

Author:

Gilles Gnacadja

Amgen

<http://math.GillesGnacadja.info/>

Title:

A Convergent and Efficient Algorithm for Calculating Equilibrium for Chemical Networks of Reversible Binding Reactions

Abstract:

We have a particular interest in chemical networks of reversible binding reactions that are complete, a qualifier that essentially affirms the conservation of the chemical species that are the building blocks of the network. These networks are pervasive in pharmacostatic, the subdiscipline of pharmacology concerned with the characterization of the equilibrium parameters and states of core interactions of physiologic and therapeutic interest. We have been on a quest for a method to calculate the equilibrium states of these networks that is generic, guaranteed to succeed, and fast; or what we called worry-free. We will report on the tangible progress we recently made in that direction.