Extended P systems for the analysis of (trans)membrane proteins populations*

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Membrane proteins have various different structures, functioning and tasks, they help in regulating the selective permeability of the membrane, the cell signaling and membrane trafficking. Membrane proteins can be classified as peripheral proteins, which are anchored to the internal or external layer of the membrane, or as integral or transmembrane proteins, which span the bilayer and face both sides of the membrane.

Several important cellular processes, such as the muscle contraction, the transmission of electric impulses in neurons, the response to environmental nutrients, etc., are regulated by the different ion concentrations inside and outside the cell, or by the activation and amplification of specific molecules (called the second messengers) inside the cell. Both phenomena are mediated by transmembrane proteins which, in the case of transporters (involved in the active or passive transport of substances), allow the selective passage of ions (or other molecules) inwards or outwards, while in the case of membrane receptors, transduce an external signal towards a downhill chain of reactions inside the cell.

The activity of different types of transmembrane proteins was previously described with P systems, starting from the known biological notions and the established mechanistic model about the functioning of single membrane proteins. In this work, we propose to widen the *single* membrane protein modelling to a global description of membrane proteins populations, in order to take care of the synergic work of *many* membrane proteins and the related effects for the cell's life.

To this aim, we present an extension of the classical notion of membrane in P systems, which consists in the use of a 3-dimensional parametric membrane surface. This new approach enables to appropriately consider the spatial distribution of protein populations over the membrane surface, and to easily describe the population by means of a finite set of circular words. Then, operations over circular words which simulate various movements of proteins upon the membrane

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surface, like insertion and deletion, permutation or interchange among words, allow to have both a dynamical and a global view of the whole membrane protein population. As a particular case, we focus our attention on transporters populations, by formalizing some biological properties characterizing the various types of transport, such as the selectivity, the direction of crossing and the flux rates.

This extended P system approach leads to several possible applications, ranging from biological-oriented to computing-oriented investigations. In the first case, one might consider the analysis of global cellular ion fluxes, the representation of the fluid mosaic model of membranes (and other recent paradigms for protein movements over a membrane), the effect of membrane proteins over the membrane curvature. In the second case, the aforementioned circular words may represent an alternative approach for the expression of symbolic membrane proteins, and thus for the analysis of the computational power and the properties of the corresponding formal model, as in the recently introduced framework of (mem)brane calculus.