

Title: Structural Basis of Analog Specificity in PKG I and II.

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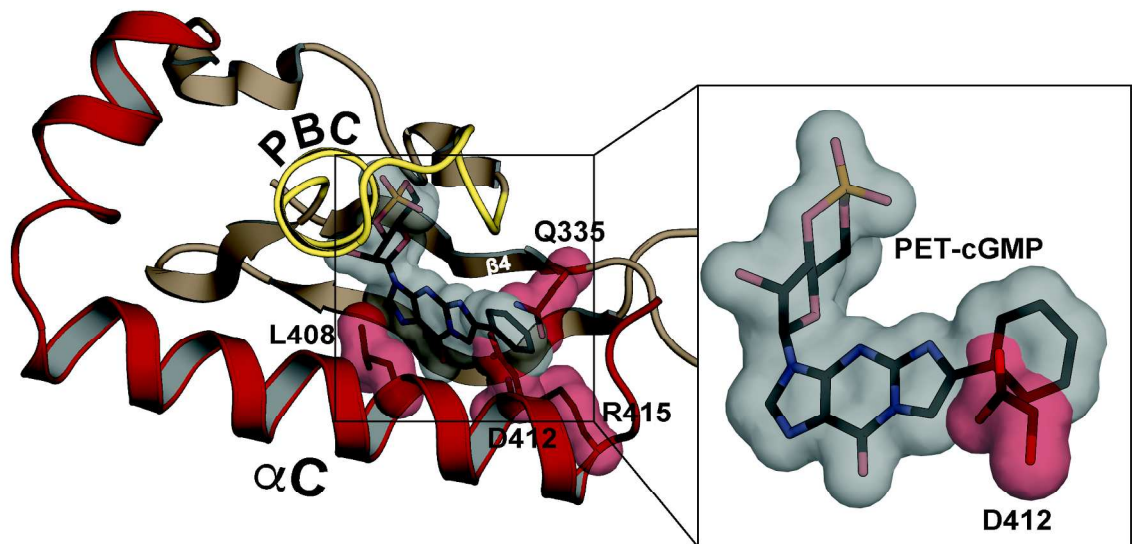


Figure S1. Structural Model of PET-cGMP bound to the PKG II CNB-B domain. PET-cGMP was modeled into the PKG II CNB-B domain by superimposing the structure of PKG I β CNB-B:PET-cGMP complex with the PKG II CNB-B:cGMP complex (PDB code: 5BV6). Only $\beta 4$ through the αC helix is shown. Key guanine binding residues and PET-cGMP are labeled and shown as *sticks*, with *transparent surfaces*. Zoomed-in view shows the steric clash between D412 and PET-cGMP.

Models of CNB-A bound with 8-pCPT-cGMP

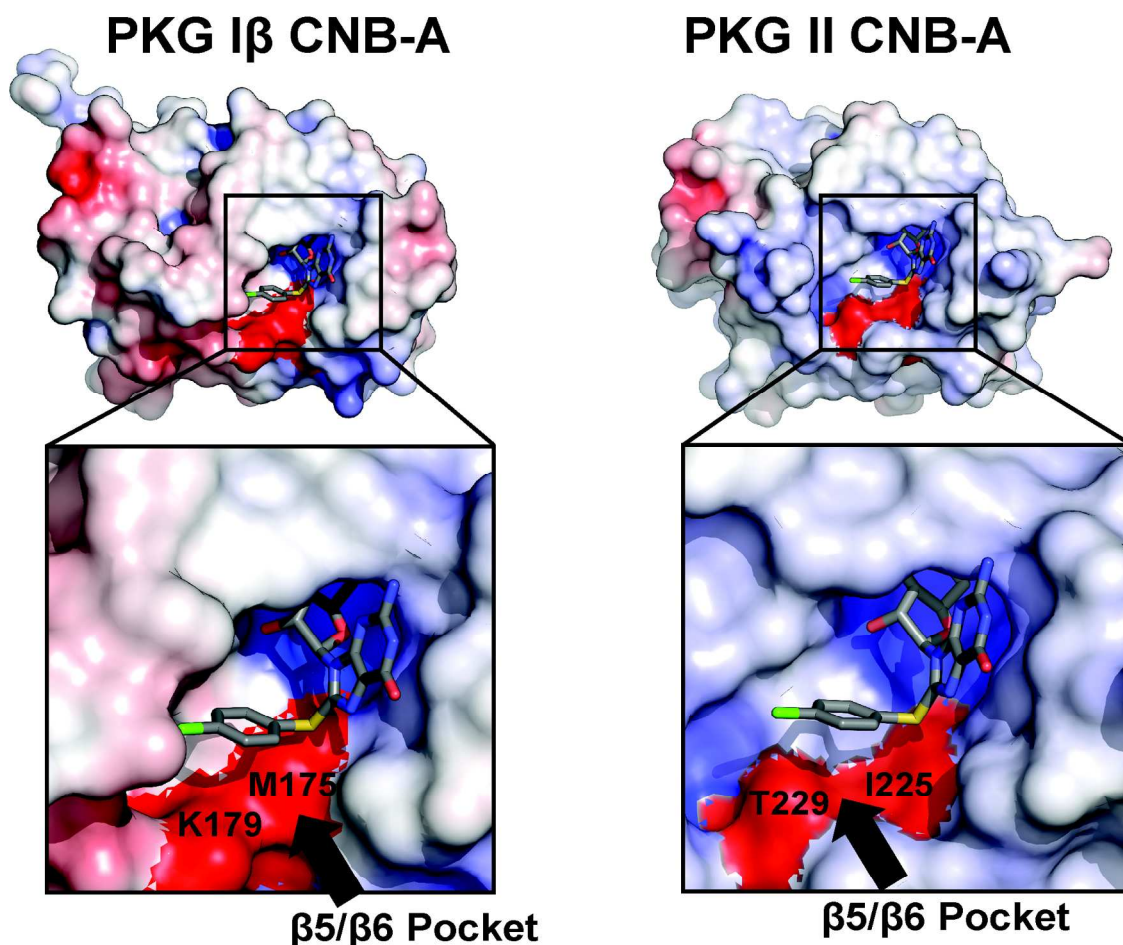


Figure S2. Structural models of PKG I β and II CNB-A domains bound to 8-pCPT-cGMP.

8-pCPT-cGMP was modeled into the PKG I β and PKG II CNB-A domains by superimposing the structure of PKG I β CNB-B:8-pCPT-cGMP complex onto respective CNB-A domains (PDB codes, 3OCP and 5C8W, respectively). The surface is colored according to the contact electrostatic potential calculated in APBS(1) except for the β 5/ β 6 residues that provide docking surface for the 8-pCPT moiety. Positively charged areas are shown in blue and negatively charged areas in red. The surfaces belonging the β 5/ β 6 residues are colored in red. Zoomed in views highlight β 5/ β 6 pockets.

Reference

1. Baker, N. A., Sept, D., Joseph, S., Holst, M. J., and McCammon, J. A. (2001) Electrostatics of nanosystems: application to microtubules and the ribosome, *Proceedings of the National Academy of Sciences of the United States of America* 98, 10037-10041.

