# February 2017
# *Complexity Community Sharing Session*
## 17 Feb (Fri) 11.00am – 1.00pm
## Seminar Room 102
(opposite The Hive) Blk 1 Innovation Centre, Level 1
16 Nanyang Drive, Singapore 637722, NTU

### *Towards in Silico Data-Driven Combination Therapy*



*A/Prof .
Sourav S. Bhowmick*

Combination therapy, where several drugs interact with multiple targets, holds tremendous promise for effective clinical outcomes in the management of chronic, complex diseases such as cancer. In this talk, we present our precarious journey towards building a novel in silico, data-driven target combination therapy framework for complex diseases. Successful realization of this framework can result in an effective platform for in silico screening of drug combinations in a rational way, by aiding early discovery of suitable combination therapy and guiding the design of further in vitro and in vivo experiments. To this end, we first construct a disease-related enriched human signaling network by integrating publicly-available disease-specific signaling networks with expression and annotation data. Next, topology and dynamics (if available) of the network, which can be noisy and incomplete, are analyzed as a whole using novel network analytics techniques to predict promising target combinations with desirable properties (e.g., synergistic in nature, good efficacy and minimum off-target effect) to regulate the activities of key disease-related molecular players. In this talk, we give an overview our framework, demonstrate world's first academic prototype of data-driven target combination prediction for breast cancer, and highlight challenges we have yet to overcome and future research directions. Results of this research have appeared in premium bioinformatics and systems biology venues such as Bioinformatics journal and ACM BCB (flagship venue of ACM SIGBio group).

*Dr. Sourav S. Bhowmick is an Assoc Prof in the School of Computer Science and Engineering (SCSE),NTU. He leads the data management research group (DANTe) in SCSE. He was a Visiting Assoc Prof at the Biological Engineering Division, Massachusetts Institute of Technology during 2007-2013. His current research interests include data management, data analytics, computational social science and network-based systems biology. He has published more than 70 papers in top-tier venues such as VLDB, IEEE ICDE, ACM WWW, ACM SIGMOD, ACM SIGIR, ACM SIGKDD, ACM MM, Bioinformatics, Biophysical Journal, IEEE TKDE, and VLDB Journal. He regularly serves as a PC member and editorial board member of leading conferences and journals in data management, data analytics, and bioinformatics. He has served as a program chair/co-chair of several international workshops and conferences. Sourav has been keynote and tutorial speaker for several international conferences. He has received Best Paper Awards at ACM CIKM 2004 and ACM BCB 2011 for papers related to evolution mining and biological network summarization, respectively. His work on computational social science was nominated for the best paper award in ACM SIGMOD 2015.*
*(Co-author) Dr. Huey Eng Chua is currently a Research Fellow at NTU. She received her Ph.D. in computational systems biology from NTU in 2015. Her current research interest is in analysis and visualization of biological networks with the goal of improving combination therapy for complex diseases such as cancer, using scalable machine learning and graph mining approaches. Her research has been published in Bioinformatics journal and ACM BCB.*

### *Prognostics Diagnostics and Therapeutics in Health - Past, Current & Future*



*Dr. Ruud Brands*

The development route for new therapeutics is a lengthy and costly process. Shortcut opportunities in such development are much wanted but not easily accepted by governmental health authorities nor by the public domain, due to failures in the past. Having tools available that would decipher the basics of diseases and to enable prediction of how these diseases may or may not develop in each of us would be a powerful asset. Biological tools like biomarkers are searched to identify specific future diseases at time points that the disease itself is not yet apparent. We target the functioning of the innate immune system's responses specifically in a patient on a given time. In-silico models are being developed to predict these responses, using clinical data to fine tune and validate the models. I will introduce you to some of above aspects of clinical therapeutic development routes from recent history, current development schemes and future options.

*Dr. Ruud Brands is a molecular cell biologist who specializes in Cellular protein trafficking, targeting and functioning in health and disease conditions. After his graduation at the University of Utrecht, he held several positions in the field of cell biology and oncology at Stanford University (Palo Alto, CA) and the Netherlands Cancer Institute. In the 90s, he was a staff member at the Dept of Biotechnology at Solvay Pharmaceuticals in the Netherlands, where he managed the R&D of the first (licensed) cell culture derived influenza vaccine. Brands was co-founder of PharmAAware in 2000, developing alkaline phosphatase for septic shock treatment. In 2005 Alloksys Life Sciences and in 2013 AMRIF were founded to further develop the rescuing alkaline phosphatase (RESCAP) platform for acute and chronic unmet medical need disease management. Since June 2015 he is associated to the Complexity Institute NTU as Senior Research Fellow where he joined an initiative of Prof Peter Sloot aiming to decipher the complexity of the innate immune system.*

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