Mechanisms of Information Transfer across Biological Membranes: G protein-Coupled Receptors

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Cell membranes

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Membrane proteins
GPCRs are excellent drug targets

GPCR activation

An “ionic lock” stabilizes inactive conformations
Molecular dynamics simulations
Spontaneous formation of the ionic lock
The cytosolic binding pocket is more stable in apo-state simulations using a crystal structure containing a G protein than a mimetic nanobody.
The ionic lock forms less frequently in apo-state simulations using a crystal structure containing a G protein than a mimetic nanobody
Future work

What is the molecular source of this differential active-state stability?
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