Interests in Chemoinformatics and Bioinformatics

- Software development of algorithmic solutions, scientific software packages and IT systems
- Model development, machine learning and computational intelligence
- Molecular modelling and simulation, molecular recognition, QSAR/QSPR
- Strategic developments
Current Research and Development Projects

**Molecular Modelling and Simulation**

- **Mesoscopic Simulation of Biomolecular Systems with Molecular Fragment Dynamics (MFD)**
  
  **Partner:** CAM-D Technologies GmbH, Essen, Germany
  Gesellschaft für naturwissenschaftliche Informatik mbH (GNWI), Oer-Erkenschwick, Germany

  **Information:**
  
  *Mesoscopic Simulation of Phospholipid Membranes, Peptides, and Proteins with Molecular Fragment Dynamics*
  A. Truszkowski, K. van den Broek, H. Kuhn, A. Zielesny and M. Epple
  (ACS Publications)

  *A molecular fragment chemoinformatics roadmap for mesoscopic simulation*
  A. Truszkowski, M. Daniel, H. Kuhn, S. Neumann, C. Steinbeck, A. Zielesny and M. Epple
  Journal of Cheminformatics (2014), 6:45
  (www.jcheminf.com/content/6/1/45)

  *Molecular simulations of peptides and proteins with Molecular Fragment Dynamics*
  A. Truszkowski, A. Fiethen, H. Kuhn, A. Zielesny and M. Epple
  Poster contribution to the „10th International Conference on Chemical Structures“ and „10th German Conference on Chemoinformatics“ from June 1 to 5, 2014, in Noordwijkerhout, The Netherlands

  *Molecular Fragment Dynamics Study of the Interaction between Zinc Ricinoleate and the Complexing Agent Methylglycinediacetic Acid as a new System for Enzyme Purification*
  K. van den Broek, A. Fiethen, A. Truszkowski, A. Zielesny and H. Kuhn
  Poster contribution to the „10th International Conference on Chemical Structures“ and „10th German Conference on Chemoinformatics“ from June 1 to 5, 2014, in Noordwijkerhout, The Netherlands

  *Extension of molecular fragment based mesoscopic simulation to the biopolymer realm*
  A. Truszkowski, A. Fiethen, H. Kuhn, A. Zielesny and M. Epple
  Poster contribution to the „28th Molecular Modeling Workshop“ from March 17 to 19, 2014, in Erlangen, Germany

- **MFD-FormulaOne** – Development of a mesoscopic simulation system for polymers, tensides, complex mixtures and biomolecular Systems with Molecular Fragment Dynamics (MFD)
  
  **Partner:** CAM-D Technologies GmbH, Essen, Germany
  Gesellschaft für naturwissenschaftliche Informatik mbH (GNWI), Oer-Erkenschwick, Germany

Software Development in Chemoinformatics and Bioinformatics
Information:

Mesoscopic Simulation of Phospholipid Membranes, Peptides, and Proteins with Molecular Fragment Dynamics
A. Truszkowski, K. van den Broek, H. Kuhn, A. Zielesny and M. Epple
(ACS Publications)

A molecular fragment cheminformatics roadmap for mesoscopic simulation
A. Truszkowski, M. Daniel, H. Kuhn, S. Neumann, C. Steinbeck, A. Zielesny and M. Epple
Journal of Cheminformatics (2014), 6:45
(www.jcheminf.com/content/6/1/45)

Molecular simulations of peptides and proteins with Molecular Fragment Dynamics
A. Truszkowski, A. Fiethen, H. Kuhn, A. Zielesny and M. Epple
Poster contribution to the „10th International Conference on Chemical Structures“ and „10th German Conference on Chemoinformatics“ from June 1 to 5, 2014, in Noordwijkerhout, The Netherlands

Molecular Fragment Dynamics Study of the Interaction between Zinc Ricinoleate and the Complexing Agent Methylglycinediacetic Acid as a new System for Enzyme Purification
K. van den Broek, A. Fiethen, A. Truszkowski, A. Zielesny and H. Kuhn
Poster contribution to the „10th International Conference on Chemical Structures“ and „10th German Conference on Chemoinformatics“ from June 1 to 5, 2014, in Noordwijkerhout, The Netherlands

Extension of molecular fragment based mesoscopic simulation to the biopolymer realm
A. Truszkowski, A. Fiethen, H. Kuhn, A. Zielesny and M. Epple
Poster contribution to the „28th Molecular Modeling Workshop“ from March 17 to 19, 2014, in Erlangen, Germany

Molecular fragment dynamics study on the water-air interface behavior of non-ionic polyoxyethylene alkyl ether surfactants
A. Truszkowski, A. Fiethen, H. Kuhn, T. Wiebringhaus, A. Zielesny and M. Epple
Poster contribution to the „9th German Conference of Chemoinformatics“ from November 10 to 12, 2013, in Fulda, Germany
Journal of Cheminformatics 2014, 6(Suppl 1):P9
(www.jcheminf.com/content/6/S1/P9)

Molecular fragment dynamics study on the water-air interface behavior of non-ionic polyoxyethylene alkyl ether surfactants
A. Truszkowski, M. Epple, A. Fiethen, A. Zielesny and H. Kuhn
Journal of Colloid and Interface Science (2013), 410, 140-145
(www.sciencedirect.com/science/article/pii/S0021979713007327)

A molecular fragment dynamics (MFD) study on the phase behavior of non-ionic surfactants
A. Truszkowski, A. Fiethen, H. Kuhn, A. Zielesny and M. Epple
Poster contribution to the „9th Zsigmondy Colloquium“ from March 6 to 8, 2013, in Essen, Germany

Molecular simulations of peptides and proteins with Molecular Fragment Dynamics (MFD)
A. Truszkowski, A. Fiethen, H. Kuhn, A. Zielesny and M. Epple
Poster contribution to the „8th German Conference of Chemoinformatics“ from November 11 to 13, 2012, in Goslar, Germany
(www.jcheminf.com/content/5/S1/P4)

Molecular fragments chemoinformatics
H. Kuhn, S. Neumann, C. Steinbeck, C. Wittekindt and A. Zielesny
Poster contribution to the „5th German Conference of Chemoinformatics“ from November 8 to 10, 2009, in Goslar, Germany
(www.jcheminf.com/content/2/S1/P14)

Machine Learning and Computational Intelligence

- **CIP – Computational Intelligence Packages** for Mathematica®: Open-source library for curve fitting, data smoothing, clustering and machine learning

Partner: Prof. Dr. Heinrich Brinck, Prof. Dr. Soeren Perrey, Westphalian University of Applied Sciences, Germany
Information: Website: www.gnwi.de

*From Curve Fitting to Machine Learning: An Illustrative Guide to Scientific Data Analysis and Computational Intelligence*
A. Zielesny
(DOI: 10.1007/978-3-642-21280-2)

Updated overview articles at website www.gnwi.de:

- Scientific Data Analysis with integrated Packages for Curve Fitting, Clustering and Machine Learning (2012)
- Document-centered Data Analysis Workflows with integrated open Mathematica Packages for Curve Fitting, Clustering and Machine Learning (2012)
Completed Research and Development Projects

**Molecular Modelling and Simulation**

- **Molecular Simulation of Peptides, Proteins and Biomembranes with Molecular Fragment Dynamics (MFD) (cooperative dissertation of Andreas Truszkowski)**

  Partner: Prof. Dr. Matthias Epple, University Duisburg-Essen, Essen, Germany  
  CAM-D Technologies GmbH, Essen, Germany  
  Gesellschaft für naturwissenschaftliche Informatik mbH (GNWI), Oer-Erkenschwick, Germany

  Completion: 2015

  Information: *Mesoscopic Simulation of Phospholipid Membranes, Peptides, and Proteins with Molecular Fragment Dynamics*
  A. Truszkowski, K. van den Broek, H. Kuhn, A. Zielesny and M. Epple  
  (ACS Publications)

  *A molecular fragment cheminformatics roadmap for mesosopic simulation*
  A. Truszkowski, M. Daniel, H. Kuhn, S. Neumann, C. Steinbeck, A. Zielesny and M. Epple  
  Journal of Cheminformatics (2014), 6:45  
  (www.jcheminf.com/content/6/1/45)

  *Molecular simulations of peptides and proteins with Molecular Fragment Dynamics*
  A. Truszkowski, A. Fiethen, H. Kuhn, A. Zielesny and M. Epple  
  Poster contribution to the „10th International Conference on Chemical Structures“ and „10th German Conference on Chemoinformatics“ from June 1 to 5, 2014, in Noordwijkerhout, The Netherlands

  *Molecular Fragment Dynamics Study of the Interaction between Zinc Ricinoleate and the Complexing Agent Methylglycinediacetic Acid as a new System for Enzyme Purification*
  K. van den Broek, A. Fiethen, A. Truszkowski, A. Zielesny and H. Kuhn  
  Poster contribution to the „10th International Conference on Chemical Structures“ and „10th German Conference on Chemoinformatics“ from June 1 to 5, 2014, in Noordwijkerhout, The Netherlands

  *Extension of molecular fragment based mesoscopic simulation to the biopolymer realm*
  A. Truszkowski, A. Fiethen, H. Kuhn, A. Zielesny and M. Epple  
  Poster contribution to the „28th Molecular Modeling Workshop“ from March 17 to 19, 2014, in Erlangen, Germany

  *Molecular simulations of peptides and proteins with Molecular Fragment Dynamics (MFD)*
  A. Truszkowski, A. Fiethen, H. Kuhn, A. Zielesny and M. Epple  
  Poster contribution to the „8th German Conference of Chemoinformatics“ from November 11 to 13, 2012, in Goslar, Germany
  (www.jcheminf.com/content/5/S1/P4)

- **Structure, stability and NMR properties of hemicucurbit[n]urils and hemicucurbit[n]uril complexes**

  Partner: Dr. Hans-Jürgen Buschmann, Deutsches Textilforschungszentrum Nord-West (DTNW), Krefeld, Germany

  Completion: 2013
Information: Geometric, electronic and NMR properties of Hemicucurbit[n]urils and their anionic Complexes
H.-J. Buschmann and A. Zielesny
Computational and Theoretical Chemistry (2013), 1022, 14-22
(www.sciencedirect.com/science/article/pii/S2210271X1300354X)

Hemicucurbit[6]uril: A macrocyclic ligand with unusual complexing properties
H.-J. Buschmann, A. Zielesny, E. Schollmeyer
Journal of Inclusion Phenomena and Macrocyclic Chemistry (2006), 54, 181-185

- Structure, stability and NMR properties of cucurbit[n]urils and cucurbit[6]uril-
spermine complexes

Partner: Dr. Hans-Jürgen Buschmann, Dr. Andreas Wego, Deutsches Textilforschungszentrum Nord-West (DTNW), Krefeld, Germany
Completion: 2005

H.-J. Buschmann, A. Wego, A. Zielesny, E. Schollmeyer
Journal of Inclusion Phenomena and Macrocyclic Chemistry (2006), 54, 241-246

Structure, Electronic Properties and NMR-Shielding of Cucurbit[n]urils
H.-J. Buschmann, A. Wego, A. Zielesny, E. Schollmeyer
Journal of Inclusion Phenomena and Macrocyclic Chemistry (2006), 54, 85-88

Understanding the Cucurbit[6]uril-Spermine-Complex: Geometry and Electronic Interactions
H.-J. Buschmann, A. Wego, A. Zielesny, E. Schollmeyer
Poster contribution to the „1st German Conference of Chemoinformatics“ from November 13 to 15, 2005, in Goslar, Germany

Software Development in Chemoinformatics and Bioinformatics

- CDK-Taverna 2.0 – Java open-source pipelining/workflow solution for cheminformatics through combination of different open-source projects (Taverna, CDK - Chemistry Development Kit, WEKA - Waikato Environment for Knowledge Analysis)

Partner: PD Dr. Christoph Steinbeck, European Bioinformatics Institute (EBI), Hinxton/Cambridge, UK
Dr. Egon Willighagen, Institute of Environmental Medicine, Karolinska Institutet, Stockholm, Sweden
Completion: 2012

Information: New developments on the cheminformatics open workflow environment CDK-Taverna
A. Truszkowski, K. V. Jayaseelan, S. Neumann, E. L. Willighagen, A. Zielesny and C. Steinbeck
Status: Highly accessed
(www.jcheminf.com/content/3/1/54)
• **GNWI.MathComponent Freeware Library** – C# 2.0 free class collection for a fast, flexible and automated mathematical interplay of an application’s classes and components at design and run time

  Partner: Gesellschaft für naturwissenschaftliche Informatik mbH (GNWI), Oer-Erkenschwick, Germany

  Completion: 2010

  Information: Website [www.gnwi.de](http://www.gnwi.de)

• **Extending CDK-Taverna: Industrial Reaction Enumerator** – Workflows for combinatorial chemistry related reaction enumeration in industrial research and development

  Partner: Gesellschaft für naturwissenschaftliche Informatik mbH (GNWI), Oer-Erkenschwick, Germany

  Completion: 2010

  Information: Development and industrial validation of a combinatorial chemistry related enumeration software library for synthesis of potential pharmaceutical drugs on the basis of the Chemistry Development Kit (CDK)

  Andreas Truszkowski

  Bachelor Thesis, University of Applied Sciences Gelsenkirchen, Germany, 2009

• **CDK-Taverna Project** - Scientific pipelining workflows in Chemoinformatics (cooperative dissertation of Thomas Kuhn)

  Partner: PD Dr. Christoph Steinbeck, Cologne University Bioinformatics Center (CUBIC), Cologne, Germany

  Completion: 2009

  Information: [CDK-Taverna: an open workflow environment for cheminformatics](http://www.biomedcentral.com/1471-2105/11/159)

  T. Kuhn, E. L. Willighagen, A. Zielesny and C. Steinbeck

  BMC Bioinformatics (2010), 11, 159

  Status: Highly accessed

  [www.biomedcentral.com/1471-2105/11/159](http://www.biomedcentral.com/1471-2105/11/159)

  **Open-Source-Workflows (in German)**

  T. Kuhn, C. Steinbeck, A. Zielesny

  Nachrichten aus der Chemie (2010), 58 (1), 40-42

  **Open Source Workflow Engine for Cheminformatics: From Data Curation to Data Analysis**

  T. Kuhn

  Dissertation, University of Cologne, Germany, 2009
Development of a chemoinformatics pipelining solution for the aggregation of natural compound data

Partner: InterMed Discovery GmbH, Dortmund, Germany
Gesellschaft für naturwissenschaftliche Informatik mbH (GNWI), Oer-Erkenschwick, Germany

Completion: 2009
Information: Confidential

Development and implementation of software solutions for combinatorial chemistry, electronic notebook applications for material sciences, life science data warehouses and Bioinformatics systems

Partner: Bayer Business Services GmbH, Science & Technology, Leverkusen, Germany
Gesellschaft für naturwissenschaftliche Informatik mbH (GNWI), Oer-Erkenschwick, Germany

Completion: 2007
Information: Confidential

Scientific Pipelining

Partner: Gesellschaft für naturwissenschaftliche Informatik mbH (GNWI), Oer-Erkenschwick, Germany

Completion: 2007
• **Chemoinformatics/Bioinformatics toolbox**

  Partner: Gesellschaft für naturwissenschaftliche Informatik mbH (GNWI), Oer-Erkenschwick, Germany

  Completion: 2006

  Information: Confidential, but see:
  
  *Development and implementation of algorithms and software components for the comparison and representation of biological sequences*
  
  Thomas Kuhn
  
  Diploma Thesis (in German), University of Applied Sciences Gelsenkirchen, Germany, 2005

• **COSI – Chemoinformatics Open Source Initiative**

  Partner: PD Dr. Christoph Steinbeck, Cologne University Bioinformatics Center (CUBIC), Cologne, Germany

  Completion: 2006

• **Bioinformatics – Data mining, modelling und algorithms (public research project at the Westphalian University of Applied Sciences, Germany)**

  Partner: Prof. Dr. Heinrich Brinck, Prof. Dr. Soeren Perrey, Westphalian University of Applied Sciences, Germany

  Completion: 2006

• **Development of information management and data mining components for the scientific IT system Wistract® – Platform for Scientific Information**

  Partner: Bayer Business Services GmbH, Science & Technology, Leverkusen, Germany
  
  Gesellschaft für naturwissenschaftliche Informatik mbH (GNWI), Oer-Erkenschwick, Germany

  Completion: 2006

  Information: *A Case Study for Information Integration and Analysis with Wistract® - A new Platform for Scientific Information*
  
  C. Schaub, A. Zielesny
  
  Proceedings of the „The International Conference for Science and Business Information (ICIC) 2005“, October 16 to 19, 2005, Nîmes, France

  *Platform for Scientific Information (in German)*
  
  C. Schaub, A. Zielesny
  
  Nachrichten aus der Chemie (2005), 53 (7/8), 786-788

  *Wistract® – Platform for Scientific Information*
  
  O. Gebert, C. Schaub, A. Zielesny
  
  Poster contribution to the „18th CIC-Workshop: New Developments in Chemoinformatics“ of the section Chemistry-Information-Computer (CIC) of the German Chemical Society from November 14 to 16, 2004, at Boppard am Rhein, Germany
• **Design and development of the application logic of the scientific IT system Wistract® – Platform for Scientific Information**

Partner: Bayer Business Services GmbH, Science & Technology, Leverkusen, Germany  
Completion: 2004  
Information: *Method for the Provision of any Type of Storage Media containing pre-recorded structured Information*  
B. Achten, F. Augustin, O. Gebert, S. Kohl, C. Schaub, M. Schimeczek, A. Zielesny  
Bayer Business Service GmbH, Leverkusen, Germany  

• **Data mining in life science related data spaces**

Partner: Bayer Business Services GmbH, Science & Technology, Leverkusen, Germany  
Completion: 2004  
Information: Confidential, but see:  
*Development, implementation and validation of an ART-based Neural Network software component for the solution of open-categorical classification problems in high dimensional scientific information spaces*  
Stefan Neumann  
Diploma Thesis (in German), University of Applied Sciences Gelsenkirchen, Germany

**QSPR of Polymer Systems**

• **Combinatorial formulation and testing for optimization of polymer adhesive systems: Integrated information management and property prediction with Soft-Computing methods**

Partner: Prof. Dr. Klaus-Uwe Koch, Prof. Dr. Holger Frenz, Westphalian University of Applied Sciences, Germany  
Completion: 2008  
Information: *Combinatorial Formulation and Testing of Adhesives*  
K. U. Koch, H. Frenz, A. Zielesny  
Poster contribution to the „International Conference on High Throughput Formulation Technologies“ of the DECHEMA from December 7 to 8, 2004, in Frankfurt am Main, Germany

• **Prediction of relevant properties of polymer adhesive systems (QSPR) with neural networks**

Partner: Prof. Dr. Klaus-Uwe Koch, Westphalian University of Applied Sciences, Germany  
Completion: 2004
Information: *Neuronal networks curtail adhesive development* (in German)
K. U. Koch, A. Zielesny
Adhesion (2004), 48(1-2), 32-37

*Prediction of Curing Times of Adhesives with Neural Networks* (in German)
K. U. Koch, A. Zielesny
Poster contribution to the „Annual Conference 2003“ of the German Chemical Society from October 6 to 11, 2003, in Munich

**Interdisciplinary Projects**

- **Concept of an innovative personalized Internet Portal for “intelligent” Job-Man Matching on the basis of modern Soft-Computing Techniques**

  Partner: Prof. Dr. Heinrich Meinhard Stindt, Bergisch Gladbach, Germany

  Completion: 2002

  Information: *Neural-Network based IT Methods for Job-Man Matching – the personalized Internet Labour Portal* (in German)
H. M. Stindt, A. Zielesny
Invited Lectures and Consulting

- **Molecular Simulation and Fragment Cheminformatics**
  
  Partner: Lecture at the European Bioinformatics Institute (EBI), Hinxton/Cambridge, UK
  
  Year: 2013

- **Foundations of Molecular Biology and Bioinformatics**
  
  Partner: Lectures of the IT4omics event series organized by Bayer Business Services (BBS), Leverkusen, Germany
  
  Year: 2013

- **The relevance of information technology for nanoscience in the 21st century**
  
  Partner: Lecture at the Association of German Engineers (VDI), Munich, Germany
  
  Year: 2008

- **Scientific Computing: Prospects for industrial companies**
  
  Partner: Lecture at the “Scientific Computing Day 2007” of Henkel KGaA, Düsseldorf, Germany
  
  Year: 2007

- **Intelligent IT systems?**
  
  Partner: Lecture at the “ScienceTech 2007” of Bayer Business Services GmbH, Science & Technology, Mettmann/Düsseldorf, Germany
  
  Year: 2007

- **Combinatorial formulation of industrial high-performance polymer systems**
  
  Partner: Lecture with Prof. Dr. Klaus-Uwe Koch, Westphalian University of Applied Sciences, at Henkel KGaA, Düsseldorf, Germany
  
  Year: 2006
• **Combinatorial formulation of high-performance adhesives for aircraft construction**
  
  Partner: Lecture with Prof. Dr. Klaus-Uwe Koch, Westphalian University of Applied Sciences, at Airbus/Composite Technology Center (CTC) GmbH, Stade, Germany
  
  Year: 2005

• **Perspectives and challenges of commercial scientific software development**
  
  Partner: Lecture at the “ScienceTech 2005” of Bayer Business Services GmbH, Science & Technology, Leverkusen, Germany
  
  Year: 2005

• **Software tools for a Proteomics IT infrastructure**
  
  Partner: Protagen AG, Dortmund, Germany
  
  Year: 2003

• **Business models and strategic directions of Chemoinformatics and Bioinformatics**
  
  Partner: Bayer Business Services GmbH, Science & Technology, Leverkusen, Germany
  
  Year: 2002/2003

• **Requirements of a life science oriented database system for object-relational data**
  
  Partner: InfoChem GmbH, München, Germany
  Microsoft GmbH, München, Germany
  
  Year: 2002

• **Scientific business computing**
  
  Partner: Protagen AG, Dortmund, Germany
  
  Year: 2002
• **Strategic developments in Chemoinformatics**

  Partner: InfoChem GmbH, München, Germany

  Year: 2001
Scientific Education

Cooperative Dissertation

- **Simulation of Peptides, Proteins and Biomembranes with Molecular Fragment Dynamics (MFD)**
  
  Student: Andreas Truszkowski  
  Partner: Prof. Dr. Matthias Epple, University Duisburg-Essen, Institute of Inorganic Chemistry, Essen, Germany  
  Year: 2015

- **Open Source Workflow Engine for Cheminformatics: From Data Curation to Data Analysis**
  
  Student: Thomas Kuhn  
  Partner: PD Dr. Christoph Steinbeck, Cologne University Bioinformatics Center, Cologne, Germany  
  Year: 2009

Master Thesis

- **Molecular Fragment Dynamics Study of Biological Membranes and Zinc Ricinoleate Layers for Enzyme Purification**
  
  Student: Karina van den Broek  
  Partner: CAM-D Technologies GmbH, Essen, Germany  
  Year: 2014

- **Enabling molecular Biosciences: Re-engineering, reaction enumeration and machine learning enhancements for the open workflow platform CDK-Taverna**
  
  Student: Andreas Truszkowski  
  Partner: Gesellschaft für naturwissenschaftliche Informatik mbH (GNWI), Oer-Erkenschwick, Germany  
  PD Dr. Christoph Steinbeck, European Bioinformatics Institute (EBI), Hinxton/Cambridge, UK  
  Year: 2011
**Bachelor Thesis**

- **Development of parallelized machine learning algorithms for biological data analysis with Mathematica**
  
  Student: Kolja Berger  
  
  Partner: Gesellschaft für naturwissenschaftliche Informatik mbH (GNWI), Oer-Erkenschwick, Germany  
  
  Year: 2014  

- **Design and development of a rich client application for the calculation of chemical descriptors based on the Chemistry Development Kit (CDK)**
  
  Student: Sebastian Fritsch  
  
  Partner: Gesellschaft für naturwissenschaftliche Informatik mbH (GNWI), Oer-Erkenschwick, Germany  
  
  Year: 2013  

- **Design and development of a rich client application for compound selection based on the Chemistry Development Kit (CDK)**
  
  Student: Hendrik Göddeke  
  
  Partner: Gesellschaft für naturwissenschaftliche Informatik mbH (GNWI), Oer-Erkenschwick, Germany  
  
  Year: 2013  

- **Programming a neural Hopfield-Network for pattern recognition**
  
  Student: Carina Goretzky  
  
  Partner: Gesellschaft für naturwissenschaftliche Informatik mbH (GNWI), Oer-Erkenschwick, Germany  
  
  Year: 2012
• **Dependency structures in protein expression data of invasive breast cancer**

  Student: Florian Boecker  
  Partner: University of Muenster, Faculty of Medicine, Institute of Bioinformatics  
  Year: 2012

• **Extension of the Chemistry Development Kit (CDK) for biomedical Modelling of Quantitative Structure-Property Relationships**

  Student: Julian Jorzik  
  Partner: Gesellschaft für naturwissenschaftliche Informatik mbH (GNWI), Oer-Erkenschwick, Germany  
  Year: 2011

• **Development and industrial validation of a combinatorial chemistry related enumeration software library for synthesis of potential pharmaceutical drugs on the basis of the Chemistry Development Kit (CDK)**

  Student: Andreas Truszkowski  
  Partner: Gesellschaft für naturwissenschaftliche Informatik mbH (GNWI), Oer-Erkenschwick, Germany  
  Bayer Business Services GmbH, Science & Technology, Leverkusen, Germany  
  Year: 2009

**Diploma Thesis**

• **Synthesis of organozinc complexes for reaction with pollutants in gas phase: Molecular modelling study of the reaction mechanism**

  Student: Thomas Veidt  
  Partner: CAM-D Technologies GmbH, Essen, Germany  
  Year: 2010
• **Alignment of molecular structures represented by Gaussian functions**
  
  Student: Christian Geiger  
  Partner: Computational Drug Discovery Group, Radboud University of Nijmegen, The Netherlands  
  Schering-Plough, Department of Molecular Design and Informatics, Oss, The Netherlands  
  Year: 2008

• **Molecular Fragment Dynamics Simulations for the Aggregation of Phospholipids at solid Surfaces**
  
  Student: Christoph Engels  
  Partner: CAM-D Technologies GmbH, Essen, Germany  
  Year: 2007

• **Quantum-chemical Investigations on Cucurbit[6]uril and α-Cyclodextrin Complexes**
  
  Student: Jan-Niklas Schäfer  
  Partner: Deutsches Textilforschungszentrum Nord-West (DTNW), Krefeld, Germany  
  Year: 2006

• **Software Design Aspects of an electronic Notebook for Materials Sciences**
  
  Student: Holger Schulte  
  Partner: Gesellschaft für naturwissenschaftliche Informatik mbH (GNWI), Oer-Erkenschwick, Germany  
  Bayer Business Services GmbH, Science & Technology, Leverkusen. Germany  
  Year: 2006
• Development and implementation of algorithms and software components for the comparison and representation of biological sequences

Student: Thomas Kuhn
Partner: Gesellschaft für naturwissenschaftliche Informatik mbH (GNWI), Oer-Erkenschwick, Germany
Bayer Business Services GmbH, Science & Technology, Leverkusen, Germany
Year: 2005

• Development, implementation and validation of an ART-based Neural Network software component for the solution of open-categorical classification problems in high dimensional scientific information spaces

Student: Stefan Neuman
Partner: Bayer Business Services GmbH, Science & Technology, Leverkusen, Germany
Year: 2004

• Integration of complex reaction mechanisms to simulation models and development of a model for hydrogenation in Trickle-Bed reactors

Student: Emrah Ergörül
Partner: Degussa AG, Marl, Germany
Year: 2004

• Partial purification, characterization and genotype determination of the acetylcholine esterase of different types of phorodon humuli

Student: Sandra Bittner
Partner: Bayer CropScience, Monheim, Germany
Year: 2003
Publications

Books

2011 From Curve Fitting to Machine Learning: An illustrative Guide to scientific Data Analysis and Computational Intelligence
A. Zielesny
(DOI: 10.1007/978-3-642-21280-2)
Supplementary information is available at website www.gnwi.de.

Open-Source and Free Software

2012 CIP - Computational Intelligence Packages (Version 1.1 and 1.2)
Mathematica® 7 (or higher) open-source library for curve fitting, data smoothing, clustering and machine learning
Website: www.gnwi.de

CDK-Taverna (Version 2.0)
Java open-source pipelining/workflow solution for cheminformatics through combination of different open-source projects (Taverna, CDK - Chemistry Development Kit, WEKA - Waikato Environment for Knowledge Analysis)
Websites: Wiki, Blog

2011 CIP - Computational Intelligence Packages (Version 1.0)
Mathematica® 7 (or higher) open-source library for curve fitting, data smoothing, clustering and machine learning
Website: www.gnwi.de

2010 MathComponent Freeware Library (Version 1.0.0.1)
C# 2.0 free class collection for a fast, flexible and automated mathematical interplay of an application’s classes and components at design and run time
Website: www.gnwi.de

Proprietary Software

2015 MFD-FormulaOne
Integrated rich-client application for mesoscopic simulation with Molecular Fragment Dynamics (MFD)
Website: www.MFD-FormulaOne.de
Online Lectures

2011  **Chemical File Formats and Line Notations**
A. Zielesny  

2011  **Storing, searching and dissemination of chemical information**
A. Zielesny  

Peer-Reviewed R&D Articles and Patents

2015  **Mesoscopic Simulation of Phospholipid Membranes, Peptides, and Proteins with Molecular Fragment Dynamics**
A. Truszkowski, K. van den Broek, H. Kuhn, A. Zielesny and M. Epple  

2014  **A molecular fragment cheminformatics roadmap for mesoscopic simulation**
A. Truszkowski, M. Daniel, H. Kuhn, S. Neumann, C. Steinbeck, A. Zielesny and M. Epple  
Journal of Cheminformatics (2014), 6:45 ([www.jcheminf.com/content/6/1/45](http://www.jcheminf.com/content/6/1/45))

2013  **Geometric, electronic and NMR properties of Hemicucurbit[n]urils and their anionic Complexes**
H.-J. Buschmann and A. Zielesny  

**Molecular fragment dynamics study on the water-air interface behavior of non-ionic polyoxyethylene alkyl ether surfactants**
A. Truszkowski, M. Epple, A. Fiethen, A. Zielesny and H. Kuhn  

2011  **New developments on the cheminformatics open workflow environment CDK-Taverna**
A. Truszkowski, K. V. Jayaseelan, S. Neumann, E. L. Willighagen, A. Zielesny and C. Steinbeck  
Status: *Highly accessed*  
([www.jcheminf.com/content/3/1/54](http://www.jcheminf.com/content/3/1/54))
2010  **CDK-Taverna: an open workflow environment for cheminformatics**
T. Kuhn, E. L. Willighagen, A. Zielesny and C. Steinbeck  
BMC Bioinformatics (2010), 11, 159  
Status: Highly accessed  
(www.biomedcentral.com/1471-2105/11/159)

H.-J. Buschmann, A. Wego, A. Zielesny, E. Schollmeyer  
Journal of Inclusion Phenomena and Macrocyclic Chemistry (2006), 54, 241-246

**Hemicucurbit[6]uril: A macrocyclic ligand with unusual complexing properties**  
H.-J. Buschmann, A. Zielesny, E. Schollmeyer  
Journal of Inclusion Phenomena and Macrocyclic Chemistry (2006), 54, 181-185

**Structure, Electronic Properties and NMR-Shielding of Cucurbit[n]urils**  
H.-J. Buschmann, A. Wego, A. Zielesny, E. Schollmeyer  
Journal of Inclusion Phenomena and Macrocyclic Chemistry (2006), 54, 85-88

2005  **Method for the Provision of any Type of Storage Media containing pre-recorded structured Information**  
B. Achten, F. Augustin, O. Gebert, S. Kohl, C. Schaub, M. Schimeczek, A. Zielesny  
Bayer Business Service GmbH  
Priority DE200410010517 (2004-03-04); DE200410032231 (2004-07-02)

2004  **Neuronal networks curtail adhesive development** (in German)  
K. U. Koch, A. Zielesny  
Adhaesion (2004), 48(1-2), 32-37

1995  **Ultrasonic absorption of nitrobenzene-isoctane mixtures of non-critical composition**  
A. Zielesny, D. Woermann  

**Diffusivity of a non-ionic surfactant/water mixture of critical composition**  
M. Lesemann, A. Zielesny, L. Belkoura, D. Woermann  

1994  **Crossover behaviour and critical amplitude of the viscosity of binary liquid mixtures of critical composition**  
A. Zielesny, D. Woermann  

**Static light scattering experiments with non-ionic surfactant/water mixtures of critical composition**  
A. Zielesny, L. Belkoura, D. Woermann  
Viscosity of two non-ionic amphiphile-water mixtures of critical composition: Study of the systems triethylene glycol monohexyl ether \((\text{C}_6\text{E}_3)\)-water and tetraethylene glycol monoocctyl ether \((\text{C}_8\text{E}_4)\)-water
A. Zielesny, S. Limberg, D. Woermann

Viscosity and diffusivity of a binary liquid mixture of critical composition: study of the system 2-butoxyethanol/water
A. Zielesny, J. Schmitz, S. Limberg, A. G. Aizpiri, S. Fusenig, D. Woermann

1990 Temperature dependence of viscosity of polystyrene/cyclohexane mixtures of critical composition
W. A. Goedel, A. Zielesny, L. Belkoura, T. Engels, D. Woermann

Other Articles

2010 Open-Source-Workflows (in German)
T. Kuhn, C. Steinbeck, A. Zielesny
Nachrichten aus der Chemie (2010), 58 (1), 40-42

2006 From Industrie to University (in German)
A. Zielesny
Nachrichten aus der Chemie (2006), 54 (11), 1172-1173
Gesellschaft Deutscher Chemiker, Berufsbilder in der Chemie, March 2008, page 44

2005 Chemistry Software Package ChemOffice Ultra 2005
A. Zielesny

Platform for Scientific Information (in German)
C. Schaub, A. Zielesny
Nachrichten aus der Chemie (2005), 53 (7/8), 786-788

Conference Lectures and Poster Contributions

2014 Molecular simulations of peptides and proteins with Molecular Fragment Dynamics
A. Truszkowski, A. Fiethen, H. Kuhn, A. Zielesny and M. Eppe
Poster contribution to the „10th International Conference on Chemical Structures” and „10th German Conference on Chemoinformatics” from June 1 to 5, 2014, in Noordwijkerhout, The Netherlands
2014 Molecular Fragment Dynamics Study of the Interaction between Zinc Ricinoleate and the Complexing Agent Methylglycinediacetic Acid as a new System for Enzyme Purification
K. van den Broek, A. Fiethen, A. Truszkowski, A. Zielesny and H. Kuhn
Poster contribution to the „10th International Conference on Chemical Structures” and „10th German Conference on Chemoinformatics” from June 1 to 5, 2014, in Noordwijkerhout, The Netherlands

Extension of molecular fragment based mesoscopic simulation to the biopolymer realm
A. Truszkowski, A. Fiethen, H. Kuhn, A. Zielesny and M. Epple
Poster contribution to the „28th Molecular Modeling Workshop” from March 17 to 19, 2014, in Erlangen, Germany

Molecular fragment dynamics study on the water-air interface behavior of non-ionic polyoxyethylene alkyl ether surfactants
A. Truszkowski, A. Fiethen, H. Kuhn, T. Wiebringhaus, A. Zielesny and M. Epple
Poster contribution to the „9th German Conference of Chemoinformatics” from November 10 to 12, 2013, in Fulda, Germany
Journal of Cheminformatics 2014, 6(Suppl 1):P9
(www.jcheminf.com/content/6/S1/P9)

2013 A molecular fragment dynamics (MFD) study on the phase behavior of non-ionic surfactants
A. Truszkowski, A. Fiethen, H. Kuhn, A. Zielesny and M. Epple
Poster contribution to the „9th Zsigmondy Colloquium” from March 6 to 8, 2013, in Essen, Germany

2012 Molecular simulations of peptides and proteins with Molecular Fragment Dynamics (MFD)
A. Truszkowski, A. Fiethen, H. Kuhn, A. Zielesny and M. Epple
Poster contribution to the „8th German Conference of Chemoinformatics” from November 11 to 13, 2012, in Goslar, Germany
(www.jcheminf.com/content/5/S1/P4)

Adsorption of amino acids in MFI-type zeolite: a computational and experimental study
K. Stueckenschneider, J. Merz, A. Zielesny, G. Schembecker
Poster contribution to the „15. European Congress on Biotechnology” from September 23 to 26, 2012, in Istanbul, Turkey

Adsorption of Alanine and Phenylalanine on MFI-type Zeolite: DFT Calculations and Experimental Results
K. Stueckenschneider, A. Zielesny, G. Schembecker
Poster contribution to the „26th Molecular Modeling Workshop” from March 12 to 14, 2012, in Erlangen, Germany

Adsorption of amino acids on MFI-type zeolite: Computational and experimental results (in German)
K. Stueckenschneider, J. Merz, A. Zielesny and G. Schembecker
Chemie Ingenieur Technik (2012), 84, No. 8, 1413
(onlinelibrary.wiley.com/doi/10.1002/cite.201250474/pdf)
Adsorption of amino acids on MFI-type zeolite: DFT calculations and experimental results
K. Stückenschneider, A. Zielesny and G. Schembecker
Poster contribution to the „7th German Conference of Chemoinformatics“ from November 6 to 8, 2011, in Goslar, Germany
(www.jcheminf.com/content/4/S1/P38)

Reaction enumeration and machine learning enhancements for the open-source pipelining solution CDK-Taverna 2.0
A. Truszkowski, S. Neumann, A. Zielesny, E. L. Willighagen and C. Steinbeck
Poster contribution to the „9th International Conference on Chemical Structures (ICCS)” from June 5 to 9, 2011, in Noordwijkerhout, The Netherlands

CDK-Taverna 2.0: migration and enhancements of an open-source pipelining solution
A. Truszkowski, S. Neumann, A. Zielesny, E. Willighagen and C. Steinbeck
Poster contribution to the „6th German Conference of Chemoinformatics” from November 7 to 9, 2010, in Goslar, Germany
(www.jcheminf.com/content/3/S1/P5)

Molecular fragments chemoinformatics
H. Kuhn, S. Neumann, C. Steinbeck, C. Wittekindt and A. Zielesny
Poster contribution to the „5th German Conference of Chemoinformatics” from November 8 to 10, 2009, in Goslar, Germany
(www.jcheminf.com/content/2/S1/P14)

Creating Chemo- & Bioinformatics Workflows: Further Developments within the CDK-Taverna Project
T. Kuhn, A. Zielesny and C. Steinbeck
Poster contribution to the „4th German Conference of Chemoinformatics” from November 9 to 11, 2008, in Goslar, Germany
Chemistry Central Journal (2009), 3 (Suppl 1): P42
(www.journal.chemistrycentral.com/content/3/S1/P42)

Creating Chemo- & Bioinformatics Workflows: Further Developments within the CDK-Taverna Project
T. Kuhn, A. Zielesny and C. Steinbeck
Poster contribution to the „8th International Conference on Chemical Structures (ICCS)” from June 1 to 5, 2008, in Noordwijkerhout, The Netherlands

Creating Chemo- and Bioinformatics Workflows – Building a Soft Computing Framework for the CDK-Taverna Project
T. Kuhn, A. Zielesny and C. Steinbeck
Poster contribution to the „3. German Conference of Chemoinformatics“ from November 11 to 13, 2007, in Goslar, Germany,
(www.journal.chemistrycentral.com/content/2/S1/P27)
2007 Intelligent IT-Systems? Challenges, Fakes and Hard Science  
S. Neumann, A. Zielesny  
Proceedings of the „2007 International Chemical Information Conference & Exhibition (ICIC)“, October 21 to 24, 2007, Sitges/Barcelona, Spain

Understanding Cucurbit[6]uril-Spermine  
H.-J. Buschmann, A. Wego, A. Zielesny, E. Schollmeyer  
Poster contribution to the 393. WE-Heraeus-Seminar „Trends in Molecular Biophysical Spectroscopy – Electronic Structure, Function, and Dynamics of Biomolecules“ from April 26 to 28, 2007, in Bad Honnef, Germany

2006 Creating Chemo- and Bioinformatics Workflows – The CDK-Taverna Project  
T. Kuhn, E. Willighagen, A. Zielesny and C. Steinbeck  
Poster contribution to the „2nd German Conference of Chemoinformatics“ from November 12 to 14, 2006, in Goslar, Germany

H.-J. Buschmann, A. Wego, A. Zielesny, E. Schollmeyer  
Poster contribution to the „1st German Conference of Chemoinformatics“ from November 13 to 15, 2005, in Goslar, Germany

Structure, Electronic Properties and NMR-Shielding of Cucurbit[n]urils  
H.-J. Buschmann, A. Wego, A. Zielesny, E. Schollmeyer  
Poster contribution to the „1st German Conference of Chemoinformatics“ from November 13 to 15, 2005, in Goslar, Germany

A Case Study for Information Integration and Analysis with Wistract® - A new Platform for Scientific Information  
C. Schaub, A. Zielesny  
Proceedings of the „2005 International Chemical Information Conference & Exhibition (ICIC)“, October 16 to 19, 2005, Nimes, France

2004 Combinatorial Formulation and Testing of Adhesives  
K. U. Koch, H. Frenz, A. Zielesny  
Poster contribution to the „International Conference on High Throughput Formulation Technologies“ of the DECHEMA from December 7 to 8, 2004, in Frankfurt am Main, Germany

Wistract® – Platform for Scientific Information  
O. Gebert, C. Schaub, A. Zielesny  
Poster contribution to the „18th CIC-Workshop: New Developments in Chemoinformatics“ of the section Chemistry-Information-Computer (CIC) of the German Chemical Society from November 14 to 16, 2004, at Boppard am Rhein, Germany

2003 Prediction of Curing Times of Adhesives with Neural Networks (in German)  
K. U. Koch, A. Zielesny  
Poster contribution to the „Annual Conference 2003“ of the German Chemical Society from October 6 to 11, 2003, in Munich
2003  **Iterated Rank based Methods for Clustering**  
S.W. Perrey, H. Brinck, A. Zielesny  

2002  **Neural-Network based IT Methods for Job-Man Matching – the personalized Internet Labour Portal** (in German)  
H. M. Stindt, A. Zielesny  

2000  **The ChemInformatics Integration Challenge**  
M. Diedrich, W. Jilge, M. Neumann, H. Rakel, A. Zielesny  
Proceedings of the „Drug Discovery Technology (DDT) 2000“, Boston, USA

1999  **Concept and Realization of Bayer's Integrated Chemistry Information System on the Corporate Intranet**  
A. Zielesny  
Proceedings of the „Chemistry and the Internet (ChemInt) 1999“, Washington DC, USA

1998  **Development of a Web-based chemical information workspace at Bayer: Review and perspectives for R&D**  
A. Zielesny, W. Jilge  

1997  **Strategies and paradigms of scientific end-user information at Bayer**  
A. Zielesny, W. T. Donner, W. Jilge  
Proceedings of the idt 97, Paris, France

1996  **Scientific PC-based end-user information workspace: New developments at Bayer**  

1995  **Use of the Beilstein Information at Bayer** (in German)  
C. Zirz, J. Sendelbach, A. Zielesny  
Proceedings of the „17. Online-Tagung der DGD“, Frankfurt am Main, May 16 to 18, 1995