

Abstract Submitted
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“Lock and key mechanism” for ligand binding with adrenergic receptors and the arising mechanical effects on the cell membrane¹ LAURA LUNGI, Department of Pharmaceutical and Applied Chemistry, Università of Siena, Italy, LUCA DESERI, Center for Nonlinear Analysis, Carnegie Mellon University — Chemicals hitting the surface of cell aggregates are known to give rise to cyclic Adenosine Mono Phosphate (cAMP), a second messenger that transduces inside the cell the effects of species that cannot get through the cell membrane. Ligands bind to a specific receptor following the so called “lock and key mechanism”; (beta)-adrenergic receptors are proteins embedded in the lipid bilayer characterized by seven transmembrane helices. Thinning and thickening in cell membranes may be initiated by conformational changes of some of three of the seven domains above. The cell response is linked to the coupling of chemical, conformational and mechanical effects. Part of the cAMP remains intracellular, whereas the remaining fractions migrates outside the cell due to membrane transporters. A new Helmholtz free energy, accounting for receptor and transporter densities, receptor conformation field and membrane elasticity is investigated. It is shown how the density of active receptors is directly related to the conformation field and it enters the resulting balance equation for the membrane stress. Balance laws for fluxes of transporters and receptors, coupled with the former because of the outgoing cAMP flux caused by the transporters, as well as for the diffusive powers must be supplied.

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Luca Deseri
Carnegie Mellon University, Center for Nonlinear Analysis

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