



Supplemental Figure 2. (A) Averaged total interaction energies of the catalytic domain with the HVR and the farnesyl, and (B) two-dimensional dynamical cross-correlation map (DCCM) of the residues motions across the protein domains for the GDP-bound K-Ras4B in the aqueous environment. (C) Averaged total interaction energies of the catalytic domain with the HVR and the farnesyl, and (D) two-dimensional DCCM of the residues motions across the protein domains for the GTP-bound K-Ras4B in the aqueous environment. The catalytic domain-HVR interaction uses the scale of interaction energy on the left (blue). The catalytic domain-farnesyl interaction uses the scale of interaction energy on the right (red). (E) Two-dimensional DCCM of the residues motions across the protein domains (left panel) and three-dimensional DCCM of the helix-to-helix motions including α_3 - α_4 , α_3 - α_5 , and α_4 - α_5 helices in the allosteric lobe (right panels) for the GDP-bound catalytic domain only K-Ras4B₁₋₁₆₆. (F) The same for the GTP-bound catalytic domain only K-Ras4B₁₋₁₆₆. For the two-dimensional DCCM, positively correlated residues with correlation coefficient, $C(i,j) = 1$ (red), anti-correlated (negatively correlated) residues with correlation coefficient, $C(i,j) = -1$ (dark purple), and un-correlated residues with correlation coefficient, $C(i,j) = 0$ (dark green) are shown. For the three-dimensional DCCM, Positively correlated residues with correlation coefficient, $C(i,j) = 0.6$ (red), anti-correlated (negatively correlated) residues with correlation coefficient, $C(i,j) = -0.6$ (dark purple), and un-correlated residues with correlation coefficient, $C(i,j) = 0$ (green) are shown.