IBSB2013 Program

# Program-at-a-glance

Tuesday, July 30	Wednesday, July 31	Thursday, August 1	Friday, August 2
	Opening Remark 8:30 – 8:40 Invited Talk 1 8:40 – 9:25	Invited Talk 4 8:30 – 9:15 Jean-Phileppe Vert	Invited Talk 6 8:30 – 9:15 Ziv Bar-Joseph
	Nathan Price Invited Talk 2 9:25 – 10:10 John P. Overington	Invited Talk 5 9:15 – 10:00 Limsoon Wong	Invited Talk 7 9:15 – 10:00 Samuel Kaski
	John P. Overington	Break 10:00 – 10:15	Break 10:00 – 10:15
	Break 10:10 – 10:25	Oral Session 4 10:15 – 11:45	
	Oral Session 1 10:25 – 12:25		Oral Session 5 10:15 – 12:15
		Lunch Break and Poster 11:45–12:30	
	Lunch Break and Poster 12:25 – 14:00		Lunch Break and Poster 12:15 – 14:00
	Invited Talk 3 14:00 – 14:45 Becca Asquith	Excursion 12:30 – 19:00	Oral Session 6 14:00 – 16:00
	Oral Session 2 14:45 – 16:45		Break 16:00 – 16:15
	Break 16:45 – 17:00		Oral Session 7 16:15 – 18:15
Reception 17:30–19:30	Oral Session 3 17:00–19:00		Clasics Densel 10.16, 10.20
			Closing Remark 18:15 – 18:30
		Banquet 19:00 –	Closing Dinner 19:30 -

# Wednesday, July 31

# Invited Talk 1 & 2 [8:40 - 10:10]

## 8:40 - 9:25 Invited Talk 1

N. Price, Biomolecular networks in the brain

# 9:25 - 10:10 Invited Talk 2

J. P. Overington,

ChEMBL - A large scale bioactivity database

Oral Session 1 [ 10:25 - 12:25 ] Chair: Daniel Gusenleitner

#### 10:25 - 10:55 IBSB-40

A. Palinkas, A. Bockmayr, S. Bulik and H.-G. Holzhutter, Constraint-based modelling of alterations in metabolic networks

#### 10:55 - 11:25 IBSB-13

W. Gottstein, Coordination of metabolism

## 11:25 - 11:55 IBSB-56

C. Wallstab, Kinetic modeling of hepatic fat accumulation and lipid droplet dynamic

### 11:55 - 12:10 IBSB-28

W. Lu, T. Tamura, J. Song, and T. Akutsu An integer programming-based method of designing synthetic metabolic networks by minimum reaction insertion

### 12:10 - 12:25 IBSB-61

Y. Zhao, M. Hayashida, H. Nagamochi, and T. Akutsu Enumeration of tree-like compounds in breadth first search order

Invited Talk 3 [ 14:00 - 14:45 ]

# 14:00 - 14:45 Invited Talk 3

B. Asquith,

Viral escape from CD8+ T Cells: evidence for a lytic effector mechanism?

Oral Session 2 [ 14:45 - 16:45 ] Chair: Christin Wallstab

#### 14:45 - 15:15 IBSB-8

A. Filipchyk, S. Grosswendt, and N. Rajewsky, Transcriptome-wide identification of miRNA binding sites in C. elegans

### 15:15 - 15:45 IBSB-59

A. L. Woelke,

Understanding selectin counter-receptor binding from electrostatic energy computations and experimental binding studies

### 15:45 - 16:15 IBSB-25

G. Korff,

Protein secondary structure assignment for protein-protein interface characterization

#### 16:15 - 16:30 IBSB-4

T. Bohnuud, Distribution of ligand-binding hot spots in flexible RNA structures

# 16:30 - 16:45 IBSB-43

P. Ruan, M. Hayashida, O. Maruyama, and T. Akutsu,

Prediction of heterodimeric protein complexes from weighted protein- protein interaction networks using novel features and kernel functions

Oral Session 3	[ 17:00 - 19:00 ]
	Chair: Yosuke Nishimura

#### 17:00 - 17:30 IBSB-9

Y. Fu, B. LaBarre, A. B. Pavel, L. Zhang, G. Benson, and S. Monti,

Detection of recurrent somatic copy number alterations in cancer

#### 17:30 - 18:00 IBSB-1

E. Ayada, A. Niida, R. Yamaguchi, S. Imoto, and S. Miyano, Application of binary contingency tables in analyzing copy number co-aberrations in cancer genome

#### 18:00 - 18:30 IBSB-55

N. Usuyama, Y. Shiraishi, S. Imoto, and S. Miyano, LDM: Detection of somatic mutations in cancer using germline variants

### 18:30 - 18:45 IBSB-24

M. Kolinski, E. Wyler, M. Schueler, G. Mastrobuoni, A. Bergfort, S. Kempa, C. Dieterich, and M. Landthaler, Popcar: protein occupancy profiling of chromatin-associated RNAs

# 18:45 - 19:00 IBSB-18

S. Iyer,

Analysis of multiple transcription factor occupancy in the human genome Invited Talk 4 & 5 [8:30 - 10:00]

# $8{:}30$ - $9{:}15$ Invited Talk 4

J.-P. Vert, On finding breakpoints in DNA copy number profiles

9:15 - 10:00 Invited Talk 5 L. Wong,

Enabling more reproducible gene expression analysis

Oral Session 4 [ 10:15 - 11:45 ]

Chair: Takanori Hasegawa

# 10:15 - 10:45 IBSB-11

M. Ghanbari, Reconstruction of gene regulatory networks by using prior knowledge

#### 10:45 - 11:15 IBSB-32

A. Mohamed, T. Hancock, and H. Mamitsuka, MetPathMineR: R package for metabolic pathway mining from gene expression

# 11:15 - 11:45 IBSB-29

Y. Maruyama, R. Yamaguchi, S. Imoto, and S. Miyano, Modeling of dynamic drug effect on gene networks

# Invited Talk 6 & 7 [ 8:30 - 10:00 ]

# 8:30 - 9:15 Invited Talk 6

Z. Bar-Joseph,

Data integration for understanding dynamic biological systems

#### 9:15 - 10:00 Invited Talk 7

S. Kaski,

Multi-view multi-task learning for drug sensitivity prediction

Oral Session 5 [ 10:15 - 12:15 ]

Chair: Teresa Wang

### 10:15 - 10:45 IBSB-45

J. M. Schmiedel, A. Sahay, N. Bluthgen, D. M. Marks, and A. van Oudenaarden,

microRNAs reduce intrinsic gene expression noise

### 10:45 - 11:15 IBSB-31

G. Moenke,

Modeling the P53 stress response system in single cells

### 11:15 - 11:45 IBSB-34

Y. Murakawa, G. Mastrobuoni, T. Yasuda, M. Schueler, C. C. Friedel, C. D. Lars Dolken, K. Rajewsky, S. Kempa, and M. Landthaler, PAR-CLIP of human RC3H1 reveals comprehensive features of target recognition and a functional role in post-transcriptional regulation of DNA damage response

# 11:45 - 12:00 IBSB-46

H. Selby, A. van der Velde, A. Labadorf, B. Chapuy, M. Shipp, and S. Monti,

A novel time series analysis of transcriptional response to targeted treatment of diffuse large B-cell lymphoma (DLBCL)

#### 12:00 - 12:15 IBSB-16

J. D. Hogan, J. L. Keenan, L. Luo, A. J. Poustka, and C. A. Bradham,

The embryonic transcriptome for the sea urchin Lytechinus variea-gatus,

Oral Session 6 [14:00 - 16:00]

Chair: Kei-ichiro Takahashi

# 14:00 - 14:30 IBSB-54

F. Uschner,

Characterizing signal transduction in S. cerevisiae osmo-sensing

#### 14:30 - 15:00 IBSB-38

C. H. Nguyen and H. Mamitsuka, Latent feature models for biological networks

### 15:00 - 15:30 IBSB-23

Y. Kataoka, T. Shimamura, S. Imoto, and Miyano, Computational detection of biological pathways related to drugsensitivity

#### 15:30 - 15:45 IBSB-26

M. Kotera, Y. Tabei, Y. Yamanishi, T. Tokimatsu, and S. Goto, Supervised learning of enzymatic reaction likeness for *de novo* reconstruction of metabolic pathways

### 15:45 - 16:00 IBSB-36

N. Nakajima and T. Akutsu, Network completion for time varying genetic networks

Oral Session 7 [ 16:15 - 18:15 ]

Chair: Thomas Spiesser

# 16:15 - 16:45 IBSB-58

T. Wang, G. Liu, M. Dumas, F. Perera, R. Miller, D. Brooks, S. Chillrud, M. Lenburg, and A. Spira,

Secondhand smoke alters the nasal epithelial gene expression profiles in adults and children

# 16:45 - 17:15 IBSB-47

Y. Shimizu, M. Kotera, T. Tokimatsu, and S. Goto, Comprehensive analysis of polyketide synthases based on domain structures,

# 17:15 - 17:45 IBSB-39

Y. Nishimura, M. Kotera, T. Tokimatsu, and S. Goto, Functional and evolutionary analysis of intragenic miRNA families in metazoan species

# 17:45 - 18:00 IBSB-6

Bridging data analysis and interactive visualizations

#### 18:00 - 18:15 IBSB-51

Y. Tan, P. Tamayo, H. Nakaya, B. Pulendran, J. Mesirov, and W. N. Haining,

Gene signatures related to B cell proliferation predict influenza vaccine-induced antibody response

I. S. Caballero,

Abstracts - Invited Talks

# Biomolecular networks in the brain

#### Nathan Price

### Abstract

The states of biomolecular networks in the brain are related to phenotypes and are reflected, in part, in the transcriptome. We have applied systems analysis of brain transcriptomes in the context of two model organisms: the honey bee (a prominent model for the links between genomics and social behavior) and the mouse (the most widely used model organism for human disease). In the bee, we show that behavior-specific neurogenomic states can be inferred from the coordinated action of transcription factors (TFs) and their predicted target genes. Our results reveal three insights concerning the relationship between genes and behavior. First, distinct behaviors are subserved by distinct neurogenomic states in the brain. Second, the neurogenomic states underlying different behaviors rely upon both shared and distinct transcriptional modules. Third, despite the complexity of the brain, simple linear relationships between TFs and their putative target genes can surprisingly be found quite abundantly in the network states underlying behavior. In the mouse, we utilized the tremendous resource of the Allen Brain Atlas to evaluate spatial expression patterns of sets of genes that have cell type-specific expression for neurons, astrocytes, and oligodendrocytes. We found that the combined spatial expression patterns of 170 neuron-specific transcripts revealed strikingly clear and symmetrical signatures for most of the brain's major subdivisions, with clear neuron-specific signatures corresponding with high fidelity to each distinct brain region. Moreover, these brain gene expression spatial signatures correspond to anatomical structures and may even reflect developmental ontogeny. Taken together, these findings hint at a wealth of information about the brain that can be probed globally at the molecular level.

# **ChEMBL** - A large scale bioactivity database

John P. Overington

## Abstract

The link between the biological and chemical worlds is of central importance in many fields, not least that of healthcare and risk assessment. A major focus in the integrative and systems level understanding of biology are genes/proteins and the networks and pathways describing their interactions and functions; similarly, within chemistry there is much interest in efficiently identifying drug-like cell-penetrant compounds that specifically interact with these targets. However there has been relatively little research explicitly directed at understanding the linkages between these two domains. Key to our work in this area has been the construction of a large and general database linking pharmacological activities of compounds through to their targets (http://www.ebi.ac.uk/chembl), and understanding how particular privileged chemotypes recognize their cognate receptors. Central to this was the development of a series of informatics approaches to efficiently curate and normalise the data, allowing far higher integration and comparison of the original data. One application of the data is to predict the polypharmacology of a given compound based on analysis of compound set target associations. The scope and contents of the ChEMBL database will be presented, alongside some application of the data to understand target modulation in complex biosystems.

# Viral escape from CD8+ T Cells: evidence for a lytic effector mechanism?

Katerina Seich al Basatena, Marjet Elemans, Fredrik Graw, Simon Frost, Roland Regoes, Chris Gkekas and Becca Asquith Dept of Immunology, Imperial College London

### Abstract

Recent evidence suggests that, in SIV and HIV-1 infection, CD8+ T cells mediate anti-viral control predominantly via non - cytolytic mechanisms. This is in apparent conflict with the observation that SIV and HIV - 1 variants that escape CD8+ T cell surveillance are frequently and reproducibly selected.We use a cellular automata model that describes spatial and temporal HIV - 1 dynamics to address the question "is the observation of escape variants evidence that CD8+ T cells kill HIV - 1 infected cells?

# On finding breakpoints in DNA copy number profiles

Jean-Philippe Vert

# Abstract

DNA reorganization, including amplification and deletion of particular genomic loci, is a hallmark of most cancers. Microarray- or sequencing-based technologies now allow to capture genome-wide profiles of DNA copy numbers, and give in particular information about locations of DNA breakpoints. In this talk, I will discuss several methods to identify breakpoints in noisy signals, and highlight in particular a method involving partial expert annotation to boost the performance of existing techniques.

# Enabling more reproducible gene expression analysis

#### Limsoon Wong

### Abstract

It is challenging to draw biological conclusions from today's microarray experiments. The main source of the difficulty is that the number of samples available for analysis is usually very small relative to the number of genes to be considered. It is often the case that many genes are statistically significant according to the wide variety of computational and statistical analysis algorithms. Yet there is little concurrence between the genes selected by different algorithms. Therefore, it is often necessary to analyze microarray experiments together with biological information to make better biological inferences.

We investigate the adequacy of current biological databases to address this need. We find a low level of consistency, comprehensiveness and compatibility among three popular pathway databases (KEGG, Ingenuity and Wikipathways). The level of consistency for genes in similar pathways across databases ranges from 0

We also introduce a series of techniques that provides both quantitative and descriptive analysis of microarray datasets by identifying specific subnetworks in pathways (from PathwayAPI) that are significant. We test our techniques on independent datasets of several diseases. For each of these diseases, we obtain two independent microarray datasets produce by distinct labs on distinct platforms. In each case, our techniques produce highly consistent lists of significant nontrivial subnetworks when they are independently applied to two independent sets of microarray data. The gene-level agreement of these significant subnetworks is much better than a number of commonly used approaches. Furthermore, the genes selected using other approaches do not form subnetworks of substantial size. Thus it is more probable that the subnetworks selected by our techniques provide the researcher with more descriptive information on the portions of the pathway actually linked to the disease.

#### CV of speaker

Limsoon Wong is KITHCT Professor of Computer Science and Professor of Pathology at the National University of Singapore. He currently works mostly on knowledge discovery technologies and their application to biomedicine. Limsoon has written about 150 research papers, some of which are among the best cited of their respective fields. He has/had served on the editorial boards of several leading journals of his fields, e.g., JBCB, TCBB, Biology Direct and Bioinformatics. He co-founded and is chairman of Molecular Connections, which has grown over the last decade into a major provider of data curation services employing over 700 curators, analysts, and engineers.

# Data integration for understanding dynamic biological systems

Ziv Bar-Joseph

## Abstract

Transcriptional gene regulation is a dynamic process and its proper functioning is essential for all living organisms. By combining the abundant static regulatory data with time series expression data using an Input-Output Hidden Markov model (IOHMM) we were able to reconstruct a dynamic representations for these networks in multiple species. The models lead to testable temporal hypotheses identifying both new regulators and their time of activation. We have recently extended these methods to allow the modeling of various aspects of post-transcriptional regulation including temporal regulation by microRNAs and linking signaling and dynamic regulatory networks. The reconstructed networks link receptors and proteins that directly interact with the environment to the observed expression outcome. I will discuss the application and experimental validation of predictions made by our methods focusing on stress response and lung development in mice. I would also mention a number of other extensions which we have used to study disease progression and the regulation of immune response.

# Multi-view multi-task learning for drug sensitivity prediction

Samuel Kaski Helsinki Institute for Information Technology HIIT Aalto University and University of Helsinki

### Abstract

In the core of personalized medicine is the computational task of predicting drug sensitivities based on genomic information. This is a supervised learning task which can be addressed by a combination of multi-view and multi-task learning. I will discuss an approach which has recently turned out to be successful, Bayesian kernelized multi-view multi-task methods for predicting sensitivities across drug profiles, and its generalizations to matrix factorization with side information.

Title List - Talks & Posters

IBSB-1 Application of binary contingency tables in analyzing copy number co-aberrations in cancer genome, E. Ayada, A. Niida, R. Yamaguchi, S. Imoto, and S. Miyano.

IBSB-2 Comparative analysis of properties and structures of natural compounds and drugs, *P. Banerjee and R. Preissner.* 

POSTER.

**IBSB-3** A bit-parallel, general integer-scoring sequence alignment algorithm, G. Benson, J. Loving, and Y. Hernandez.

POSTER.

**IBSB-4** Distribution of ligand-binding hot spots in flexible RNA structures, *T. Bohnuud.* 

POSTER & SHORT TALK (Oral Session 2).

**IBSB-5** Clinical pathoscope: Rapid alignment and filtration for accurate pathogen identification using unassembled sequence data, *A. Byrd, J. Perez-Rogers, and E. Johnson.* 

POSTER.

**IBSB-6** Bridging data analysis and interactive visualizations, *I. S. Caballero*.

POSTER & SHORT TALK (Oral Session 7).

IBSB-7 Naïve bayes gene set enrichment analysis, Z. Chen, T. P. Hancock, and H. Mamitsuka.

POSTER.

IBSB-8 Transcriptome-wide identification of miRNA binding sites in C. elegans, A. Filipchyk, S. Grosswendt, and N. Rajewsky.

LONG TALK (Oral Session 2).

- **IBSB-9** Detection of recurrent somatic copy number alterations in cancer, Y. Fu, B. LaBarre, A. B. Pavel, L. Zhang, G. Benson, and S. Monti. POSTER & LONG TALK (Oral Session 3).
- IBSB-10 VNTRSeek analysis of the genome of a khoisan individual using a computational pipeline for VNTR detection, Y. Gelfand, J. Loving, Y. Hernandez, and G. Benson.

POSTER.

 $\label{eq:BSB-11} \begin{array}{ll} \mbox{Reconstruction of gene regulatory networks by using prior knowledge,} \\ M. \ Ghanbari. \end{array}$ 

LONG TALK (Oral Session 4).

IBSB-12 Statistical inference of Ig germline gene-segment haplotype from highthroughput Ig gene sequencing, *H. Gomez and T. Kepler.* 

POSTER.

POSTER & LONG TALK (Oral Session 3).

**IBSB-13** Coordination of metabolism, *W. Gottstein.* 

#### POSTER & LONG TALK (Oral Session 1).

IBSB-14 Genomic signatures of carcinogenicity, D. Gusenleitner, S. Auerbach, D. Sherr, and S. Monti.

POSTER.

- IBSB-15 Prediction of protein-RNA residue-base contacts using twodimensional conditional random field with the lasso, *M. Hayashiday, M. Kamaday, J. Songz, and T. Akutsu.* POSTER.
- IBSB-16 The embryonic transcriptome for the sea urchin Lytechinus varieagatus, J. D. Hogan, J. L. Keenan, L. Luo, A. J. Poustka, and C. A. Bradham.

POSTER & SHORT TALK (Oral Session 5).

IBSB-17 A RNA-seq-based screen for skeletal patterning genes in sea urchin embryos, J. D. Hogan, J. L. Keenan, L. Luo, J. Coulombe-Huntington, A. J.

Poustka, and C. A. Bradham.

POSTER.

IBSB-18 Analysis of multiple transcription factor occupancy in the human genome, S. Iyer.

POSTER & SHORT TALK (Oral Session 3).

IBSB-19 Analysis on the similarity between oncogenic virus and human proteins in cancer pathways, Z. Jin, M. Kotera, and S. Goto.

POSTER.

**IBSB-20** Developing latent genotypes for genome-wide association studies, *I. Johnston and L. E. Carvalho.* 

POSTER.

IBSB-21 Light-weight modular constraint enforcement for scientific workflow systems, M. M. Kańduła and D. P. Kreil.

POSTER.

IBSB-22 Sparse multiple graph integration for label propagation, M. Karasuyama and H. Mamitsuka.

POSTER.

IBSB-23 Computational detection of biological pathways related to drugsensitivity, Y. Kataoka, T. Shimamura, S. Imoto, and Miyano.

POSTER & LONG TALK (Oral Session 6).

IBSB-24 Popcar: Protein occupancy profiling of chromatin-associated RNAs, M. Kolinski, E. Wyler, M. Schueler, G. Mastrobuoni, A. Bergfort, S. Kempa, C. Dieterich, and M. Landthaler.

POSTER & SHORT TALK (Oral Session 3).

IBSB-25 Protein secondary structure assignment for protein-protein interface characterization, G. Korff.

#### POSTER & LONG TALK (Oral Session 2).

IBSB-26 Supervised learning of enzymatic reaction likeness for de novo reconstruction of metabolic pathways, M. Kotera, Y. Tabei, Y. Yamanishi, T. Tokimatsu, and S. Goto.

POSTER & SHORT TALK (Oral Session 6).

IBSB-27 Recent progress and opportunities in selected projects through the programme's international student exchange, D. P. Kreil.

#### POSTER.

- IBSB-28 An integer programming-based method of designing synthetic metabolic networks by minimum reaction insertion, W. Lu, T. Tamura, J. Song, and T. Akutsu. POSTER & SHORT TALK (Oral Session 1).
- IBSB-29 Modeling of dynamic drug effect on gene networks, Y. Maruyama, R. Yamaguchi, S. Imoto, and S. Miyano. POSTER & LONG TALK (Oral Session 4).
- **IBSB-30** A clustering approach to associate drug side effects to drug indications,

S. Mizutani and S. Goto.

POSTER.

**IBSB-31** Modeling the P53 stress response system in single cells, *G. Moenke*.

LONG TALK (Oral Session 5).

IBSB-32 MetPathMineR: R package for metabolic pathway mining from gene expression data, A. Mohamed, T. Hancock, and H. Mamitsuka.

POSTER & LONG TALK (Oral Session 4).

IBSB-33 KEGG OC: automatically constructed comprehensive ortholog clusters based on taxonomic relation, Y. Moriya, T. Tokimatsu, M. Kotera, and S. Goto.

POSTER.

**IBSB-34** PAR-CLIP of human RC3H1 reveals comprehensive features of target recognition and a functional role in post-transcriptional regulation of DNA damage response,

Y. Murakawa, G. Mastrobuoni, T. Yasuda, M. Schueler, C. C. Friedel, C. D. Lars Dolken, K. Rajewsky, S. Kempa, and M. Landthaler.

LONG TALK (Oral Session 5).

IBSB-35 Reaction modules: conserved sequences of reactions in metabolic pathways,

A. Muto, M. Kotera, T. Tokimatsu, Z. Nakagawa, S. Goto, and M. Kanehisa.

POSTER.

- IBSB-36 Network completion for time varying genetic networks, N. Nakajima and T. Akutsu. POSTER & SHORT TALK (Oral Session 6).
- IBSB-37 In silico analysis of histone modification dynamics at ash1 binding regions in D. melanogaster, Y. Natsume-Kitatani and H. Mamitsuka.

POSTER.

IBSB-38 Latent feature models for biological networks, C. H. Nguyen and H. Mamitsuka. POSTER & LONG TALK (Oral Session 6).

IBSB-39 Functional and evolutionary analysis of intragenic miRNA families in metazoan species, Y. Nishimura, M. Kotera, T. Tokimatsu, and S. Goto.

POSTER & LONG TALK (Oral Session 7).

- **IBSB-40** Constraint-based modelling of alterations in metabolic networks, A. Palinkas, A. Bockmayr, S. Bulik, and H.-G. Holzhutter. LONG TALK (Oral Session 1).
- **IBSB-41** Integrated modelling of metabolism and gene regulation, A. Palinkas, A. Bockmayr, S. Bulik, and H.-G. Holzhutter. POSTER.
- IBSB-42 Orthology and paralogy in polyketide biosynthetic gene clusters of pathogenic fungi, J. H. Ramirez-Prado, M. Kanehisa, and S. Goto.

POSTER.

IBSB-43 Prediction of heterodimeric protein complexes from weighted proteinprotein interaction networks using novel features and kernel functions,

P. Ruan, M. Hayashida, O. Maruyama, and T. Akutsu. SHORT TALK (Oral Session 2).

- IBSB-44 Comparative analysis of metatranscriptome and metagenome of soil microbiome, T. Satoh, Y. Moriya, T. Tokimatsu, S. Goto, and N. Miyashita. POSTER.
- IBSB-45 microRNAs reduce intrinsic gene expression noise, J. M. Schmiedel, A. Sahay, N. Bluthgen, D. M. Marks, and A. van Oudenaarden.

LONG TALK (Oral Session 5).

IBSB-46 A novel time series analysis of transcriptional response to targeted treatment of diffuse large B-cell lymphoma (DLBCL),
H. Selby, A. van der Velde, A. Labadorf, B. Chapuy, M. Shipp, and S. Monti.

POSTER & SHORT TALK (Oral Session 5).

**IBSB-47** Comprehensive analysis of polyketide synthases based on domain structures,

Y. Shimizu, M. Kotera, T. Tokimatsu, and S. Goto.

POSTER & LONG TALK (Oral Session 7).

IBSB-48 SBML-Pedigree: A web-based framework for modeling hierarchical populations of SBML models, *T. W. Spiesser.* 

POSTER.

IBSB-49 Generating gene set networks from microarray data, K. Takahashi, I. Takigawa, and H. Mamitsuka.

POSTER.

IBSB-50 Completing method for ortholog-based GPR metabolic network by gene essentiality, *T. Tamura and T. Akutsu.* 

POSTER.

IBSB-51 Gene signatures related to B cell proliferation predict influenza vaccine-induced antibody response, Y. Tan, P. Tamayo, H. Nakaya, B. Pulendran, J. Mesirov, and W. N. Haining.

POSTER & SHORT TALK (Oral Session 7).

**IBSB-52** A novel tool for gene-specific fusion detection, Y. Tan, B. Chapuy, and S. Monti.

POSTER.

IBSB-53 Classification of plant type III polyketide synthase-related secondary metabolites for predicting their biosynthetic pathways, *T. Tokimatsu, M. Kotera, and S. Goto.* 

#### POSTER.

**IBSB-54** Characterizing signal transduction in *S. cerevisiae* osmo-sensing, *F. Uschner.* 

LONG TALK (Oral Session 6).

IBSB-55 LDM: Detection of somatic mutations in cancer using germline variants,

N. Usuyama, Y. Shiraishi, S. Imoto, and S. Miyano. POSTER & LONG TALK (Oral Session 3).

IBSB-56 Kinetic modeling of hepatic fat accumulation and lipid droplet dynamic, C. Wallstab.

LONG TALK (Oral Session 1).

**IBSB-57** Mathematical modeling of lipid droplet dynamics in hepatocytes, *C. Wallstab.* 

POSTER.

**IBSB-58** Secondhand smoke alters the nasal epithelial gene expression profiles in adults and children,

T. Wang, G. Liu, M. Dumas, F. Perera, R. Miller, D. Brooks, S. Chillrud, M. Lenburg, and A. Spira.

POSTER & LONG TALK (Oral Session 7).

**IBSB-59** Understanding selectin counter-receptor binding from electrostatic energy computations and experimental binding studies, *A. L. Woelke*.

LONG TALK (Oral Session 2).

IBSB-60 The role of Glu286 in CcO function as a potential proton gate explored by electrostatic energy computations combined with molecular dynamics, A. L. Woelke.

### POSTER.

IBSB-61 Enumeration of tree-like compounds in breadth first search order, Y. Zhao, M. Hayashida, H. Nagamochi, and T. Akutsu. POSTER & SHORT TALK (Oral Session 1).