Editorial

iMedPub Journals
www.imedpub.com

Chemical Informatics
ISSN 2470-6973

2017
Vol.3 No.1:3

Chemistry, Informatics and Systems Biology

Diego Liberati*

Department of Electronics, Information and Bioengineering, Polytechnic of Milan, Milan Leonardo 32, 20133 Milano, Italy

***Corresponding author:** Diego Liberati, Department of Electronics, Information and Bioengineering, Polytechnic of Milan, Milan Leonardo 32, 20133 Milano, Italy, Tel: +390223993481; E-mail: diego.liberati@polimi.it

Received date: November 20, 2017; **Accepted date:** November 22, 2017; **Published date:** November 28, 2017

Citation: Liberati D. Chemistry, Informatics and Systems Biology. Chem Inform 2017, Vol.3 No. 1: 3.

Editorial

Chemistry is (also) information: as a matter of example, our DNA is a chemical matter, where everything about each of ourself - in power - is written, dynamically expressing itself epigenetically by interacting with the neigh borough. Also our slow control system is chemistry, being related to hormones; and even the fast one, though apparently electric, the neural one, does in fact rely on chemistry both in junctions, through neurotransmitters, and even in propagation, by means of Sodium and Potassium active pumping through the axon membrane.

It is thus not surprising the increasing importance of information technologies, especially informatics, in Chemistry: this same journal is a nice review of most of them, permeating most of the chemical publications nowadays. Some are recent: QSAR for instance, an application of inductive artificial intelligence to infer properties of a candidate new molecule taking into account what is known about its radicals; thus complementing - *in silico* - and forecasting the standard deductive and experimental approach to this Science (Of course, informatics is precious also in standard design and modeling of the properties of a compound).

One of the growing fields in which such a novel informatics approach to Chemistry is paramount is Systems Biology, aiming to better understand the dynamics of key biochemical species in living organisms. A couple of paradigmatic examples could be the following ones.

The inner dynamics of a molecule while interacting with its milieu is often of interest in appreciating its biochemical properties: a quite recent paper [1] uses the Gillespie classical continuation for dynamical systems simulation in order to appreciate the behaviour of Sos-Ras oncogenic-oncosuppresive behaviour in their cytoplasmic interaction in proximity of the cell membrane. Besides confirming the opening and closing of the two "arms" of the stereochemical characteristic of Son-of-sevenless, according to its "willing" to accept, refuse or keep the Ras stimulus, one interesting yielding of such paper, and in general of this kind of approach, is the ability to forecast behaviours not yet observed in nature: in that case, a mutant not yet described was taken into account whose properties has been forecasted and then confirmed when finally discovered.

At a just a bit higher level, an even more recent paper [2] describes the dynamics of the Tumor Necrosis Factor when released by irradiated cells and internalized in non-irradiated cells, when able to locally tri-merize in proximity of their membrane, triggering the so-called bystander effect: two paths are thus possibly alternatively elicited, one yielding apoptosis, mainly mediated by Caspase, the other one to survival, mainly mediated by NF-κB. Interestingly enough, both path appears to need at least two steps of the same sign in order to become irreversible, showing a kind of fault tolerance in each choice, aiming at confirming the inner state of the very cell in subsequent though close times, in order to be sure of its "will" to determinate each fate.

Such few examples do already show how informatics - and systems and control theory techniques indeed, specifically - is very powerful in order to help *in silico* understanding and modeling of chemical properties *in vivo*, thus predicting behaviours then confirmed in both *in vivo* observations and *in vitro* standard experimentation: Chemistry, at the basis of the information needed for our lives, with the help of Informatics - and related disciplines - allows to investigate the very processes yielding to our pathophysiological behaviour, enabling modeling and forecasting pathologies and possible therapies, whose application could then also be more easily monitored.

References

1. Sacco E, Farina M, Greco C, Lamperti S, Busti S, et al. (2012) Regulation of hSos1 activity is a system-level property generated by its multi-domain structure. Biotechnology Advances 30: 154-168.
2. Mezza D, Pappalettera M, Liberati D (2016) A quantitative numerical model for TNF-α mediated cellular Apoptosis. Biology Engineering and Medicine 1: 5-8.