Structure and dynamics of the fibronectin-III domains of *Aplysia californica* cell adhesion molecules

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Electronic Supplementary Information

ANIMATIONS

Movie S1. Animation (AVI movie) showing a representative atomistic MD trajectory (250 ns, simulated using explicit water molecules) of apCAM's Fn1-Fn2 tandem. The frames of this trajectory have been aligned to C_α atoms of the Fn1 domain in order to visualize its equilibrium structural fluctuations.
This animation is available online at: http://dx.doi.org/10.1039/C4CP05307A

Movie S2. Animation (AVI movie) showing a representative atomistic MD trajectory (250 ns, simulated using explicit water molecules) of apCAM's Fn1-Fn2 tandem. The frames of this trajectory have been aligned to C_α atoms of the Fn2 domain in order to visualize its equilibrium structural fluctuations.
This animation is available online at: http://dx.doi.org/10.1039/C4CP05307A

FIGURES

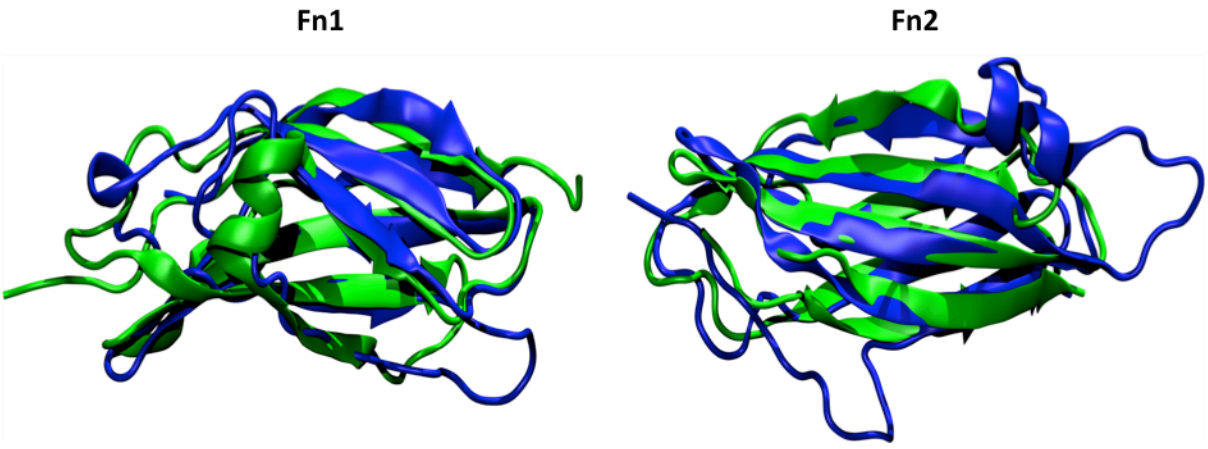

Figure S1, Related to Figure 2. Comparison of Fn-III domain structures for the initial homology-based apCAM model and for the NCAM crystal structure template. The homology-based apCAM Fn-III structures are shown in blue, and the NCAM crystal structure is shown in green. The RMSD separating apCAM and NCAM is 2.55 Å for Fn1 and 2.10 Å for Fn2.

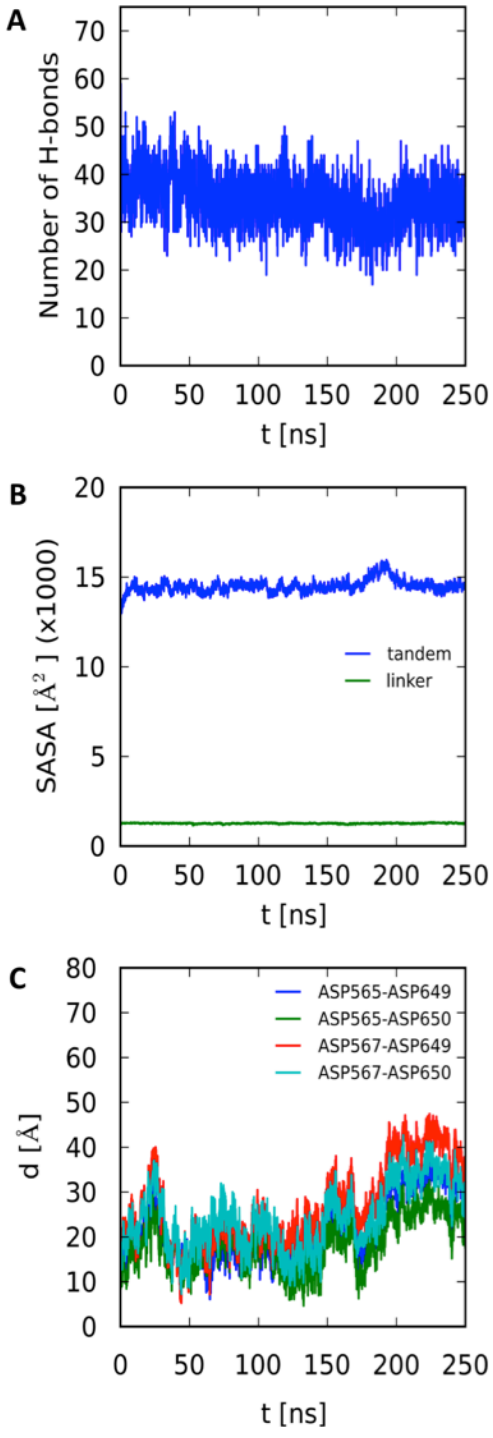

Figure S2, Related to Figure 4. Structural stability of the entire Fn1-Fn2 tandem along the 250 ns atomistic MD simulation with explicit water molecules. (A) The number of hydrogen bonds, (B) the solvent accessible solvent area, and (C) distances between negatively charged Asp residues that play a role in restricting the relative Fn1-Fn2 orientations and inter-domain contacts.

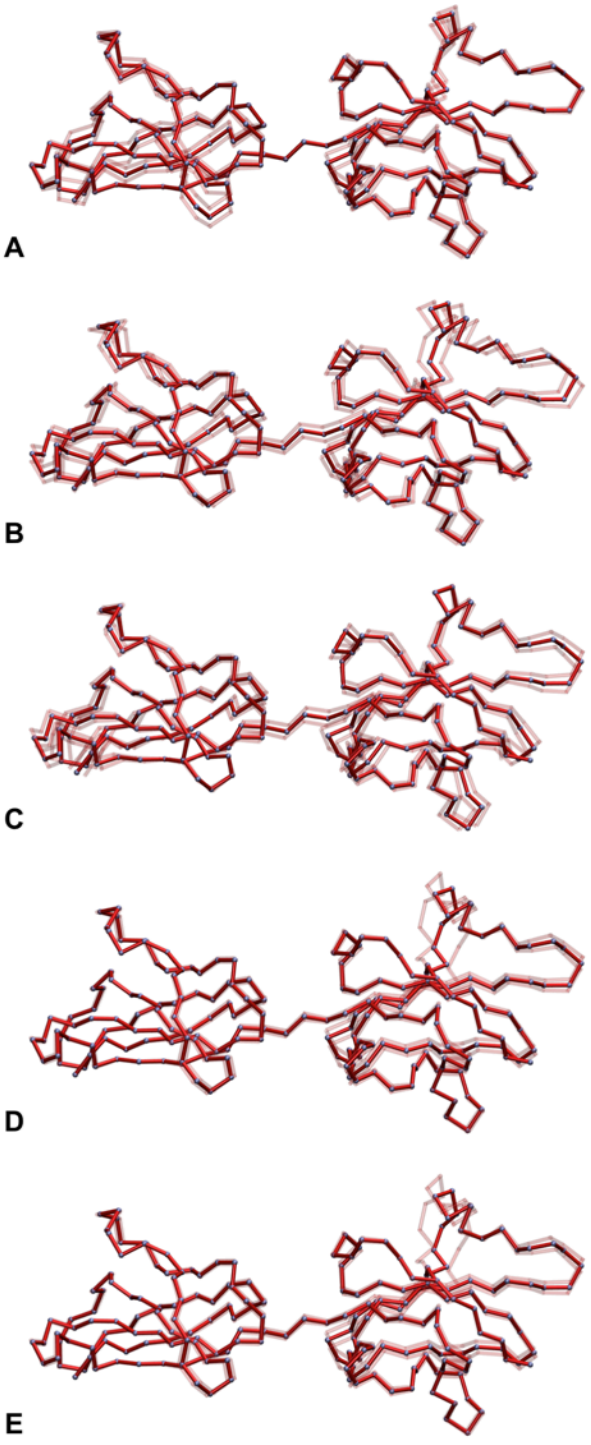

Figure S3. Illustration of the Elastic Network Model (ENM) modes 6 to 10 (panels A to E, see also Fig. 8). Maximum (+) and (-) amplitudes for the first five non-zero modes as calculated for the representative structure of the apCAM Fn1-Fn2 tandem.

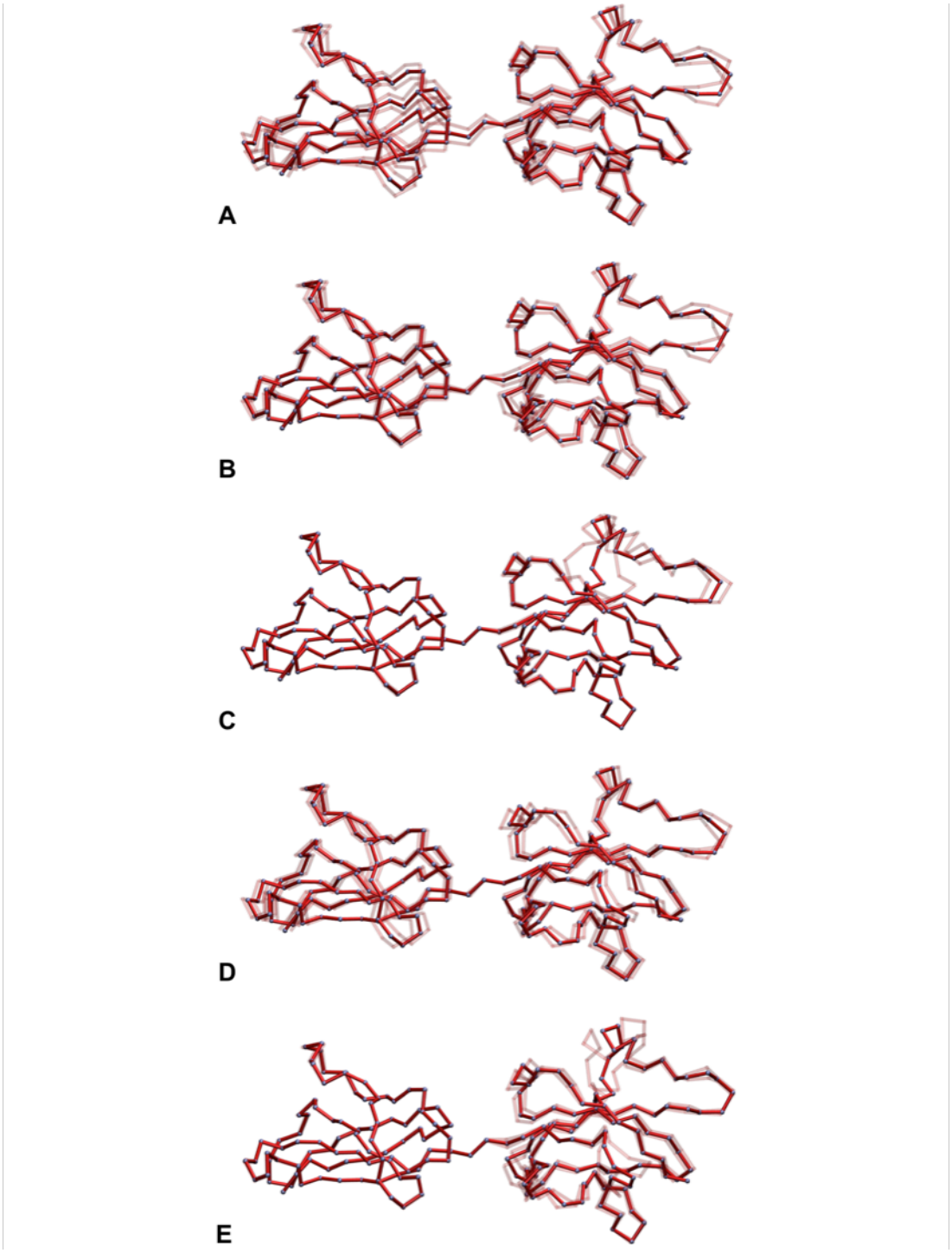

Figure S4. Illustration of the ENM modes 11 to 15 (panels A to E, see also Fig. 8). Maximum (+) and (-) amplitudes for the second group of five non-zero modes as calculated for the representative structure of the apCAM Fn1-Fn2 tandem.