

RULE BASED MODELLING OF BIOCHEMICAL NETWORKS

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New technologies and improvements in established techniques in biology have lead to a massive increase in the amount of knowledge on molecular reactions, and in turn to a need for new techniques for modelling biological networks. A major challenge in biochemical modelling is created by the number of functionally important sites in macromolecules that can be modified. Any attempt to describe the resulting network at the level of individual reactions faces a combinatorial explosion of potential reaction possibilities. In many cases there are more potential reactions than there are molecules in the cell. Rule based modelling addresses this problem by describing partial complexes instead of biochemical entities which helps to control the combinatorial explosion problem from which traditional modelling methods suffer. Kappa is a rule based modelling language designed specifically for use in the biological domain, which is capable of modelling reaction binding sites and post-translational modifications. Such modelling can aid our understanding of how existing system behaviour results from the interactions of its molecular constituents. The resulting models are easy to modify and can be used to explore how phenotypes map to genotypes, for example by simulating the effects of a reduction in the concentration of a specific protein. Such work can help us in understanding adaptive landscapes, the distribution of mutational effects and epistasis.