



Institute of  
Molecular and  
Cell Biology

## SEMINAR ANNOUNCEMENT

DATE: 15 March 2012, Thursday  
TIME / VENUE: 2:00PM @ Level 3, IMCB Seminar Room 3-46, Proteos, Biopolis  
SPEAKER: Dr. Hiroaki Kitano  
TITLE OF SEMINAR: **Systems biomedicine and their computational platforms**

### Dr. Hiroaki Kitano

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Discovery of drugs and appropriate therapeutic interventions are complex enterprises. It is inherently complex as biological systems evolved to be complex in order to cope with broad range of perturbations and to maintain various functionalities. Multiple coordinated interventions are key for successful drugs to coming decades. The inherent difficulties lies in robustness and fragility associated with disease out break and progression as well as host response to therapeutic interventions.

The talk addresses issues in the current drug discovery processes, and argue that more systematic approach need to be taken with principles behind. One option is the use of multi-component multi-target drugs. However, it requires powerful computational approach to overcome its combinatorial explosion problems. It also requires principles that guide the discovery process. Experimental approach such as gTOW (genetic Tug-of-War) shall uncover various mechanistic issues that causes discrepancies between computational and experimental results.

At the same time, it requires systematic and well designer engineering process to make the whole enterprise successful and economically viable. Nevertheless, lack of common platform hinders efficient development of tools that can potentially speed up drug discovery process. This talk outlines principles for systems drug discovery, addresses experimental issues, and efforts to develop unified and versatile software platform to enhance the process. The Garuda alliance was initiated to resolve this problem. (<http://www.garuda-alliance.org/>) HD-Physiology project aims at development on an integrated and mechanisms-based ADME/PK-PD-Tox and multi-layer heart model within the Garuda platform.

[ Related publications ]

Standard formation (SBML <http://www.sbml.org/> , SBGN <http://www.sbgm.org/> , etc): Le Novère, N., et al. The Systems Biology Graphical Notation. Nature Biotechnology. 27(8), 735-741, 2009. Kitano, H.; Funahashi, A.; Matsuoka, Y.; Oda, K. Using process diagrams for the graphical representation of biological networks. Nature Biotechnology. 23(8), 961 – 966, 2005. Hucka, M.; Finney, A.; Sauro, H.M.; Bolouri, H.; Doyle, J.C.; Kitano, H.; et al. The Systems Biology Markup Language (SBML): A Medium for Representation and Exchange of Biochemical Network Models. Bioinformatics. 19(4), 524-531, 2003.

Software and Social Platform: Kitano, H.; et al. Social engineering for virtual big science in systems biology. Nature Chemical Biology. 7(6), 323-326, 2011. Ghosh, S.;et al. Software for systems biology: from tools to platforms. Nature Reviews Genetics. 12(12), 821-832, 2011. Ghosh, S.;Matsuoka, Y.; Kitano, H. Connecting the dots: role of standardization and technology sharing in biological simulation. Drug Discover Today. 15(23/24), 1024-1031, 2010.

*Host: Prof. Wanjin Hong*

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