

Dr. Georg Hinselmann



Background

- 10/2006 - 03/2011: Research assistant, Cognitive Systems, University of Tübingen
- 08/2009 - 10/2009: Internship, EMBL-EBI (group of Dr. Christoph Steinbeck), Cambridge
- 10/2000 - 09/2006: Studies of Computer Science (Bioinformatics), University of Tübingen
- 09/2000 - 06/2002: Working student, Festo AG & Co. KG, Esslingen am Neckar
- 11/1999 - 08/2000: Military service, German mountain troopers, Kempten
- 06/1999: High school diploma (Abitur), Schelztor-Gymnasium, Esslingen am Neckar

Publications

- [1] 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](#)]
- [2] Georg Hinselmann, Andreas Jahn, Nikolas Fechner, Lars Rosenbaum, and Andreas Zell. Approximation of graph kernel similarities for chemical graphs by kernel principal component analysis. In Clara Pizzuti, Marylyn D. Ritchie, and Mario Giacobini, editors, *Evolutionary Computation, Machine Learning and Data Mining in Bioinformatics*, volume 6623 of *Lecture Notes in Computer Science*, pages 123--134. Springer Berlin Heidelberg, 2011.
- [3] Georg Hinselmann, Andreas Jahn, Lars Rosenbaum, and Andreas Zell. Fast data mining with sparse chemical graph fingerprints by estimating the probability of unique patterns. In Michel Verleysen, editor, *Proceedings of 19th European Symposium on Artificial Neural Networks (ESANN 2011)*, pages 417--422, Bruges, Belgium, 2011.
- [4] Georg Hinselmann, Lars Rosenbaum, Andreas Jahn, Nikolas Fechner, Claude Ostermann, and Andreas Zell. Large-scale learning of structure-activity relationships using a linear support vector machine and problem-specific metrics. *Journal of Chemical Information and Modeling*, 52:203--213, 2011.
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- [6] Andreas Jahn, Georg Hinselmann, Lars Rosenbaum, Nikolas Fechner, and Andreas Zell. Boltzmann-enhanced flexible atom-pair kernel with dynamic dimension reduction. *Molecular Informatics*, 30(4):307--315, 2011.
- [7] Andreas Jahn, Lars Rosenbaum, Georg Hinselmann, and Andreas Zell. 4D Flexible Atom-Pairs: An efficient probabilistic conformational space comparison for ligand-based virtual screening. *Journal of Cheminformatics*, 3(23), 2011.
- [8] Lars Rosenbaum, Georg Hinselmann, Andreas Jahn, and Andreas Zell. Interpreting linear support vector machine models with heat map atom and bond coloring. *Journal of Cheminformatics*, 3:11, 2011.
- [9] Verena Schattel, Georg Hinselmann, Andreas Jahn, Andreas Zell, and Stefan Laufer. A modeling and benchmark data set for the inhibition of c-jun n-terminal kinase-3. *Journal of Chemical Information and Modeling*, 51:670--679, 2011.
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- [11] Nikolas Fechner, Georg Hinselmann, Andreas Jahn, Lars Rosenbaum, and Andreas Zell. A Free-Wilson-like approach to analyze QSAR models based on graph decomposition kernels. *Molecular Informatics*, 29:491--497, 2010. [[DOI](#) | [link](#)]
- [12] Nikolas Fechner, Georg Hinselmann, and Jörg Kurt Wegner. *Handbook of Chemoinformatics Algorithms*, chapter Molecular Descriptors, pages 89--143. Chapman &

Hall/CRC Mathematical & Computational Biology, 2010.

- [13] Nikolas Fechner, Andreas Jahn, Georg Hinselmann, and Andreas Zell. Estimation of the applicability domain of kernel-based machine learning models for virtual screening. *Journal of Cheminformatics*, 2(1):2, 2010. [[DOI](#) | [link](#)]
- [14] Georg Hinselmann, Nikolas Fechner, Andreas Jahn, Matthias Eckert, and Andreas Zell. Graph kernels for chemical compounds using topological and three-dimensional local atom pair environments. *Neurocomputing*, 74(1-3):219--229, 2010. [[DOI](#) | [link](#)]
- [15] Andreas Jahn, Georg Hinselmann, Nikolas Fechner, and Andreas Zell. Optimal assignment methods for ligand-based virtual screening. *Journal of Cheminformatics*, 1(14), August 2009. [[DOI](#) | [link](#) | [pdf](#)]
- [16] Georg Hinselmann, Andreas Jahn, Nikolas Fechner, and Andreas Zell. Chronic rat toxicity prediction of chemical compounds using kernel machines. In *Evolutionary Computation, Machine Learning and Data Mining in Bioinformatics: 7th European Conference (EvoBio 2009)*, volume 5483, pages 25--36, Tübingen, Germany, April 2009. Springer. [[link](#)]
- [17] Nikolas Fechner, Andreas Jahn, Georg Hinselmann, and Andreas Zell. Atomic local neighborhood flexibility incorporation into a structured similarity measure for qsar. *Journal of Chemical Information and Modeling*, 49(3):549--560, March 2009.
- [18] Carsten Henneges, Georg Hinselmann, S Jung, J Madlung, W Schütz, A Nordheim, and Andreas Zell. Ranking methods for the prediction of frequent top scoring peptides from proteomics data. *Journal of Proteomics & Bioinformatics*, 2(5):226--235, 2009. [[link](#)]