Dr. Nikolas Fechner

Background

- Oct. 2000 - Jun. 2006: Studies of Computer Science (Bioinformatics) at the University of Tübingen
- since Aug. 2006 Research assistant at the Center of Bioinformatics (ZBIT), University of Tübingen
- Aug.-Oct. 2009 Internship in the Group of Dr. Christoph Steinbeck at the EBI-EMBL, Cambridge, UK

Research Interests

- Chemoinformatics
- Proteochemometrics
- Machine Learning in Chemo-/Bioinformatics
- Problem-Specific Kernel Methods

Current Projects

- JOELib2: A Java based cheminformatics (computational chemistry) library
- Optimal Assignment Kernels (OAK) for chemical compounds
- BlueDesc: A ready-to-use executable jar that calculates the molecular descriptors available in JOELib and CDK

Publications

Book Chapters

Molecular Descriptors
Nikolas Fechner, Georg Hinselmann, and Joerg K. Wegner
Handbook of Chemoinformatics Algorithms
Chapman & Hall/CRC Mathematical & Computational Biology, 2010, pp. 89-143

Journal Publications

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, 491-497
Abstract DOI: 10.1002/minf.201000053

Estimation of the applicability domain 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

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),441-455

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**, in press

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

Atomic local neighborhood flexibility incorporation into a structured similarity measure for QSAR
Nikolas Fechner, Andreas Jahn, Georg Hinselmann and Andreas Zell
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)* , Springer-Verlag Berlin Heidelberg, **2009**, 5483, 25-36
DOI: 10.1007/978-3-642-01184-9_3

Comparison of Different Approaches to Vibration-based Terrain Classification
Christian Weiss, Nikolas Fechner, Matthias Stark and Andreas Zell
Proceedings of the 3rd European Conference on Mobile Robots (ECMR 2007), Freiburg, Germany, September 19-21, **2007**, pp. 7-12

Abstracts

Assessing the selectivity of serine proteases inhibitors using structural similarity
Nikolas Fechner, Andreas Jahn, Georg Hinselmann and Andreas Zell
in *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
in *Chemistry Central Journal*, **2009**, *3(Suppl 1)*, P11.
Abstract, DOI: 10.1186/1752-153X-3-S1-P11

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

Estimating the applicability domain of kernel based QSPR models using classical descriptor vectors
Nikolas Fechner, Georg Hinselmann, Christina Schmiedl and Andreas Zell
in *Chemistry Central Journal*, **2008**, *2(Suppl 1)*, P2.
Abstract, DOI: 10.1186/1752-153X-2-S1-P2

Beyond descriptor vectors: QSAR modelling using structural similarity
Andreas Zell, Georg Hinselmann, Nikolas Fechner and Andreas Jahn
in *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
A. Jahn, N. Fechner, G. Hinselmann and Andreas Zell,
4. German Conference on Cheminformatics, 9-11. November 2008, Goslar

Altered Ligands for Heterodimers of Toll-Like Receptors 1 and 2
K.-H. Wiesmüller, S. Voss, G. Hinselmann, N. Fechner, R. Spohn and Andreas Zell,
12th Japanese-German Symposium on Peptide Science, Akabori, Japan.

Beyond Descriptor Vectors: QSAR Modelling with structural similarity measures
G. Hinselmann, N. Fechner, A. Jahn and A. Zell
3. German Conference on Cheminformatics, 11-13. November 2007, Goslar

Poster

Kernel-based Estimation of the Applicability Domain of QSAR models
N. Fechner, G. Hinselmann, A. Jahn, A. Zell

presented on the German Conference on Chemoinformatics 2009

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

Two-Step Hierarchical Assignments on Molecular Graphs
A. Jahn, N. Fechner, 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

Altered Ligands for Heterodimers of Toll-Like Receptors 1 and 2
S. Voss, D. Bächle, R. Spohn, G. Hinselmann, N. Fechner, A. Zell, A.J. Ulmer and K.-H. Wiesmüller,
presented at the IEIIS 2008, Edingburgh, Scottland

Estimating the Applicability Domain of Kernel based QSPR Models using Classical Descriptor Vectors
N. Fechner, G. Hinselmann, C. Schmiedl, A. Zell
presented on the German Conference on Chemoinformatics 2007

Structural Similarity Measures with Kernel Properties for Ligand based Virtual Screening
N. Fechner, G. Hinselmann, A. Zell
presented on the NAD Workshop 2007 at Rauischholzhausen

Implicitly Defined Substructure Fingerprints for Support Vector Machines
N. Fechner, G. Hinselmann, A. Zell
presented on the German Conference on Chemoinformatics 2006

In Silico Lead-Structure Proposal with Filters using Support Vector Machines and Implicit Defined Substructure Fingerprints
N. Fechner, G. Hinselmann, A. Zell
presented on the German Conference on Bioinformatics 2006

Address, Phone, Fax, Email

Eberhard-Karls-Universität Tübingen
Wilhelm-Schickard-Institut für Informatik
Lehrstuhl Rechnerarchitektur
Sand 1
D - 72076 Tübingen

Germany

Tel: (+49/0) 7071 / 29 77174
Fax: (+49/0) 7071 / 29 5091
Email: nikolas.fechner@uni-tuebingen.de