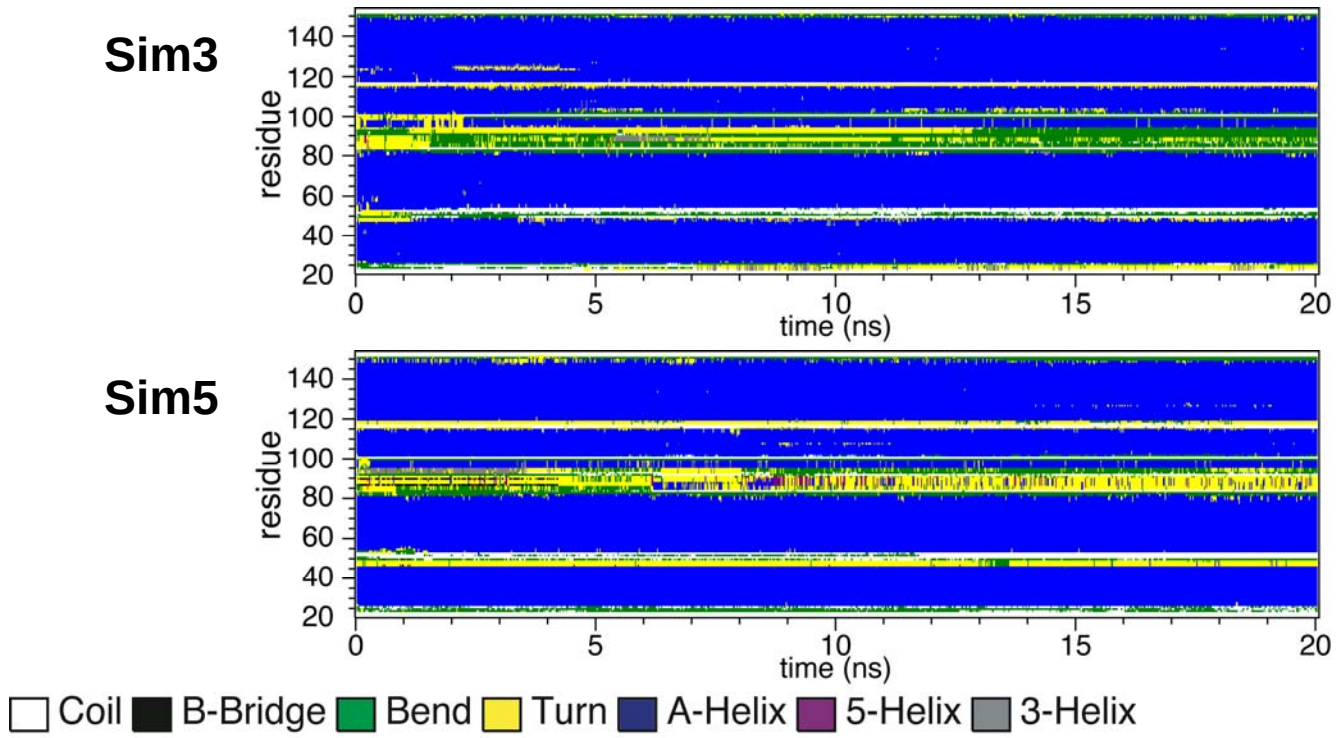



*Fig S4:* Time evolution of the secondary structure of the VS in AT Simulations 1, 2, 3 and 5.