Short Communication

Network chemistry, network toxicology, network informatics, and network behavioristics: A scientific outline

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Abstract

In present study, I proposed some new sciences: network chemistry, network toxicology, network informatics, and network behavioristics. The aims, scope and scientific foundation of these sciences are outlined.

Keywords network chemistry; network toxicology; network informatics; network behavioristics; scientific foundation; aims and scope; new sciences.

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1 Introduction

Like network biology (Barabasi and Oltvai, 2004; Zhang, 2011, 2012; Find details on network biology at http://www.iaees.org/publications/journals/nb/nb.asp), and network pharmacology (Hopkins, 2007, 2008), network science has been successfully used in some areas of sciences. Using network theory and methodology to improve traditional sciences is proved to be an effective approach. In present study, I try to propose some new sciences, i.e., network chemistry, network toxicology, network informatics, and network behavioristics, and to outline the aims, scope and scientific foundation of these sciences, in order to lay the foundation for further studies in the future.

2 Proposed New Sciences

2.1 Network chemistry

The aims of network chemistry are to analyze interactions between chemicals/molecules/compounds in the complex chemical networks, to study the evolution of chemical networks, and to control these chemical networks, etc. At the level of molecular biology and biochemistry, some of the research scopes of network chemistry coincide with that of network biology (Goemann et al., 2011; Huang and Zhang, 2012; Li and

Zhang, 2013; Rahman et al., 2013). Graph theory, network science, systematics, chemistry, and computational science, etc., are scientific foundation of network chemistry.

2.2 Network toxicology

In a sense, network toxicology is a branch of network chemistry. However, network toxicology further considers environmental factors also. Network toxicology aims to study the mechanisms of toxicant's flow in the networks like ecosystems, etc., and to control the flow according to findings on these mechanisms. Graph theory, network science, systematics, ecology/environmental sciences, health science, and computational science, etc., are scientific foundation of network toxicology.

2.3 Network informatics

Network informatics aims to exploit the mechanisms of information dissemination in the networks like social networks, ecosystems, the human brain, etc., and to improve the efficacy of information dissemination based on findings on these mechanisms. Graph theory, network science, systematics, information science, and computational science, etc., are all scientific foundation of network informatics.

2.4 Network behavioristics

Network behavioristics is closely related to sleforganizology and agent-based modeling (Zhang, 2012, 2013, 2014a, 2014b, 2016; Zhang and Liu, 2015). It aims to exploit the co-evolution mechanisms of behavioral rules of nodes in the networks as human/animal communities, ecosystems, etc. Graph theory, network science, systematics, agent-based modeling, selforganizology, and computational science, etc., are scientific foundation of network behavioristics.

3 Summary

The present study just proposed the basic concepts and outlined the new sciences. The aims, scope, and methodology, etc., of these sciences are expected to be further revised, improved and developed in the future.

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References

Barabasi AL, Oltvai ZN. 2004. Network biology: understanding the cell's functional organization. Nature Reviews Genetics, 5: 101-113

Goemann B, Wingender E, Potapov AP. 2011. Topological peculiarities of mammalian networks with different functionalities: transcription, signal transduction and metabolic networks. Network Biology, 1(3-4): 134-148

Hopkins AL. 2007. Network pharmacology. Nature Biotechnology, 25(10): 1110-1111.

Hopkins AL. 2008. Network pharmacology: the next paradigm in durg discovery. Nature Chemical Biololgy, 4(11): 682-690

Huang JQ, Zhang WJ. 2012. Analysis on degree distribution of tumor signaling networks. Network Biology, 2(3): 95-109

Li JR, Zhang WJ. 2013. Identification of crucial metabolites/reactions in tumor signaling networks. Network Biology, 3(4): 121-132

Rahman KMT, Md. Islam F, Banik RS, et al. 2013. Changes in protein interaction networks between normal and cancer conditions: Total chaos or ordered disorder? Network Biology, 3(1): 15-28

Zhang WJ. 2011. Network Biology: an exciting frontier science. Network Biology, 1(1): 79-80

Zhang WJ. 2012. Computational Ecology: Graphs, Networks and Agent-based Modeling. World Scientific, Singapore

Zhang WJ. 2013. Selforganizology: A science that deals with self-organization. Network Biology, 3(1):1-14

Zhang WJ. 2014a. A framework for agent-based modeling of community assembly and succession. Selforganizology, 1(1): 16-22

Zhang WJ. 2014b. Selforganizology: A more detailed description. Selforganizology, 1(1): 31-46

Zhang WJ. 2016. Selforganizology: The Science of Self-Organization. World Scientific, Singapore

Zhang WJ, Liu GH. 2015. Coevolution: A synergy in biology and ecology. Selforganizology, 2(2): 35-38