Complete Networks of Reversible Binding Reactions

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Presentation Abstract

A binding reaction is a chemical reaction that transforms two or more reactants into a single product. Networks of reversible binding reactions describe many pathogenic and therapeutic mechanisms that are studied in pharmacology. Determining the equilibrium state is a recurrent issue in that context. Toward an effort to do so systematically, we propose the class of complete networks of reversible binding reactions and characterize their equilibrium states. Completeness consists of structural and kinetic requirements that are applicable in the motivating context. The structural requirement is that there is a notion of composition that is intrinsic to the network and defines species, and that reactions preserve composition. The kinetic requirement is that the law of mass action applies, and that certain coherence equations constrain rate constants along reaction pathways with same outcome. In a complete network, the nonnegative stoichiometric compatibility classes are convex polytopes defined by equations that express the conservation of composition. Within each class, there exists a unique equilibrium state; it is detailed-balanced and characterized by a positive polynomial system with rather interesting features, and it is globally attracting. Global attraction is obtained in part from the fact that the boundary of the class is weakly repelling, a property which is proved with the Vol'pert Strict Positivity Theorem.

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