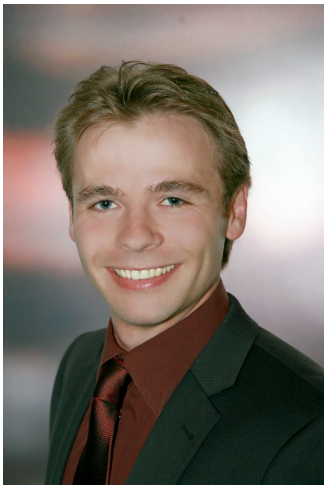
Dr. Andreas Jahn



Background

- 11/2008: FIZ CHEMIE Berlin-Preis 2008 for the best diploma thesis.
- since 04/2008: Research assistant at the Center of Bioinformatics (ZBIT), University of Tübingen
- 04/2006 - 03/2008: Student assistant at the Department of Computer Architecture
- Oct. 2002 - Mar. 2008: Studies of Computer Science (Bioinformatics) at the University of Tübingen
- 09/2001 - 05/2000: Military service, German mountain troopers, Kempten
- 06/2001: Abitur at the Gymnasium am Rosenberg, Oberndorf a.N.

Research Interests

- Software Engineering
- Data Mining
- Machine Learning
- Ligand-based Virtual Screening

Current Projects

- Optimal Assignment Kernels (OAK) for chemical compounds
- Conformational space encoding for virtual screening and machine learning (4D FAP)
- Molecular flexibility encoding for virtual screening and machine learning
- Graph kernel approximations for linear support vector machines

Awards

- FIZ CHEMIE Berlin-Preis 2008

Publications

4D Flexible Atom-Pairs: An efficient probabilistic conformational space comparison for ligand-based virtual screening
Andreas Jahn, Lars Rosenbaum, Georg Hinselmann, and Andreas Zell
Journal of Cheminformatics, **2011**, 3:23

Boltzmann-enhanced Flexible Atom-Pair Kernel with Dynamic Dimension Reduction
Andreas Jahn, Georg Hinselmann, Lars Rosenbaum, Nikolas Fechner, and Andreas Zell
Molecular Informatics, **2011**, 30 (4), pp 307-315

Efficient machine learning on molecular graphs by estimating the probability of unique patterns
Georg Hinselmann, Andreas Jahn, Lars Rosenbaum, and Andreas Zell
In *Proceedings of 11th European Symposium on Artificial Neural Networks (ESANN 2011)*, Bruges, Belgium, **2011**, accepted for publication

Approximation of graph kernel similarities for chemical graphs by kernel principal component analysis
Georg Hinselmann, Andreas Jahn, Lars Rosenbaum, Nikolas Fechner, and Andreas Zell
In *Evolutionary Computation, Machine Learning and Data Mining in Bioinformatics: 9th European Conference (EvoBio 2011)*, Springer, **2011**, accepted for publication

Interpreting linear support vector machine models with heat map atom and bond coloring
Lars Rosenbaum, Georg Hinselmann, Andreas Jahn, and Andreas Zell
Journal of Cheminformatics, **2011**, 3:11

jcompoundmapper: An open source java library and command-line tool for chemical fingerprints
Georg Hinselmann, Lars Rosenbaum, Andreas Jahn, Nikolas Fechner, and Andreas Zell
Journal of Cheminformatics, **2011**, 3:3

A modeling and benchmark data set for the inhibition of c-jun n-terminal kinase-3
Verena Schattel, Georg Hinselmann, Andreas Jahn, Andreas Zell, and Stefan Laufer
Journal of Chemical Information and Modeling, **2011**, accepted for publication

Large-scale learning of structure-activity relationships using a linear support vector machine and problem-specific metrics
Georg Hinselmann, Lars Rosenbaum, Andreas Jahn, Nikolas Fechner, Claude Ostermann, and Andreas Zell
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A Free-Wilson-like approach to analyze QSAR models based on graph decomposition kernels
Nikolas Fechner, Georg Hinselmann, Andreas Jahn, Lars Rosenbaum, and Andreas Zell
Molecular Informatics, **2010**, 29 (6-7), pp 491-497
Abstract, DOI: 10.1002/minf201000053

Probabilistic Modeling of Conformational Space for 3D Machine Learning Approaches
Andreas Jahn, Georg Hinselmann, Nikolas Fechner, Carsten Henneges, and Andreas Zell
Molecular Informatics, **2010**, 29 (5), pp 441-455
Abstract, DOI: 10.1002/minf201000036

Graph Kernels for Chemical Compounds Using Topological and Three-Dimensional Local Atom Pair Environments
Georg Hinselmann, Nikolas Fechner, Andreas Jahn, and Andreas Zell
Elsevier Neurocomputing, **2010**, *74, pp 219-229*
DOI: 10.1016/j.neucom.2010.03.008

Estimation of the applicability doman of kernel-based machine learning models for virtual screening
Nikolas Fechner, Andreas Jahn, Georg Hinselmann, and Andreas Zell
Journal of Cheminformatics, **2010**, 2:2
Abstract, PDF, DOI: 10.1186/1758-2946-2-2

Optimal assignment methods for ligand-based virtual screening
Andreas Jahn, Georg Hinselmann, Nikolas Fechner, and Andreas Zell
Journal of Cheminformatics, **2009**, 1:14
Abstract, PDF, DOI: 10.1186/1758-2946-1-14

Incorporating molecular flexibility into three-dimensional structural kernels
Andreas Jahn
Chemistry Central Journal, **2009**, *3(Suppl 1)*:O11.
Abstract, DOI: 10.1186/1752-153X-3-S1-O11

Two-step hierarchical assignments on molecular graphs
Andreas Jahn, Nikolas Fechner, Georg Hinselmann, and Andreas Zell
Chemistry Central Journal, **2009**, *3(Suppl 1)*:P13.
Abstract, DOI: 10.1186/1752-153X-3-S1-P13

Assessing the selectivity of serine proteases inhibitors using structural similarity
Nikolas Fechner, Andreas Jahn, Georg Hinselmann, and Andreas Zell
Chemistry Central Journal, **2009**, *3(Suppl 1)*:P10.
Abstract, DOI: 10.1186/1752-153X-3-S1-P10

An extension of the pharmacophore kernel using radial atomtype fingerprints 

Georg Hinselmann, Matthias Eckert, Thomas Holder, Andreas Jahn, Nikolas Fechner, and Andreas Zell
Chemistry Central Journal, **2009**, *3(Suppl 1)*:P11.
Abstract, DOI: 10.1186/1752-153X-3-S1-P11

Atomic local neighborhood flexibility incorporation into a structured similarity measure for QSAR

Nikolas Fechner, Andreas Jahn, Georg Hinselmann, and Andreas Zell
in *Journal of Chemical Information and Modeling*, **2009**, 49 (3), pp 549-560
DOI: 10.1021/ci800329r

Chronic Rat Toxicity Prediction of Chemical Compounds using Kernel Machines

Georg Hinselmann, Andreas Jahn, Nikolas Fechner, and Andreas Zell
in *Lecture Notes in Computer Science (EvoBIO 2009)*, **2009**, 5483, 25-36

Beyond descriptor vectors: QSAR modelling using structural similarity 

Andreas Zell, Georg Hinselmann, Nikolas Fechner, and Andreas Jahn
Chemistry Central Journal, **2008**, *2(Suppl 1)*:S3.
Abstract, DOI: 10.1186/1752-153X-2-S1-S3

Presentations

Incorporating Molecular Flexibility into three-dimensional Structural Kernels

Jahn, A.; Fechner, N. H.; Hinselmann, G. and Zell, A.
4. German Conference on Chemoinformatics, 09.-11. November 2008, Goslar [pdf]

Beyond Descriptor Vectors: QSAR Modelling with structural similarity measures

Hinselmann, G.; Fechner, N. H.; Jahn, A. and Zell, A.
3. German Conference on Chemoinformatics, 11-13. November 2007, Goslar [pdf, ~14MB including a demo movie]

Poster

Two-Step Hierarchical Assignments on Molecular Graphs

A. Jahn, N. Fechner, G. Hinselmann, A. Zell
presented on the German Conference on Chemoinformatics 2008

Assessing the Selectivity of Serine Proteases Inhibitors using Structural Similarity

N. Fechner, A. Jahn, G. Hinselmann, A. Zell
presented on the German Conference on Chemoinformatics 2008

Extending Pharmacophore Kernels with Radial Fingerprint Environments

G. Hinselmann, M. Eckert, T. Holder, A. Jahn, N. Fechner, A. Zell
presented on the German Conference on Chemoinformatics 2008

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