Supplemental Data

Recognition of the Activated States of Gα13

by the rgRGS Domain of PDZRhoGEF

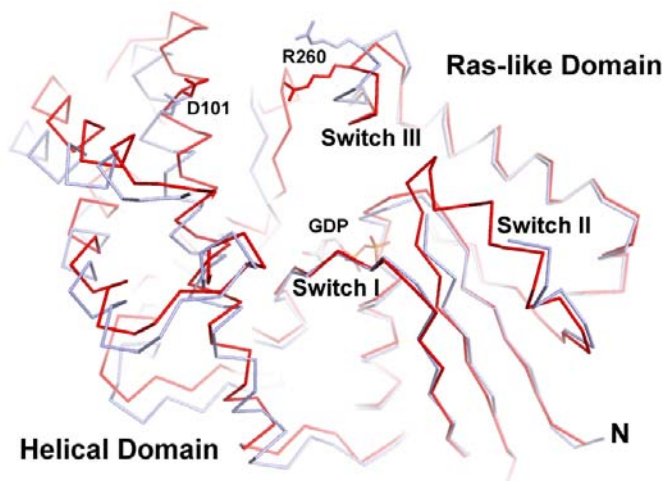**Zhe Chen, William D. Singer, Shahab M. Danesh, Paul C. Sternweis, and Stephen R. Sprang**

Figure S1. Cα Traces of Gα13•GDP Alone (blue) and in a Complex with PRG-rgRGS Domain, Superimposed Using their Ras-like Domains

Interaction with PRG-rgRGS may constrain Gα13•GDP in an active conformation, by pulling the helical and Ras domains together. In the structure of uncomplexed Gα13•GDP (Kreutz et al., 2006), these are rotated 8° further apart. The distance between Asp-101 and Arg-260, which is unique to the G12 class Gα subunits and drawn here as ball-and-stick models, increases to 21 Å, compared with 16 Å when complexed with PRG-rgRGS.
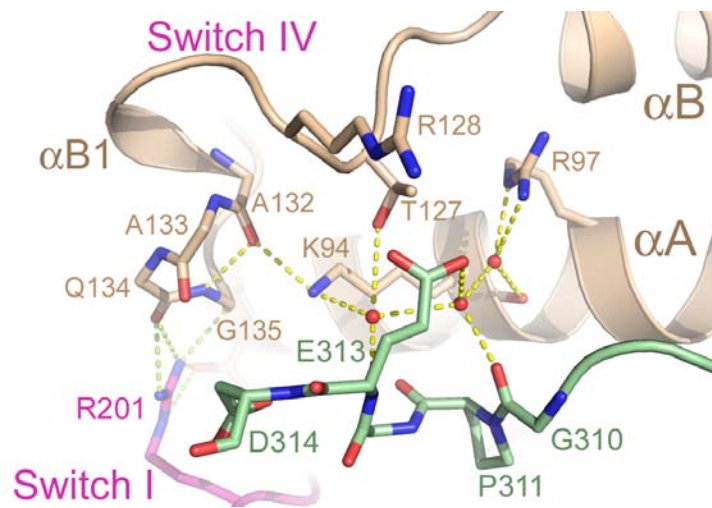
Figure S2. Ribbon Diagram Depicting the Interaction Between the N-Terminal Subdomain of PRG-rgRGS and Switch IV of Gα13

Residues involved in this interface are represented as ball and stick models and colored as in Figure 1C. Hydrogen bonds are drawn as dotted lines and colored yellow. Switch IV (the αB-αC loop) in Gα subunits is not well conserved. For Gα13, it possesses two additional short helices (αB1 and αB2) and is referred to as the "helical insert". This segment interacts with the N-terminus of PRG-rgRGS and Arg-201 from switch I of Gα13 (Figure 4D) in the GTPγS complex structure. Side chains of Thr-127 and Arg-128 from switch IV form van der Waals contacts with the side chain of r-Glu-313 from PRG-rgRGS. The backbone of Ala-133 from switch IV also forms van der Waals contacts with the side chain of r-Asp-314 from PRG-rgRGS. The hydroxyl group of the Thr-127 side chain forms a hydrogen bond with a water molecule, which is hydrogen bonded to the backbone amide group of r-Glu-313 in PRG-rgRGS.
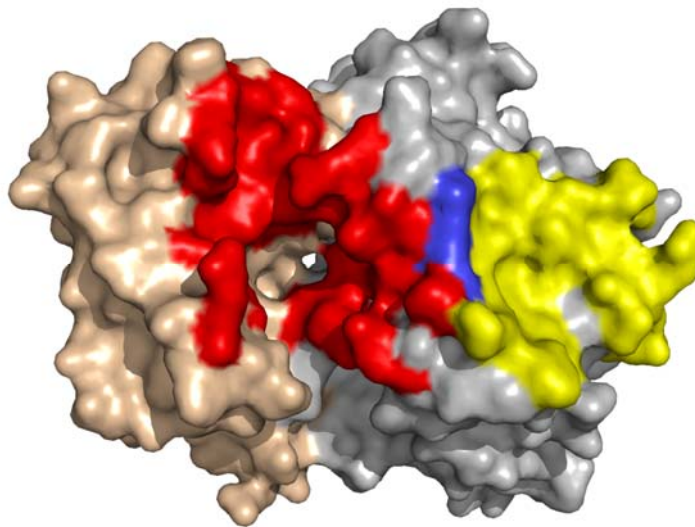

Figure S3. The N-Terminal and the RGS-box Subdomains of PRG-rgRGS Bind at Distinct, Largely Nonoverlapping Surfaces on Gα13

The solvent accessible surface of Gα13 is colored as in Figure 1C. Residues on Gα13 contacting the N-terminal subdomain of PRG-rgRGS are colored red. Residues on Gα13 contacting the RGS-box are colored yellow. Arg-227 from switch II of Gα13, which forms contacts with both subdomains of PRG-rgRGS, is colored blue.