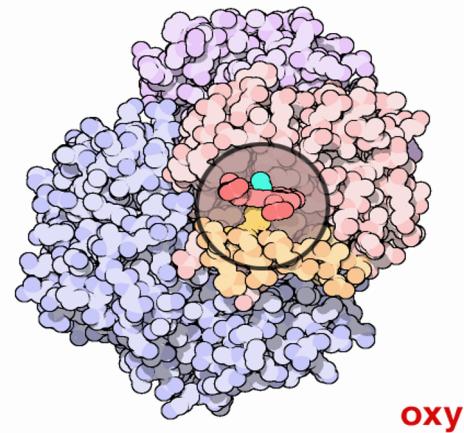
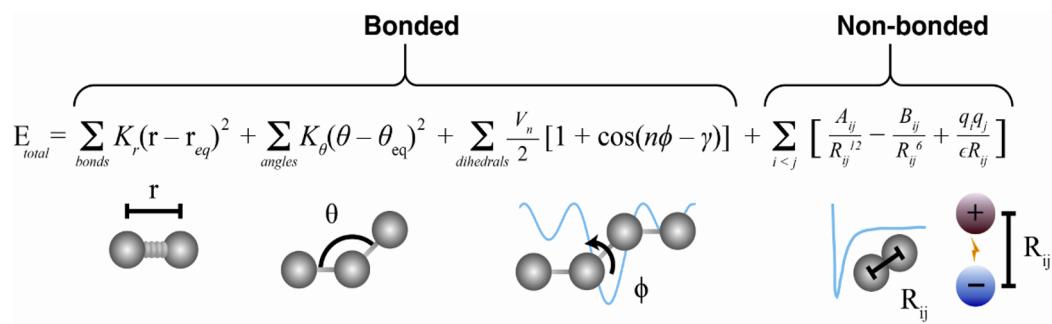
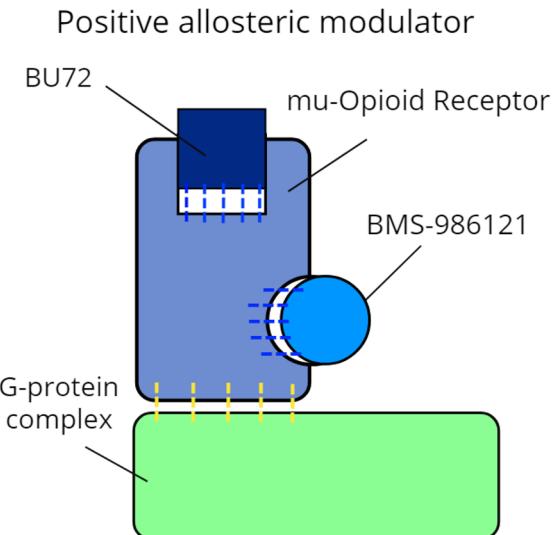
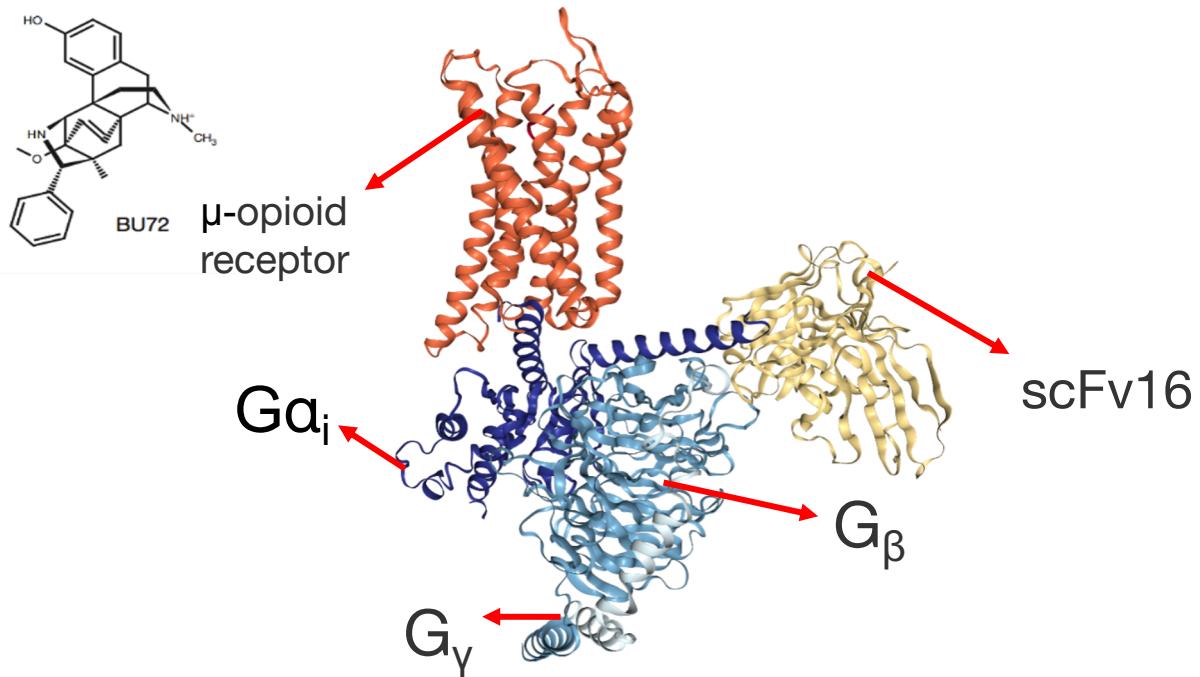


Correlating the allosteric modulation to the protein-protein interaction can provide information about cell signaling



Oxygen binding at the four heme sites in hemoglobin <http://pdb101.rcsb.org/motm/41>

Membrane protein simulations require HPCs

- $> 2.3 \times 10^5$ atoms
- Lipid bilayer bound
- Ran in NAMD 2.11
- 21 perturbed systems (ligands and mutants)
- 30 ns production
~1 month benchmark
- 4 Tb data stored

