Combinatorially Complex Equilibrium Model Selection

Tom Radivoyevitch March 14, 2009

1 Introduction

A conceptual overview of this package is given in the ccems help page. Please read that first, then the help for ems and mkg. An example of how this package can be used to design subsequent experiments is given in RtExpDes.pdf in doc.

This package is being developed according to its author's research in the dNTP supply enzymes ribonucleotide reductase (a hexamer), thymidine kinase (a tetramer) and on deck, deoxycytidine kinase (a dimer). Simple enzyme-substrate-inhibitor monomer enzyme models are not in this set. Thus, there are no such examples herein, and the software should not be expected to work on any. The software is expected to work in situations where there is one ligand binding the protein, possibly at two different binding sites (of variable binding status) per monomer, and with no limit on the j-mer size j. Developments to broader conditions will develop in the future, but only one step at a time, as the author's specific research demands it.