Predicting drug-target interaction networks from the integration of chemical, genomic, and pharmacological spaces

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In silico prediction of drug-target interactions from heterogeneous biological data is critical in the search for drugs and therapeutictargets for known diseases such as cancers. In this study, we investigate the correlation between the chemical space of compound structures, the genomic space of genes/proteins, the pharmacological space of phenotypic effects, and the topology of drug-target interaction networks. We then develop a new method to predict unknown drug-target interactions from chemical, genomic, and pharmacological data on a large scale. The originality of the proposed method lies in the formalization of the drug-target interaction inference as a supervised learning problem for a bipartite graph, the lack of need for 3D structure information of the target proteins, and in the integration of chemical, genomic, and pharmacological spaces in a unified framework. In the results, we make predictions for four classes of important drug-target interactions involving enzymes, ion channels, GPCRs, and nuclear receptors. Our comprehensively predicted drug-target interaction networks enable us to suggest many potential drug-target interactions and to increase research productivity toward genomic drug discovery.

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EDUCATIONS/TRAINING

2005	Kyoto University Graduate School of Science, Japan, PhD.

POSITIONS AND HONORS

2005-2006	Postdoctral Fellow, Center for Computational Biology, École Nationale Supérieure des Mines de Paris, France
2006-2007	Assistant Professor, Institute for Chemical Research, Kyoto University, Japan
2008-2012	Permanent Researcher, Center for Computational Biology, Mines ParisTech, France
2008-2012	Permanent Researcher, Unit of Bioinformatics, Biostatistics, Epidemiology and Computational Systems Biology of Cancer, Curie Institute, France
2012 - Present	Associate Professor, Institute for Advanced Study, Kyushu University, Japan
2012 - Present	Associate Professor, Medical Institute of Bioregulation, Kyushu University, Japan
2003	The ICR Award (ICR: Institute for Chemical Research, Kyoto University)

RECENT PUBLICATIONS

1. Yamanishi Y, Pauwels E and Kotera M. Drug side-effect prediction based on the integration of chemical and biological spaces. ***Journal of Chemical Information and Modeling*** 52: 3284-3292, 2012.
2. Takarabe M, Kotera M, Nishimura Y, Goto S and Yamanishi Y. Drug target prediction using adverse event report systems: a pharmacogenomic approach ***Bioinformatics*** 28: i611-i618, 2012.
3. Mizutani S, Pauwels E, Stoven V, Goto S and Yamanishi Y. Relating drug-protein interaction network with drug side-effects ***Bioinformatics*** 28: i522-i528, 2012.
4. Tabei Y, Pauwels E, Stoven V, Takemoto K and Yamanishi Y. Identification of chemogenomic features from drug-target interaction networks using interpretable classifiers. ***Bioinformatics*** 28: i487-i494, 2012.
5. Kotera M, Yamanishi Y, Moriya Y, Kanehisa M and Goto S. GENIES: gene network inference engine based on supervised analysis ***Nucleic Acids Research*** 40: W162-W167, 2012.
6. Yamanishi Y, Pauwels E, Saigo H and Stoven V. Extracting sets of chemical substructures and protein domains governing drug-target interactions ***Journal of Chemical Information and Modeling***, 51: 1183-1194, 2011.
7. Yamanishi Y, Kotera M, Kanehisa M and Goto S. Drug-target interaction prediction from chemical, genomic and pharmacological data in an integrated framework ***Bioinformatics*** 26: i246-i254, 2010.
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9. Yamanishi Y, Araki M, Gutteridge A, Honda W and Kanehisa M. Prediction of drug-target interaction networks from the integration of chemical and genomic spaces ***Bioinformatics*** 24: i232-i240, 2008.