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Supplementary Information

Structure and Dynamics of Mono- *vs.* Doubly-Lipidated Rab5 in Membranes

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Table S1. Dimension of simulations boxes and simulated systems

Membrane system	Component	Number of lipids (ratio)	Lateral (x,y) dimensions / nm
Pure POPC	POPC	2 x 273 (100%)	15.7 x 14.9
Ternary	POPC	2 x 166 (40%)	14.8 x 14.4
	CHOL	2 x 166 (40%)	
	PSM	2 x 83 (20%)	
Six-component	POPC	2 x 90 (17.8%)	16.9 x 16.6
	CHOL	2 x 150 (29.7%)	
	PSM	2 x 50 (9.9%)	
	POPE	2 x 135 (26.7%)	
	POPS	2 x 55 (10.9%)	
	PI(3)P	2 x 25 (5.0%)	

Simulation z-direction box dimensions
12.8 nm HVR,
16.4 nm GG-Rab5(GDP), 16.4 nm GG-Rab5(GTP),
16.9 nm G-Rab5(GDP), 17.0 nm G-Rab5(GTP).

The exact number of water molecules and ions were in the charged six-component membrane
$HVR^{206-215}$ 65586 water/186 chloride/440 sodium
GG-Rab5(GDP) 94096 water/266 chloride/524 sodium
GG-Rab5(GTP) 94426 water/267 chloride/526 sodium
G-Rab5(GDP) 94805 water/268 chloride/526 sodium
G-Rab5(GTP) 97284 water/275 chloride/534 sodium

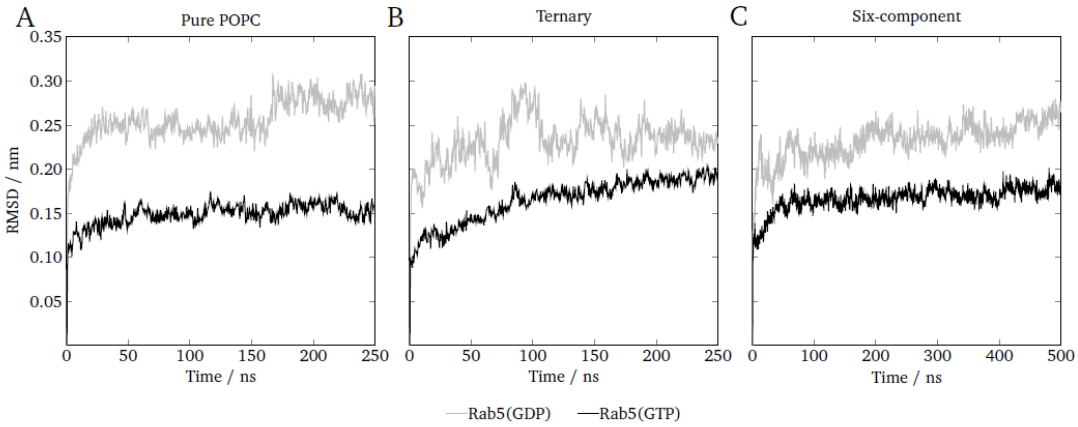

Figure S1. Top: RMSD of the double-GG Rab5 Cα atoms from the initial configuration over the complete MD simulation in A) pure POPC, B) the ternary mixture, and C) in the six-component membrane. Data are averaged over three independent simulations for Rab5(GDP) or Rab5(GTP) in each membrane system.

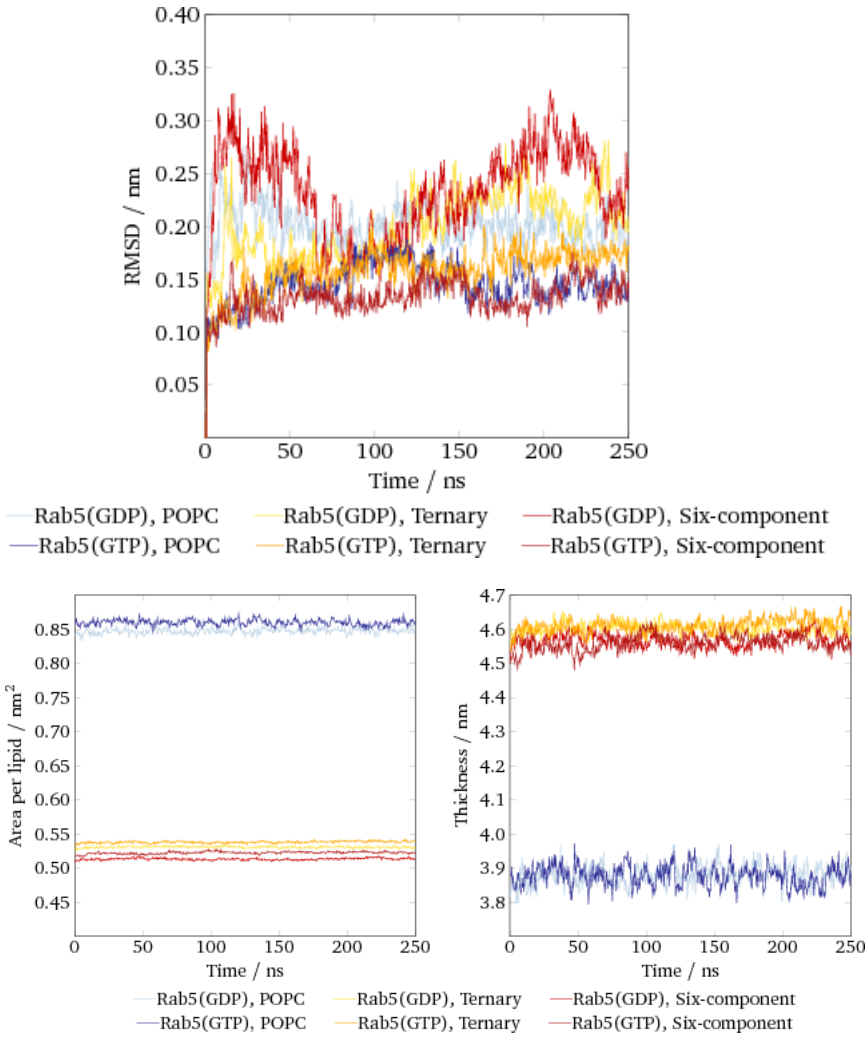

Figure S2. RMSD (top), area per lipid molecule and bilayer thickness (bottom) for mono-geranylgeranylated Rab5 in GTP-and GDP-bound states in membranes of different composition (POPC, ternary and six-component membranes; see text for details).

33

34