

# Dr. Clemens Wrzodek



## Background

- 03/2009-06/2013 Research assistant and PhD student in computer science at the Center for Bioinformatics (ZBIT), University of Tübingen
- 1999-2011 Software development as freelancer. References include Smart Software Development Ltd. London, Deutsche Managementgesellschaft für Gesundheit (DMGG), da Vinci Diabetes Care GmbH, Professor Dr. Baum GmbH
- 2009 Diploma in computer science. Thesis: Modelling of transcriptional networks by integrating expression data and promoter analysis
- 2008 Internship as patent attorney at Stolz & Partner, Munich
- 10/2007-02/2009 Continued studies of computer science at the University of Tübingen.
- 07/2006-07/2007 Studies of computer sciences at the San Diego State University, CA, USA
- 10/2003-07/2006 Studies of computer science (bioinformatics) at the University of Tübingen
- Until 10/2003 Gymnasium (high school) Waldschule Degerloch in Stuttgart

## Research Interests

My main research focuses on developing novel algorithms and software tools that break fresh ground and improve today's capabilities in analyzing complex datasets. In particular:

- Data mining algorithms (clustering methods, evolutionary algorithms and linear regression). Applied, e.g., for the analysis and detection of gene-regulatory relationships (ModuleMaster, SABINE)
- Novel data structures and innovative approaches for the integration of *omics* data from multiple different layers, including integrated analysis and visualization (InCroMAP)
- Machine learning and distributed computing to enhance feature identification in computational epigenetics (CpG island feature generator)
- Systems biology, especially analysis, visualization and modeling of regulatory, metabolic and signaling networks (see [JSBML](#), KEGGtranslator, BioPAX2SBML)
- Ontologies and the Semantic Web (OWL, RDF)
- Software engineering in general

## Current Projects

International projects, funded by the European Union:

- EU IMI MARCAR: towards novel biomarkers for cancer risk assessment. In cooperation with (among others) Novartis, Bayer, Boehringer Ingelheim, UCB and Lundbeck

The following projects are all funded by the Federal Ministry of Education and Research (*Bundesministerium für Bildung und Forschung*, [BMBF](#), Germany):

- Spher4Sys: a systems-biology-based approach for preclinical lead compound development using an in-vivo like spheroid test system. This project contributes to the medical systems biology network [MedSys](#).
- German National Genome Research Network (*Nationales Genomforschungsnetz*, NGFN-Plus): medical genome research with focus on Parkinson's disease.

Other projects:

- [Path2Models](#): a systems-biology project that aims at large-scale generation of quantitative and qualitative models from pathways.

## Software products

Main projects:

- InCroMAP: Integrated analysis of Cross-platform MicroArray and Pathway data.
- KEGGtranslator: Visualizing and translating the KEGG PATHWAY database
- CpG island feature generator: Generating features to distinct between methylated and unmethylated CpG islands
- ModuleMaster: A new tool to decipher transcriptional regulatory networks

Contributions:

- BioPAX2SBML: Translation of BioPAX into SBML including the Qualitative Models extension.
- [JSBML](#): A flexible Java library for working with SBML.
- SBMLsimulator: An efficient Java™ solver implementation for SBML.
- ProDGe: Investigating protein-protein interactions at the domain level.
- SBML2LaTeX: Conversion of SBML files into human-readable reports.
- SABINE: Prediction of the binding specificity of transcription factors using support vector regression.
- ZBIT Bioinformatics Toolbox: A web-based Galaxy framework for bioinformatics tools.

## Awards and honors

- 2001/2002: 1<sup>st</sup> price in the first round, 1<sup>st</sup> price in the second round and reaching the finals of the 20<sup>th</sup> German Federal Competition for Informatics (20. BWINF) as one of 2.5% of all participants.
- 2002/2003: 1<sup>st</sup> price in the first round and 1<sup>st</sup> price in the second round of the 21<sup>st</sup> German Federal Competition for Informatics (21. BWINF).
- 2008: Diploma thesis was awarded the [EVE Award for Evolutionary Biology](#) ("EvE-Förderpreis für Evolutionsbiologie") of the Volkswagen Foundation.

## Publications

- [1] Michael Römer, Johannes Eichner, Andreas Dräger, Clemens Wrzodek, Finja Wrzodek, and Andreas Zell. ZBIT Bioinformatics Toolbox: a Web-Platform for Systems Biology and Expression Data Analysis. *PLoS ONE*, 11(2):e0149263, February 2016. [ [DOI](#) | [link](#) ]
- [2] Nicolas Rodriguez, Alex Thomas, Leandro Watanabe, Ibrahim Y. Vazirabad, Victor Kofia, Harold F. Gómez, Florian Mittag, Jakob Matthes, Jan D. Rudolph, Finja Wrzodek, Eugen Netz, Alexander Diamantikos, Johannes Eichner, Roland Keller, Clemens Wrzodek, Sebastian Fröhlich, Nathan E. Lewis, Chris J. Myers, Nicolas Le Novère, Bernhard Ø. Palsson, Michael Hucka, and Andreas Dräger. JSBML 1.0: providing a smorgasbord of options to encode systems biology models. *Bioinformatics*, June 2015. [ [DOI](#) | [arXiv](#) | [link](#) | [pdf](#) ]
- [3] Johannes Eichner, Lars Rosenbaum, Clemens Wrzodek, Hans-Ulrich Häring, Andreas Zell, and Rainer Lehmann. Integrated enrichment analysis and pathway-centered visualization of metabolomics, proteomics, transcriptomics, and genomics data by using the InCroMAP software. *Journal of Chromatography B*, May 2014. [ [DOI](#) | [link](#) ]
- [4] Johannes Eichner, Clemens Wrzodek, Michael Römer, Heidrun Ellinger-Ziegelbauer, and Andreas Zell. Evaluation of toxicogenomics approaches for assessing the risk of nongenotoxic carcinogenicity in rat liver. *PLoS ONE*, 9(5):e97678, May 2014. [ [DOI](#) | [link](#) ]

- [5] Elif B. Unterberger, Johannes Eichner, Clemens Wrzodek, Harri Lempiäinen, Raphaëlle Luisier, Rémi Terranova, Ute Metzger, Simon Plummer, Thomas Knorpp, Albert Braeuning, Jonathan Moggs, Markus Templin, Valerie Honndorf, Martial Piotto, Andreas Zell, and Michael Schwarz. Metabolic Programs Orchestrated by the Activated Ha-ras and  $\beta$ -Catenin Oncoproteins in Mouse Liver Tumors. *International Journal of Cancer*, March 2014. [ [DOI](#) | [link](#) ]
- [6] Johannes Eichner, Florian Topf, Andreas Dräger, Clemens Wrzodek, Dierk Wanke, and Andreas Zell. TFpredict and SABINE: Sequence-Based Prediction of Structural and Functional Characteristics of Transcription Factors. *PLoS ONE*, 8(12):e82238, December 2013. [ [DOI](#) | [link](#) | [link](#) ]
- [7] Finja Büchel, Nicolas Rodriguez, Neil Swainston, Clemens Wrzodek, Tobias Czauderna, Roland Keller, Florian Mittag, Michael Schubert, Mihai Glont, Martin Golebiewski, Martijn van Iersel, Sarah M. Keating, Matthias Rall, Michael Wybrow, Henning Hermjakob, Michael Hucka, Douglas B Kell, Wolfgang Müller, Pedro Mendes, Andreas Zell, Claudine Chaouiya, Julio Saez-Rodriguez, Falk Schreiber, Camille Laibe, Andreas Dräger, and Nicolas Le Novère. Path2Models: large-scale generation of computational models from biochemical pathway maps. *BMC Systems Biology*, 7(1):116, November 2013. [ [DOI](#) | [link](#) | [pdf](#) ]
- [8] Finja Büchel, Sandra Saliger, Andreas Dräger, Stephanie Hoffmann, Clemens Wrzodek, Andreas Zell, and Philipp J. Kahle. Parkinson's disease: dopaminergic nerve cell model is consistent with experimental finding of increased extracellular transport of  $\alpha$ -synuclein. *BMC Neuroscience*, 14(136), November 2013. [ [DOI](#) | [link](#) | [pdf](#) ]
- [9] Finja Büchel, Florian Mittag, Clemens Wrzodek, Andreas Zell, Thomas Gasser, and Manu Sharma. Integrative pathway-based approach for genome-wide association studies: identification of new pathways for rheumatoid arthritis and type 1 diabetes. *PLoS ONE*, 8(10), September 2013. [ [DOI](#) | [link](#) ]
- [10] Johannes Eichner, Nadine Kossler, Clemens Wrzodek, Arno Kalkuhl, Dorthe Bach Toft, Nina Ostefeldt, Virgile Richard, and Andreas Zell. A Toxicogenomic Approach for the Prediction of Murine Hepatocarcinogenesis Using Ensemble Feature Selection. *PLoS ONE*, 8(9):e73938, September 2013. [ [DOI](#) | [link](#) ]
- [11] Clemens Wrzodek, Finja Büchel, Manuel Ruff, Andreas Dräger, and Andreas Zell. Precise generation of systems biology models from KEGG pathways. *BMC Systems Biology*, 7(1):15, January 2013. [ [DOI](#) | [link](#) | [pdf](#) ]
- [12] Clemens Wrzodek, Johannes Eichner, Finja Büchel, and Andreas Zell. InCroMAP: Integrated analysis of Cross-platform MicroArray and Pathway data. *Bioinformatics*, 29(4):506–508, December 2012. [ [DOI](#) | [arXiv](#) | [link](#) | [pdf](#) ]
- [13] Harri Lempiäinen, Philippe Couttet, Federico Bolognani, Arne Müller, Valérie Dubost, Raphaëlle Luisier, Espinola Alberto Del Rio, Veronique Vitry, Elif B Unterberger, John P Thomson, Fridolin Treindl, Ute Metzger, Clemens Wrzodek, Florian Hahne, Tulipan Zollinger, Sarah Brasa, Magdalena Kalteis, Magali Marcellin, Fanny Giudicelli, Albert Braeuning, Laurent Morawiec, Natasa Zamurovic, Ulrich Längle, Nico Scheer, Dirk Schübeler, Jay Goodman, Salah-Dine Chibout, Jennifer Marlowe, Diethilde Theil, David J Heard, Olivier Grenet, Andreas Zell, Markus F Templin, Richard R Meehan, C. Roland Wolf, Clifford R Elcombe, Michael Schwarz, Pierre Moulin, Rémi Terranova, and Jonathan G Moggs. Identification of *Dlk1-Dio3* imprinted gene cluster non-coding RNAs as novel candidate biomarkers for liver tumor promotion. *Toxicological Sciences*, 131(2):375–386, October 2012. [ [DOI](#) | [arXiv](#) | [link](#) | [pdf](#) ]
- [14] Clemens Wrzodek, Johannes Eichner, and Andreas Zell. Pathway-based visualization of cross-platform microarray datasets. *Bioinformatics*, 28(23):3021–3026, September 2012. [ [DOI](#) | [arXiv](#) | [link](#) | [pdf](#) ]
- [15] Finja Büchel, Clemens Wrzodek, Florian Mittag, Andreas Dräger, Johannes Eichner, Nicolas Rodriguez, Nicolas Le Novère, and Andreas Zell. Qualitative translation of relations from BioPAX to SBML qual. *Bioinformatics*, 28(20):2648–2653, August 2012. [ [DOI](#) | [link](#) | [pdf](#) ]
- [16] Clemens Wrzodek, Finja Büchel, Georg Hinselmann, Johannes Eichner, Florian Mittag, and Andreas Zell. Linking the epigenome to the genome: Correlation of different features to DNA methylation of CpG islands. *PLoS ONE*, 7(4):e35327, 04 2012. [ [DOI](#) | [link](#) ]
- [17] Finja Büchel, Clemens Wrzodek, Florian Mittag, Andreas Dräger, Adrian Schröder, and Andreas Zell. ProDGe: investigating protein-protein interactions at the domain level.

- Technical report, Nature Precedings, August 2011. [ [DOI](#) | [link](#) | [pdf](#) ]
- [18] Adrian Schröder, Johannes Wollnik, Clemens Wrzodek, Andreas Dräger, Michael Bonin, Oliver Burk, Maria Thomas, Wolfgang E. Thasler, Ulrich M. Zanger, and Andreas Zell. Inferring statin-induced gene regulatory relationships in primary human hepatocytes. *Bioinformatics*, 27(18):2473--2477, July 2011. [ [DOI](#) | [link](#) | [pdf](#) ]
- [19] Andreas Dräger, Nicolas Rodriguez, Marine Dumousseau, Alexander Dörr, Clemens Wrzodek, Nicolas Le Novère, Andreas Zell, and Michael Hucka. JSBML: a flexible Java library for working with SBML. *Bioinformatics*, 27(15):2167--2168, June 2011. [ [DOI](#) | [link](#) | [pdf](#) ]
- [20] Adrian Schröder, Clemens Wrzodek, Johannes Wollnik, Andreas Dräger, Dierk Wanke, Kenneth W. Berendzen, and Andreas Zell. Inferring transcriptional regulators for sets of co-expressed genes by multi-objective evolutionary optimization. In *IEEE Congress on Evolutionary Computation (CEC 2011)*, New Orleans, USA, June 2011. IEEE. [ [DOI](#) | [link](#) ]
- [21] Clemens Wrzodek, Andreas Dräger, and Andreas Zell. KEGGtranslator: visualizing and converting the KEGG PATHWAY database to various formats. *Bioinformatics*, 27(16):2314--2315, June 2011. [ [DOI](#) | [link](#) ]
- [22] Clemens Wrzodek, Adrian Schröder, Andreas Dräger, Dierk Wanke, Kenneth W. Berendzen, Marcel Kronfeld, Klaus Harter, and Andreas Zell. ModuleMaster: A new tool to decipher transcriptional regulatory networks. *Biosystems*, 99(1):79--81, January 2010. [ [DOI](#) | [link](#) ]
- [23] Simon Rieche, Klaus Wehrle, Leo Petrak, and Clemens Wrzodek. Cerco: Supporting range queries with a hierarchically structured peer-to-peer system. In *Proceedings of 31st IEEE Conference on Local Computer Networks (LCN 2006)*, Tampa, Florida, USA, November 2006. [ [link](#) ]

## Theses

- [1] Clemens Wrzodek. *Inference and integration of biochemical networks with multilayered omics data*. PhD thesis, University of Tuebingen, Tübingen, Germany, June 2013. [ [link](#) ]
- [2] Clemens Wrzodek. Modeling transcriptional regulatory networks by integrating expression data and promoter analysis. Diplomarbeit, University of Tuebingen, November 2008.
- [3] Clemens Wrzodek. Range queries in hierarchically structured peer-to-peer systems. Studienarbeit, University of Tuebingen, 2006.

## Selected Posters

- Clemens Wrzodek, Johannes Eichner and Andreas Zell. Bioinformatics tools and research. *Presented at the MARCAR consortium meeting, Dundee, 2011.*
- Clemens Wrzodek, Andreas Dräger and Andreas Zell. KEGGtranslator: visualizing and converting the KEGG PATHWAY database to various formats. *Presented at the national genome research net (NGFN) meeting 2011.*
- Andreas Dräger, Nicolas Rodriguez, Marine Dumousseau, Alexander Dörr, Clemens Wrzodek, Roland Keller, Sebastian Fröhlich, Nicolas Le Novère, Andreas Zell and Michael Hucka JSBML: a flexible and entirely Java-based library for working with SBML. Presented at *Computational Modeling in BIology Network (COMBINE) 2011*, and at the *12th International Conference on Systems Biology (ICSB) 2011* in Heidelberg. [ [details](#) | [pdf](#) ]
- Nicolas Rodriguez, Marine Dumousseau, Andreas Dräger, Clemens Wrzodek, Alexander Dörr, Sarah M. Keating, Akiya Jouraku, Nicolas Le Novère, Andreas Zell and Michael Hucka JSBML: a flexible and entirely Java-based library for working with SBML. *Presented at the International Conference on Systems Biology (ICSB) 2010*. [ [details](#) | [pdf](#) ]
- Clemens Wrzodek, Adrian Schröder, Andreas Dräger, Dierk Wanke, Kenneth Berendzen, Marcel Kronfeld, Klaus Harter and Andreas Zell. ModuleMaster: deciphering transcriptional regulatory networks. *Presented at the national genome research net (NGFN) meeting 2009 and the meeting of Students in Evolution and Ecology (StEvE) 2009.*

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