Dr. Jörg Kurt Wegner

Background

- Full Curriculum Vitae (at Wikipedia): german, english
- 10/1995 - 07/2000 Studies of Chemistry at Eberhard-Karls-University Tübingen
- 10/1997 - 01/1998 Practical seminar for "*applied rhetoric - a scientific lecture*" from Prof. G. Ueding and K. Steinke
- 06/1998 - 09/1998 Internship at the CIB (Computereinsatz und Informatik in der Biomedizin) GmbH, Berlin-Buch
- 04/1999 - 09/1999 Minor field of study:
  algorithms (sorting- and search algorithms, graphs, trees and text search algorithms), neuronal networks,
  evolutionary algorithms (genetic algorithms, evolutionary strategies, genetic programming)
- 29/11/1999 - 03/12/1999 Seminar "*sequence-, structure-, function-analysis. Working fields of applied bioinformatics*"
- 08/2000 - 02/2001 Master thesis (Diplomarbeit) at the Computer Chemistry Center (Prof. J. Gasteiger, Erlangen) and Institute of Physical Chemistry (Prof. Gauglitz, Tübingen) "*Investigations of the automated comparison of infrared spectra in consideration of band shapes and band shifts*"

- Since 03/2001 Research assistant at the Department of Computer Architecture of Tübingen University
- Estimated PhD thesis end: October 2005

Research Interests

- Cheminformatics (JOELib@SourceForge, JOELib@Freshmeat)
- Data/Graph Mining (Regression, Classification, Clustering), Information Theory, Optimization
- Algorithms: Maximum Common Substructure Search (MCS), Feature Selection/Feature Extraction
- Virtual Screening, Library Design

Current Projects

- direct cooperation with ALTANA Pharma AG, Konstanz, Germany

Terminated Projects

- SOL: Search and Optimization of Lead Structures

Journal Publications

Data and Graph Mining in Chemical Space for ADME and Activity Data Sets
J. K. Wegner, H. Fröhlich, H. Mielenz A. Zell
QSAR Comb. Sci., **2005**, *accepted*.

Kernel Functions for Attributed Molecular Graphs -A New Similarity Based Approach To ADME Prediction in Classification and Regression
H. Fröhlich, J. K. Wegner, F. Sieker, A. Zell
QSAR Comb. Sci., **2005**, *accepted*.

Towards Optimal Descriptor Subset Selection with Support Vector Machines in Classification and Regression
H. Fröhlich, J. K. Wegner, A. Zell
QSAR Comb. Sci., **2004**, *23*, 311-318.
DOI: 10.1002/qsar.200410011

Feature selection for Descriptor based Classification Models: Part I – Theory and GA-SEC Algorithm
J. K. Wegner, H. Fröhlich, A. Zell
Journal of Chemical Information and Computer Science (JCICS), **2004**, *44*, 921-930.
DOI: 10.1021/ci0342324

Feature selection for Descriptor based Classification Models: Part II – Human Intestinal Absorption (HIA)
J. K. Wegner, H. Fröhlich, A. Zell
Journal of Chemical Information and Computer Science (JCICS), **2004**, *44*, 931-939.
DOI: 10.1021/ci034233w

Prediction of Aqueous Solubility and Partition Coefficient Optimized by a Genetic Algorithm Based Descriptor Selection Method
J. K. Wegner, A. Zell
Journal of Chemical Information and Computer Science (JCICS), **2003**, *43*(3), 1077-1084.
DOI: 10.1021/ci034006u

The Compressed Feature Matrix - A fast method for feature based substructure search
S.F.Badreddin Abolmaali, Jörg K. Wegner, Andreas Zell
Journal of Molecular Modeling, **2003**, *9*(4), 235-241.
DOI: 10.1007/s00894-003-0126-0

Presentations/Publications on Conferences and Workshops

Optimal Assignment Kernels For Attributed Molecular Graphs
H. Fröhlich, J. K. Wegner, F. Sieker, A. Zell
The 22nd International Conference on Machine Learning (ICML 2005), Bonn, Germany, 7-11 August, **2005**.
Full scientific program

Assignment Kernels For Chemical Compounds
H. Fröhlich, J. K. Wegner, A. Zell
International Joint Conference on Neural Networks (IJCNN), in Montréal, Québec, Canada, July 31-August 4, **2005**.
Full scientific program

Comparing Vector Versus Structural Coding for Predicting ADMETox Data Sets
J. K. Wegner, H. Fröhlich, A. Zell
The 7th International Conference on Chemical Structures, in Noordwijkerhout, The Netherlands, CA, June 5–9, **2005**. Session: Structure-Activity and Structure-Property Prediction (Chair: Markus Wagener). Organisations: CINF, CSA Trust, CSJ, GDCh, KNCV, RSC, and SCS
Full scientific program

Difference in vector-based and graph-based coding for ADME prediction.
J. K. Wegner, A. Zell
The 229th ACS National Meeting, in San Diego, CA, March 13-17, **2005**. Session: ADME/tox Informatics (Chair: O. F. Güner). Organisation: American Chemical Society (ACS)-Division of Computers in Chemistry
Abstract, Session program, Full 'Division of Chemical Information' (CINF) scientific program, Full scientific program

Relevance of feature selection for clustering molecules.
J. K. Wegner, F. Sieker, A. Zell
The 229th ACS National Meeting, in San Diego, CA, March 13-17, **2005**. Session: Applications of Information Theory in Chemistry (Chair: V. Shanmugasundaram and G. M Maggiora). Organisation: American Chemical Society (ACS)-Division of Computers in Chemistry
Abstract, Session program, Full 'Division of Chemical Information' (CINF) scientific program, Full scientific program

JOELib - An open source chemoinformatics library for data mining and graph mining on molecular structures.

J. K. Wegner
invited presentation at eCheminfo **2004**, 8-19 November, Applications of Cheminformatics and Modelling to Drug Discovery. Session: Open Source (Chair: G. Morris). Organisation: Douglas Connect
Abstract, Full scientific program (HTML, PDF)

Data Mining and Generalisation Ability on Molecular Structures.

J. K. Wegner, H. Mielenz
CIC Workshop **2004** - Neue Entwicklungen in der Chemoinformatik, 14.-16. November, Germany . Session: Pharmazeutische Chemoinformatik (Chair: G. Schneider). Organisation: Gesellschaft Deutscher Chemiker (GDCh)
Full scientific program (HTML, PDF)

Data preparation and feature selection for chemical data sets - Building 'general' models.

J. K. Wegner
invited presentation at Analytica Conference **2004**, 11.-13. May, Munich, Germany.
Session: Molecular Informatics for a Deeper Insight (Chair: C. Steinbeck). Organisation:

- Gesellschaft Deutscher Chemiker (GDCh)
- Gesellschaft für Biochemie und Molekularbiologie (GBM)
- Deutsche Vereinte Gesellschaft für Klinische Chemie und Laboratoriumsmedizin (DGKL)

Full scientific program

Poster Publications

Relevance of feature selection for clustering

Jörg K. Wegner, Holger Fröhlich, Florian Sieker, Andreas Zell
International Workshop New Approaches in Drug Design & Discovery, Marburg, Germany, March 21-24, **2005**.
Poster

Building QSAR models using shannon entropy and a genetic algorithm

Jörg K. Wegner, Andreas Zell
17. Molecular-Modelling Workshop, Erlangen, Germany, May 27-28, **2003**.
Poster

JOELib-Eine plattformunabhängige computational chemistry-Bibliothek in Java

Jörg K. Wegner, Andreas Zell
16. Molecular-Modelling Workshop, Erlangen, Germany, May 07-08, **2002**.
Poster

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