Computational Methods Aiding Early-Stage Drug Design
Dagstuhl Seminar 13212

	Monday **20.5.2013**	**Tuesday** **21.5.2013**	**Wednesday** **22.5.2013**	**Thursday** **23.5.2013**	**Friday** **24.5.2013**
7:30-8:45	Breakfast	Breakfast	Breakfast	Breakfast	Breakfast
9:00-12:00	Introduction: Hinrich Göhlmann Sepp Hochreiter Coffee at 10:45	Andreas Bender (60) Completing the Compound-Target Bioactivity Matrix via Compound Databases and Computer Algorithms Gianluca Pollastri (60) *Recursive Neural Networks for Undirected Graphs and Neural Network Pairwise Interaction Fields for annotating 2D and 3D small molecules* Coffee at 10:45	Günter Klambauer (30) Detecting differentially expressed genes in RNA-Seq drug design studies Wolfgang Huber (60) *Systematic mapping of synthetic genetic interactions with combinatorial RNAi* Leo Lahti (60) *Intestinal microbiota, individuality and health* Coffee at 10:45	Samuel Kaski (60) *Multi-view learning for drug sensitivity prediction* Dhammika Amaratunga (30) Enriched methods for classification of high-dimensional data Adetayo Kasim (30) *Semi-supervised investigation of association of gene expression with structural fingerprints of chemical compounds* Coffee at 10:45	Jelle J. Goemann (60) *False discovery proportions of gene lists prioritized by the user* Oswaldo Trelles (30) *Scaling Bioinformatics algorithms in the Cloud* Stefan Kramer (60) *New Algorithms for Graphs and Small Molecules: Exploiting Structural Graph Neighborhoods and Target Label Dependencies* Coffee at 10:45
12:15-14:00	Lunch	Lunch	Lunch	Lunch	Lunch
14:00-15:30	Justin Lamb (60) *Library-Scale Gene-Expression Profiling and Digital Open Innovation*	Ulrich Bodenhofer (30) Similarity-based clustering of compounds and its application to knowledge discovery from kernel-based QSAR models Johannes Mohr (60) *A Maximum Common Subgraph Kernel Method for Predicting the Chromosome Aberration Test*	Excursion	Murat Iskar (60) *Drug-induced transcriptional modules in mammalian biology: implications for drug repositioning and resistanc* Ziv Shkedy (30) Integrated analysis of gene expression, chemical structure and bioassay data	Departure
15:30-16:00	Coffee	Coffee		Coffee	
16:00-17:30	*Jörg Wegner (60)* *Large scale Chemogenomics/L1000 orthogonal gene ranking and how to bridge SystemsBiology with MedicinalChemistry in Pharma*	Chas Bountra (60) *Protein family focused, structure enabled chemical probes, to accelerate the discovery of new targets* Willem Talloen (30) *The nature of gene signature development*		Bie Verbist (30) *Minor Variant Detection In Virology with Model Based Clustering* Javier Cabrera (60) *Shrinking methods and their applications to estimation with special focus on networks*	
18:00	Diner	Diner		Diner	