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An in silico Approach for Exploring the Intercellular Communication in Cancer Cells

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Abstract : Intercellular communication is a necessary condition for cellular functions and it allows a group of cells to survive as a population. Throughout this interaction, the cells work in a coordinated and collaborative way which facilitates their survival. In the case of cancerous cells, these take advantage of intercellular communication to preserve their malignancy, since through these physical unions they can send signs of malignancy. The Wnt/β-catenin signaling pathway plays an important role in the formation of intercellular communications, being also involved in a large number of cellular processes such as proliferation, differentiation, adhesion, cell survival, and cell death. The modeling and simulation of cellular signaling systems have found valuable support in a wide range of modeling approaches, which cover a wide spectrum ranging from mathematical models; e.g., ordinary differential equations, statistical methods, and numerical methods– to computational models; e.g., process algebra for modeling behavior and variation in molecular systems. Based on these models, different simulation tools have been developed from mathematical ones to computational ones. Regarding cellular and molecular processes in cancer, its study has also found a valuable support in different simulation tools that, covering a spectrum as mentioned above, have allowed the in silico experimentation of this phenomenon at the cellular and molecular level. In this work, we simulate and explore the complex interaction patterns of intercellular communication in cancer cells using the Cellulat bioinformatics tool, a computational simulation tool developed by us and motivated by two key elements: 1) a biochemically inspired model of self-organizing coordination in tuple spaces, and 2) the Gillespie's algorithm, a stochastic simulation algorithm typically used to mimic systems of chemical/biochemical reactions in an efficient and accurate way. The main idea behind the Cellulat simulation tool is to provide an in silico experimentation environment that complements and guides in vitro experimentation in intra and intercellular signaling networks. Unlike most of the cell signaling simulation tools, such as E-Cell, BetaWB and Cell Illustrator which provides abstractions to model only intracellular behavior, Cellulat is appropriate for modeling both intracellular signaling and intercellular communication, providing the abstractions required to model –and as a result, simulate– the interaction mechanisms that involve two or more cells, that is essential in the scenario discussed in this work. During the development of this work we made evident the application of our computational simulation tool (Cellulat) for the modeling and simulation of intercellular communication between normal and cancerous cells, and in this way, propose key molecules that may prevent the arrival of malignant signals to the cells that surround the tumor cells. In this manner, we could identify the significant role that has the Wnt/β-catenin signaling pathway in cellular communication, and therefore, in the dissemination of cancer cells. We verified, using in silico experiments, how the inhibition of this signaling pathway prevents that the cells that surround a cancerous cell are transformed.

Keywords : cancer cells, in silico approach, intercellular communication, key molecules, modeling and simulation
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