SUPPORTING INFORMATION

Computational Design of Myristoylated Cell Penetrating Peptides Targeting Oncogenic K-Ras.G12D at the Effector Binding Membrane Interface

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Figure S1: Snapshots for simulation of K-Ras at a POPC membrane doped with R9 peptides (no myr anchor).

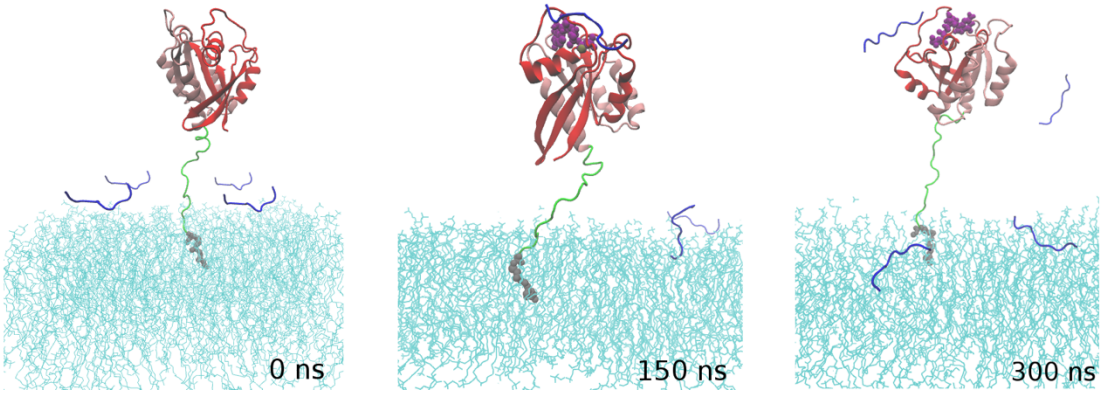

Figure S2: Simulation of K-Ras at a POPC membrane doped with far_R9. (left) Time evolution of distance between the center of mass of the K-Ras4B core domain and the membrane center. (middle) Frequency of K-Ras4B: myr_R9 contacts (protein residue atoms within 4 Å of myr_R9 atoms) over the last 300 ns simulations. (right) Contour maps of D_z and θ.

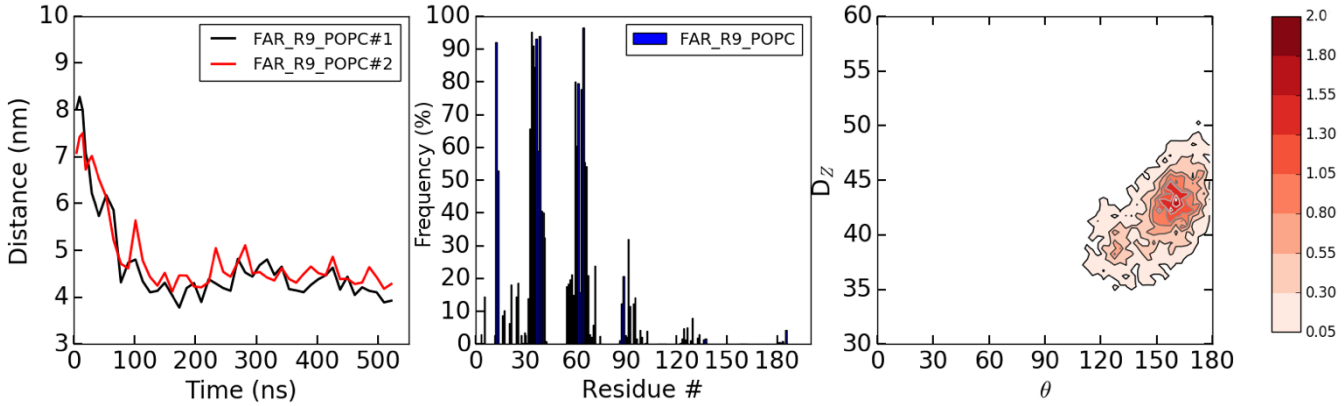

Figure S3: Simulation of K-Ras at a POPC membrane doped with myr_CRD peptide (143-RKTFLKLA-150). (left) Time evolution of distance between the center of mass of the K-Ras4B core domain and the membrane center. (middle) Frequency of K-Ras4B: myr_CRD peptide contacts over the last 300 ns simulations. (right) Contour maps of D_z and θ.

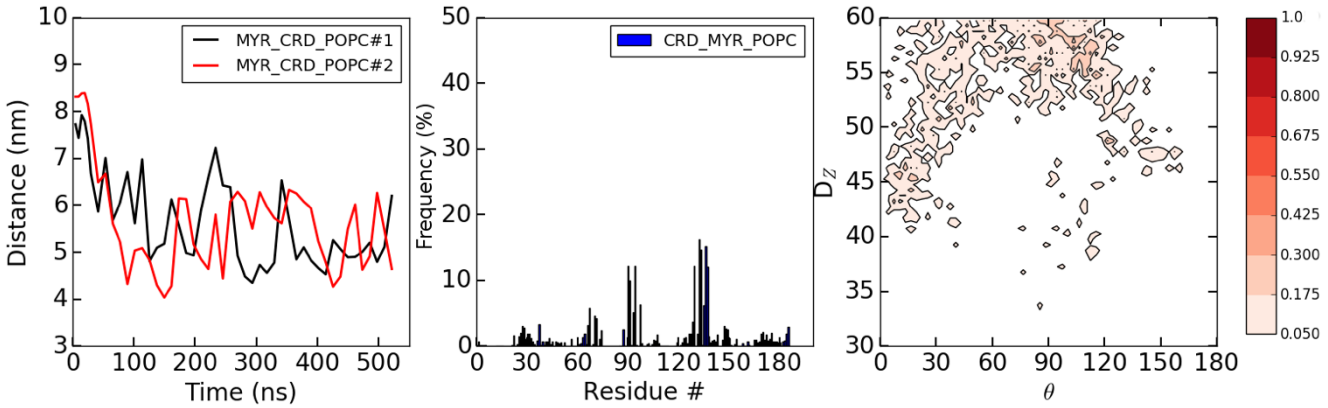

Figure S4: Simulation of K-Ras at a POPC membrane doped with myr_Cyclorasin. (left) Time evolution of distance between the center of mass of the K-Ras4B core domain and the membrane center. (middle) Frequency of K-Ras4B: myr_Cyclorasin contacts over the last 300 ns simulations. (right) Contour maps of D_z and θ.