

Figure S1. Representative Scheme of sliding binding-box docking. NA structure (N1) is shown in cartoon. Panel (A) displays the binding pocket of NA and the x, y, and z axis in the sliding binding-box docking process. Panel (B) provides the scheme of the grid box setup process. Box with red lines indicate overlapped parts in z-direction, box with blue lines represent the top box numbered with 13. Panel (C) and (D) represent the bottom (number 1) and top (number 13) grid boxes in the real sliding-binding box procedure, respectively.

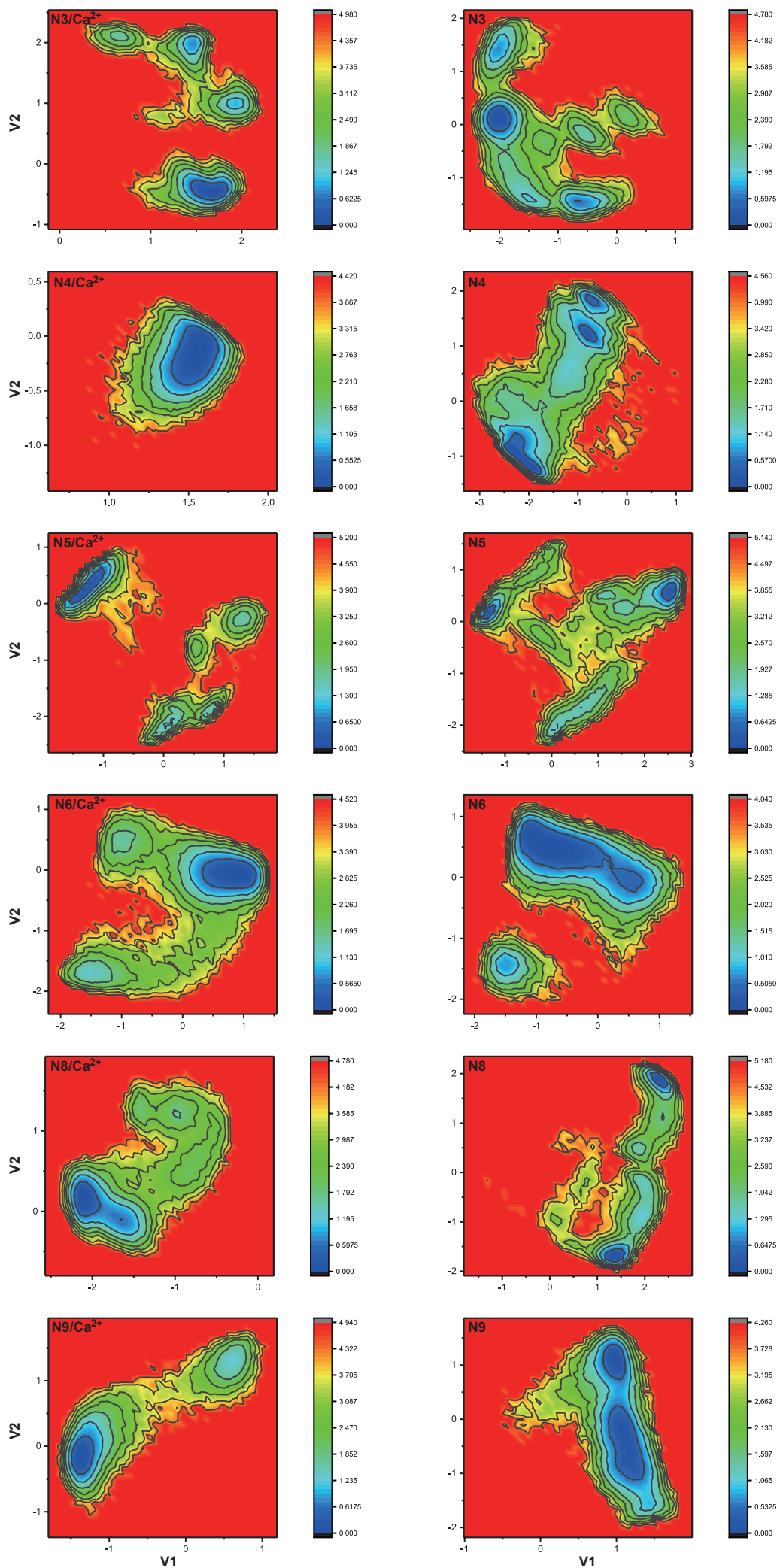


Figure S2. Free energy landscapes of the 340-loop in N3, N4, N5, N6, N8, and N9 calcium-bound and calcium-free systems were obtained using dihedral principle component analysis (dPCA).