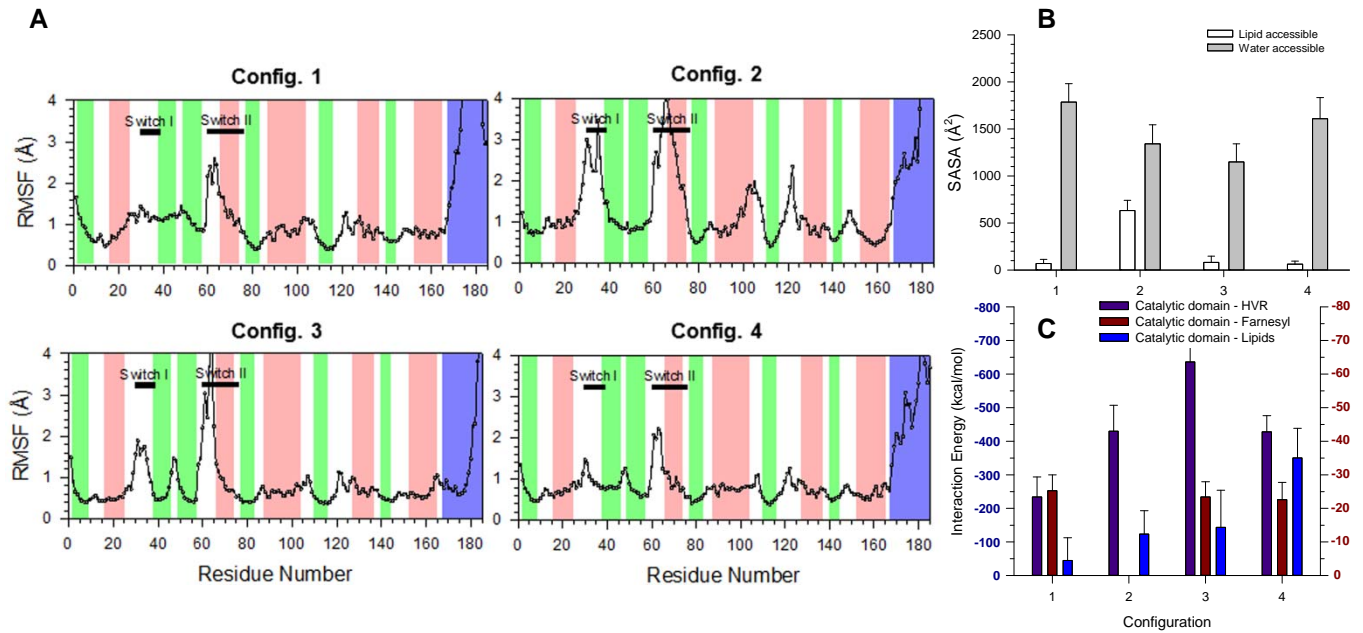
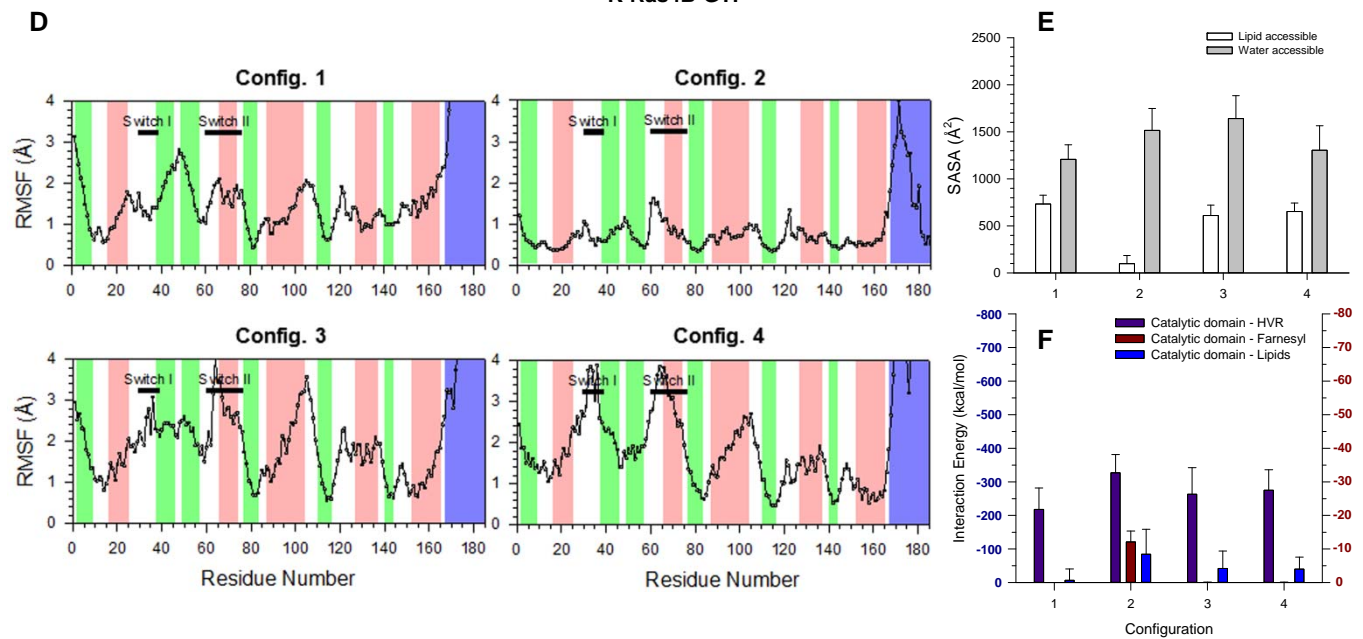


K-Ras4B-GDP



K-Ras4B-GTP



Supplemental Figure 4. (A) The average root-mean-squared fluctuations (RMSF) from the starting point for C α atoms, (B) lipid (white bars) and water (gray bars) accessible surface areas for the HVR, and (C) averaged total interaction energies of the catalytic domain with the HVR, the farnesyl, and lipids for the GDP-bound K-Ras4B at the lipid bilayer. (D) The average RMSF from the starting point for C α atoms, (E) lipid (white bars) and water (gray bars) accessible surface areas for the HVR, and (F) averaged total interaction energies of the catalytic domain with the HVR, the farnesyl, and lipids for the GTP-bound K-Ras4B at the lipid bilayer. In the RMSF plots, the green and pink backgrounds denote the β -sheet and α -helix secondary structures of K-Ras4B, respectively, and the blue background represents the HVR. In the bar graphs of interaction energy, the interactions of the catalytic domain with HVR and lipids use the scale of interaction energy on the left (blue). The catalytic domain-farnesyl interaction uses the scale of interaction energy on the right (red).