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Title:

Polynomial Systems in Receptor Pharmacology

Abstract:

Pharmacology studies interactions between biological processes and therapeutic agents. It is usually viewed as consisting of two subdisciplines: pharmacokinetics (what the body does to the drug) and pharmacodynamics (what the drug does to the body). Receptor pharmacology is a common foundation, which, at the beginning of the research pipeline, is concerned with "pharmacostatics", the in vitro equilibrium states of key biochemical interactions involving receptors. At the core of the applicable mathematical models are certain systems of polynomial equations. Established practices are to solve these systems in closed form at all cost (or give up). Sometimes the assumptions intended to justify such simplifications are dubious. Sometimes the simple, closed-form formulas are incapable of revealing experimentally observed features. As a result, candidate molecules can be assessed overoptimistically or discarded prematurely. This presentation will discuss efforts to develop methods to solve these polynomial systems systematically with a priori assurance of convergence, and a related success case of simulating and explaining an unforeseen experimental observation.