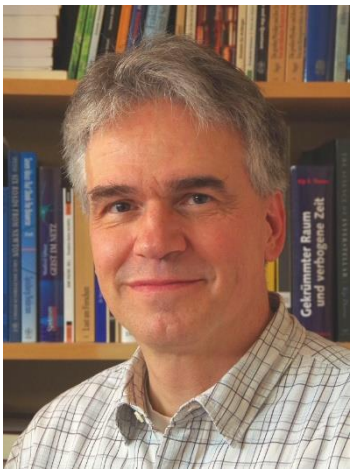


Prof. Dr. Achim Zielesny

Westphalian University of Applied Sciences
Institute for Bioinformatics and Chemoinformatics (IBCI)

August-Schmidt-Ring 10
D-45665 Recklinghausen, Germany

Phone +49-2361-915530
E-Mail achim.zielesny@w-hs.de

Date 2024/02/16

Interests in Cheminformatics and Bioinformatics

- Software development of algorithmic solutions, scientific software packages and IT systems
- Molecular modeling and simulation, molecular recognition, QSAR/QSPR
- Model development, machine learning und computational intelligence
- Strategic developments

Publications

Peer-Reviewed R&D Articles

2023 **DECIMER.ai: an open platform for automated optical chemical structure identification, segmentation and recognition in scientific publications**
K. Rajan, H. O. Brinkhaus, M. I. Agea, A. Zielesny and C. Steinbeck
Nature Communications (2023), 14:5045
(online)

Notes on molecular fragmentation and parameter settings for a dissipative particle dynamics study of a $C_{10}E_4$/water mixture with lamellar bilayer formation
F. Bänsch, C. Steinbeck and A. Zielesny
Journal of Cheminformatics (2023), 15:23
(online)

Open data and algorithms for open science in AI-driven molecular informatics
H.-O. Brinkhaus, K. Rajan, J. Schaub, A. Zielesny, C. Steinbeck
Current Opinion in Structural Biology (2023), 79:102542
(online)

MORTAR: a rich client application for in silico molecule fragmentation
F. Bänsch, J. Schaub, B. Sevindik, S. Behr, J. Zander, C. Steinbeck and A. Zielesny
Journal of Cheminformatics (2023), 15:1
(online)

2022 **Scaffold Generator: a Java library implementing molecular scaffold functionalities in the Chemistry Development Kit (CDK)**
J. Schaub, J. Zander, A. Zielesny, C. Steinbeck
Journal of Cheminformatics (2022), 14:79
(online)

Notes on the Treatment of Charged Particles for Studying Cyclotide/Membrane Interactions with Dissipative Particle Dynamics
F. Bänsch, C. Steinbeck and A. Zielesny
Membranes (2022), 12(6):619
(online)

DECIMER - Hand-drawn molecule images dataset
H.-O. Brinkhaus, A. Zielesny, C. Steinbeck, K. Rajan
Journal of Cheminformatics (2022), 14:36
(online)
Zenodo repository: online

2022 **RanDepict - Random Chemical Structure Depiction Generator**
H.-O. Brinkhaus, K. Rajan, A. Zielesny and C. Steinbeck
Journal of Cheminformatics (2022), 14:31
(online)

Performance of chemical structure string representations for chemical image recognition using transformers


K. Rajan, C. Steinbeck and A. Zielesny
Digital Discovery (2022), 1:84-90
(online)

2021 **DECIMER 1.0: deep learning for chemical image recognition using transformers**
K. Rajan, A. Zielesny and C. Steinbeck
Journal of Cheminformatics (2021), 13:61
(online)

Quantitative Estimation of Cyclotide-Induced Bilayer Membrane Disruption by Lipid Extraction with Mesoscopic Simulation
K. van den Broek, M. Epple, L. S. Kersten, H. Kuhn and A. Zielesny
Journal of Chemical Information and Modeling (2021), 61, 3027-3040
(online)

STOUT: SMILES to IUPAC names using neural machine translation
K. Rajan, A. Zielesny and C. Steinbeck
Journal of Cheminformatics (2021), 13:34
(online)

Description and Analysis of Glycosidic Residues in the Largest Open Natural Products Database
J. Schaub, A. Zielesny, C. Steinbeck and M. Sorokina
Biomolecules (2021), 11, 486
(online)

DECIMER-Segmentation: Automated extraction of chemical structure depictions from scientific literature
K. Rajan, H. O. Brinkhaus, M. Sorokina, A. Zielesny and C. Steinbeck
Journal of Cheminformatics (2021), 13:20
(online)

Molecule Set Comparator (MSC) – A CDK-based open rich-client tool for molecule set similarity evaluations
K. Rajan, J.-M. Hein, C. Steinbeck and A. Zielesny
Journal of Cheminformatics (2021), 13:5
(online)

2020 **Too sweet: cheminformatics for deglycosylation in natural products**
J. Schaub, A. Zielesny, C. Steinbeck and M. Sorokina
Journal of Cheminformatics (2020), 12:67
(online)

2020 **DECIMER - Towards Deep Learning for Chemical Image Recognition**
K. Rajan, A. Zielesny and C. Steinbeck
Journal of Cheminformatics (2020), 12:65
(online)

A review of optical chemical structure recognition tools
K. Rajan, H. O. Brinkhaus, A. Zielesny and C. Steinbeck
Journal of Cheminformatics (2020), 12:60
(online)

MFsim - an open Java all-in-one rich-client simulation environment for mesoscopic simulation
K. van den Broek, M. Daniel, M. Epple, J.-M. Hein, H. Kuhn, S. Neumann, A. Truszkowski and A. Zielesny
Journal of Cheminformatics (2020), 12:29
(online)

2019 **ErtlFunctionalGroupsFinder: automated rule-based functional group detection with the Chemistry Development Kit (CDK)**
S. Fritsch, S. Neumann, J. Schaub, C. Steinbeck and A. Zielesny
Journal of Cheminformatics (2019), 11:37
(online)

2018 **SPICES: a particle-based molecular structure line notation and support library for mesoscopic simulation**
K. van den Broek, M. Daniel, M. Epple, H. Kuhn, J. Schaub and A. Zielesny
Journal of Cheminformatics (2018), 10:35
(online)

Jdpd: an open Java simulation kernel for molecular fragment dissipative particle dynamics
K. van den Broek, H. Kuhn and A. Zielesny
Journal of Cheminformatics (2018), 10:25
(online)

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
Journal of Chemical Information and Modeling (2015), 55(5), 983-997
(online)

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
(online)

2013 **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
(online)

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
(online)

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
Journal of Cheminformatics (2011), 3, 54
(online)

2010 **CDK-Taverna: an open workflow environment for cheminformatics**
T. Kuhn, E. L. Willighagen, A. Zielesny and C. Steinbeck
BMC Bioinformatics (2010), 11, 159
(online)

2006 **Structure, Stability, Electronic Properties and NMR-Shielding of the Cucurbit[6]uril-Spermine-Complex**
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

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-isooctane mixtures of non-critical composition**
A. Zielesny, D. Woermann
J. Chem. Soc., Faraday Trans. (1995), 91 (21), 3889-3892

Diffusivity of a non-ionic surfactant/water mixture of critical composition
M. Lesemann, A. Zielesny, L. Belkoura, D. Woermann
J. Chem. Phys. (1995), 102 (1), 414-418

1994 **Crossover behaviour and critical amplitude of the viscosity of binary liquid mixtures of critical composition**
A. Zielesny, D. Woermann
J. Chem. Soc., Faraday Trans. (1994), 90 (15), 2215-2222

Static light scattering experiments with non-ionic surfactant/water mixtures of critical composition
A. Zielesny, L. Belkoura, D. Woermann
Ber. Bunsen-Ges. Phys. Chem. (1994), 98 (4), 579-584

Viscosity of two non-ionic amphiphile-water mixtures of critical composition: Study of the systems triethyleneglycolmonohexyl ether (C_6E_3)-water and tetraethyleneglycolmonooctyl ether (C_8E_4)-water
A. Zielesny, S. Limberg, D. Woermann
Ber. Bunsen-Ges. Phys. Chem. (1994), 98 (2), 195-201

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
Int. J. Thermophys. (1994), 15 (1), 67-94

1990 **Temperature dependence of viscosity of polystyrene/cyclohexane mixtures of critical composition**
W. A. Goedel, A. Zielesny, L. Belkoura, T. Engels, D. Woermann
Ber. Bunsen-Ges. Phys. Chem. (1990), 94 (1), 17-24

Patent

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
Patent WO2005086039A2 (2005-09-15), US2008021798A1, JP2007528543A
Application EP2005001748W (2005-02-19)
Priority DE102004010517A (2004-03-04), DE102004032231A (2004-07-02)

Textbook

2016 **From Curve Fitting to Machine Learning: An illustrative Guide to scientific Data Analysis and Computational Intelligence**
Second revised and extended Edition
A. Zielesny
Springer: Intelligent Systems Reference Library, Volume 109, 2016
Supplementary information available on GitHub.

2011 **From Curve Fitting to Machine Learning: An illustrative Guide to scientific Data Analysis and Computational Intelligence**
A. Zielesny
Springer: Intelligent Systems Reference Library, Volume 18, 2011
Supplementary information available on GitHub.

Preprint R&D Articles *(not peer-reviewed)*

2024 **An automated Calculation Pipeline for Differential Pair Interaction Energies with Molecular Force Fields using the Tinker Molecular Modeling Package**
F. Bänsch, M. Daniel, H. Lanig, C. Steinbeck, A. Zielesny
ChemRxiv. Preprint: online

2023 **Complex formation of Cucurbit[6]uril with DABCO and DABCO derivatives: An experimental and DFT study**
A. Wego, A. Zielesny
ChemRxiv. Preprint: online

DECIMER.ai - An open platform for automated optical chemical structure identification, segmentation and recognition in scientific publications
K. Rajan, H. O. Brinkhaus, M. I. Agea, A. Zielesny, C. Steinbeck
ChemRxiv. Preprint: online

2022 **Open data and algorithms for open science in AI-driven molecular informatics**
H. O. Brinkhaus, K. Rajan, J. Schaub, A. Zielesny, C. Steinbeck
ChemRxiv. Preprint: online

MORTAR - A Rich Client Application for in silico Molecule Fragmentation
F. Bänsch, J. Schaub, B. Sevindik, S. Behr, J. Zander, C. Steinbeck, A. Zielesny
ChemRxiv. Preprint: online

DECIMER - Hand-drawn molecule images dataset
H.-O. Brinkhaus, A. Zielesny, C. Steinbeck, K. Rajan
ChemRxiv. Preprint: online
Zenodo repository: online

Scaffold Generator - A Java library implementing molecular scaffold functionalities in the Chemistry Development Kit (CDK)
J. Schaub, J. Zander, A. Zielesny, C. Steinbeck
ChemRxiv. Preprint: online

RanDepict - Random Chemical Structure Depiction Generator
H.-O. Brinkhaus, K. Rajan, A. Zielesny, C. Steinbeck
ChemRxiv. Preprint: online

2021 **Performance of chemical structure string representations for chemical image recognition using transformers**
K. Rajan, C. Steinbeck, A. Zielesny
ChemRxiv. Preprint: online

DECIMER 1.0: Deep Learning for Chemical Image Recognition using Transformers
K. Rajan, A. Zielesny and C. Steinbeck
ChemRxiv. Preprint: online

2021 **Quantitative estimation of cyclotide-induced bilayer membrane disruption by lipid extraction with mesoscopic simulation**
K. van den Broek, M. Epple, L. S. Kersten, H. Kuhn and A. Zielesny
ChemRxiv. Preprint: online

DECIMER Segmentation - Automated Extraction of Chemical Structure Depictions from Scientific Literature
K. Rajan, H. O. Brinkhaus, M. Sorokina, A. Zielesny and C. Steinbeck
ChemRxiv. Preprint: online

2020 **STOUT: SMILES to IUPAC names using Neural Machine Translation**
K. Rajan, A. Zielesny and C. Steinbeck
ChemRxiv. Preprint: online

Too sweet: cheminformatics for deglycosylation in natural products
J. Schaub, A. Zielesny, C. Steinbeck and M. Sorokina
Preprint: online

DECIMER - Towards Deep Learning for Chemical Image Recognition
K. Rajan, A. Zielesny and C. Steinbeck
ChemRxiv. Preprint: online

Open-Source Software

2023 **MFsim (Versions 2.6.1.0, 2.6.0.0)**
An open Java all-in-one rich-client simulation environment for mesoscopic simulation
Available on GitHub.

Jdpd (Versions 1.6.1.0)
An open Java Simulation Kernel for Molecular Fragment Dissipative Particle Dynamics (DPD)
Available on GitHub.

2022 **MFsim (Versions 2.5.0.0)**
An open Java all-in-one rich-client simulation environment for mesoscopic simulation
Available on GitHub.

Jdpd (Versions 1.6.0.0)
An open Java Simulation Kernel for Molecular Fragment Dissipative Particle Dynamics (DPD)
Available on GitHub.

2021 **MFsim (Versions 2.4.0.0, 2.3.0.0)**
An open Java all-in-one rich-client simulation environment for mesoscopic simulation
Available on GitHub.

Jdpd (Versions 1.5.0.0, 1.4.0.0)
An open Java Simulation Kernel for Molecular Fragment Dissipative Particle Dynamics (DPD)
Available on GitHub.

2020 **MSC (Version 1.0)**
Molecule Set Comparator
Available on GitHub.

MFsim (Version 2.2.4.0)
An open Java all-in-one rich-client simulation environment for mesoscopic simulation
Available on GitHub.

CIP - Computational Intelligence Packages (Version 3.1)
Mathematica® 11 (or higher) open-source library for curve fitting, data smoothing, clustering and machine learning
Available on GitHub.

2019 **ErtlFunctionalGroupsFinder (Versions 1.0.3.0, 1.0.2.0, 1.0.1.0, 1.0.0.0)**
Ertl algorithm for automated functional groups detection and extraction of organic molecules implemented on the basis of the Chemistry Development Kit (CDK)
Available on GitHub.

Jdpd (Versions 1.3.0.0, 1.2.0.0, 1.1.1.0)
An open Java Simulation Kernel for Molecular Fragment Dissipative Particle Dynamics (DPD)
Available on GitHub.

2018 **SPICES (Version 1.0.0.0)**
A particle-based Molecular Structure Line Notation and Support Library for Mesoscopic Simulation
Available on GitHub.

Jdpd (Versions 1.1.0.0, 1.0.2.0, 1.0.1.0 and 1.0.0.0)
An open Java Simulation Kernel for Molecular Fragment Dissipative Particle Dynamics (DPD)
Available on GitHub.

CIP - Computational Intelligence Packages (Version 3.0)
Mathematica® 11 (or higher) open-source library for curve fitting, data smoothing, clustering and machine learning
Available on GitHub.

MathCompiler (Version 1.0.0.0)
A C# high-performance mathematical function compiler for efficient and fast calculation of function values of arbitrary complex single-line mathematical formulas at design and runtime.
Available on GitHub.

2016 **CIP - Computational Intelligence Packages (Version 2.0)**
Mathematica® 10 (or higher) open-source library for curve fitting, data smoothing, clustering and machine learning
Available on GitHub.

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
Available on GitHub.

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: 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
Available on GitHub.

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
Project support was stopped in 2018, see successor project "MathCompiler" above.

Online Lectures

2011 **Chemical File Formats and Line Notations**
A. Zielesny
in C. Steinbeck (ed.), Introduction to Cheminformatics: The Biomedical & Life Sciences Collection, Henry Stewart Talks Ltd, London (online) , 2011 (last reviewed: 2022)

Storing, searching and dissemination of chemical information
A. Zielesny
in C. Steinbeck (ed.), Introduction to Cheminformatics: The Biomedical & Life Sciences Collection, Henry Stewart Talks Ltd, London (online) , 2011 (last reviewed: 2022)

Other Articles

2023 **Decomposition of molecules into biofunctional units** (in German)
F. Bänsch, S. Behr, J. Schaub, B. Sevindik, C. Steinbeck, A. Zielesny
Research and Development at the Westphalian University
Research Report 2022

Molecular interactions for biomolecular mesoscopic simulations (in German)
F. Bänsch, M. Daniel, C. Steinbeck, A. Zielesny
Research and Development at the Westphalian University
Research Report 2022

2022 **DECIMER – Artificial intelligence for optical chemical structure recognition**
K. Rajan, C. Steinbeck, A. Zielesny
Research and Development at the Westphalian University
Research Report 2018 – 2021

Mesoscopic simulation of large (bio)molecular systems
K. van den Broek, A. Zielesny
Research and Development at the Westphalian University
Research Report 2018 – 2021

2021 **DECIMER – Artificial intelligence for recognising the structures of chemical molecules** (in German)
K. Rajan, C. Steinbeck, A. Zielesny
Research and Development at the Westphalian University of Applied Sciences
Research Report 2020

2019 **Mesoscopic Simulation of large (bio)molecular Systems** (in German)
K. van den Broek, A. Zielesny
Research and Development at the Westphalian University of Applied Sciences
Research Report 2018

2015 **A virtual Microscope into the biomolecular Nanoworld** (in German)
K. van den Broek, A. Truszkowski, A. Zielesny
Research and Development at the Westphalian University of Applied Sciences
Research Report 2014

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
J. Chem. Inf. Model. (2005), 45 (5), 1474-1477

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

2023 **DECIMER.ai developments and automated chemical literature mining for COCONUT 2.0**
K. Rajan, H.-O. Brinkaus, M. I. Agea, V. C. Nainala, N. Sharma, A. Zielesny and C. Steinbeck
Lecture at the „ ACS Fall Meeting" from August 13 to 17, 2023, in San Francisco, USA

Training data diversification for data-driven OCSR applications with RanDepict
H.-O. Brinkhaus, K. Rajan, M. I. Agea, A. Zielesny, C. Steinbeck
Poster contribution to the „ ACS Fall Meeting" from August 13 to 17, 2023, in San Francisco, USA

MORTAR – A Rich Client Application for in silico Molecule Fragmentation
F. Bänsch, J. Schaub, B. Sevindik, S. Behr, J. Zander, C. Steinbeck, A. Zielesny
Poster contribution to the „35th Molecular Modeling Workshop" from March 13 to 15, 2023, in Erlangen, Germany

A Calculation Pipeline for Differential Molecule Pair Interaction Energies
F. Bänsch, M. Daniel, H. Lanig, C. Steinbeck, A. Zielesny
Poster contribution to the „35th Molecular Modeling Workshop" from March 13 to 15, 2023, in Erlangen, Germany

2022 **The DECIMER (Deep lEarning for Chemical IMagE Recognition) project**
K. Rajan, H.-O. Brinkhaus, A. Zielesny, C. Steinbeck
Lecture at the „ ACS Fall Meeting" from August 21 to 25, 2022, in Chicago, USA

The DECIMER (Deep lEarning for Chemical IMagE Recognition) project
K. Rajan, H.-O. Brinkhaus, A. Zielesny, C. Steinbeck
Poster contribution to the „12th International Conference on Chemical Structures" from June 12 to 16, 2022, in Noordwijkerhout, The Netherlands

The DECIMER (Deep lEarning for Chemical IMagE Recognition) project
K. Rajan, H.-O. Brinkhaus, A. Zielesny, C. Steinbeck
Lecture at the „17th German Conference on Cheminformatics" from May 8 to 10, 2022, in Garmisch-Partenkirchen, Germany

In silico deglycosylation with the Sugar Removal Utility (SRU)
J. Schaub, A. Zielesny, C. Steinbeck, M. Sorokina
Poster contribution to the „17th German Conference on Cheminformatics" from May 8 to 10, 2022, in Garmisch-Partenkirchen, Germany

MORTAR - An open rich-client framework for in silico molecule fragmentation
F. Bänsch, J. Schaub, C. Steinbeck, A. Zielesny
Poster contribution to the „17th German Conference on Cheminformatics" from May 8 to 10, 2022, in Garmisch-Partenkirchen, Germany

2020 **A new Approach to DPD Repulsion Parameter Estimation**
F. Bänsch, M. Daniel, H. Lanig, C. Steinbeck and A. Zielesny
Poster contribution to the „34th Molecular Modeling Workshop" from February 17 to 19, 2020, in Erlangen, Germany

Rule-based in-silico Fragmentation for the Analysis of Natural Product Chemical Space
J. Schaub, F. Bänsch, A. Zielesny and C. Steinbeck
Poster contribution to the „34th Molecular Modeling Workshop" from February 17 to 19, 2020, in Erlangen, Germany

2019 **Towards a comprehensive open computational support cycle for Molecular Fragment Dissipative Particle Dynamics (DPD)**
F. Bänsch, M. Daniel, J. Schaub, C. Steinbeck, A. Zielesny
Poster contribution to the „15th German Conference on Cheminformatics" from November 3 to 5, 2019, in Mainz, Germany

ErtlFunctionalGroupsFinder: automated rule-based functional group detection with the Chemistry Development Kit (CDK)
J. Schaub, S. Fritsch, S. Neumann, C. Steinbeck, A. Zielesny
Poster contribution to the „15th German Conference on Cheminformatics" from November 3 to 5, 2019, in Mainz, Germany

2018 **Steps towards an open all-in-one rich-client Environment for particle-based Mesoscopic Simulation**
K. van den Broek, H. Kuhn, A. Zielesny and M. Epple
Poster contribution to the „14th German Conference on Cheminformatics" from November 11 to 13, 2018, in Mainz, Germany

PSMILES – A particle-based Molecular Structure Representation for Mesoscopic Simulation
K. van den Broek, M. Daniel, M. Epple, J. Schaub, H. Kuhn and A. Zielesny
Poster contribution to the „11th International Conference on Chemical Structures" from May 27 to 31, 2018, in Noordwijkerhout, The Netherlands

2017 **Mesoscopic Simulations: New Membrane Models & Studying the Mechanism of the Cyclotide Kalata B1 and it's Mutants**
K. van den Broek, H. Kuhn, A. Zielesny and M. Epple
Poster contribution to the „13th German Conference on Chemoinformatics" from November 5 to 7, 2017, in Mainz, Germany

Improved Plasma Membrane Models as Test Systems for the Membrane Disrupting Activity of Kalata B1
K. van den Broek, S. Albrecht, H. Kuhn, A. Zielesny and M. Epple
Poster contribution to the „31th Molecular Modeling Workshop" from March 27 to 29, 2017, in Erlangen, Germany

2016 **Mesoscopic simulation of the membrane disrupting activity of the cyclotide Kalata B1**
K. van den Broek, H. Kuhn, A. Zielesny and M. Epple
Poster contribution to the „12th German Conference on Chemoinformatics" from November 6 to 8, 2016, in Fulda, Germany

2016 **Mesoscopic Simulation of the Membrane Disrupting Activity of the Cyclotide Kalata B1**
K. van den Broek, H. Kuhn, A. Zielesny and M. Epple
Poster contribution to the „30th Molecular Modeling Workshop" from April 4 to 6, 2016, in Erlangen, Germany

2015 **Mesoscopic Simulation of Biomolecular Systems**
A. Zielesny, K. van den Broek, M. Epple, H. Kuhn, A. Truszkowski
Lecture at the „11th German Conference on Chemoinformatics" from November 8 to 10, 2015, in Fulda, Germany
Journal of Cheminformatics 2016, 8(Suppl 1):O8

2014 **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 on Chemoinformatics" from November 10 to 12, 2013, in Fulda, Germany
Journal of Cheminformatics 2014, 6(Suppl 1):P9
(online)

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 on Chemoinformatics" from November 11 to 13, 2012, in Goslar, Germany
Journal of Cheminformatics (2013), 5(Suppl 1): P4
(online)

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
(online)

2011 **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 on Chemoinformatics" from November 6 to 8, 2011, in Goslar, Germany
Journal of Cheminformatics (2012), 4(Suppl 1): P38
(online)

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

2010 **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 on Chemoinformatics" from November 7 to 9, 2010, in Goslar, Germany
Journal of Cheminformatics (2011), 3 (Suppl 1): P5
(online)

2009 **Molecular fragments chemoinformatics**
H. Kuhn, S. Neumann, C. Steinbeck, C. Wittekindt and A. Zielesny
Poster contribution to the „5th German Conference on Chemoinformatics" from November 8 to 10, 2009, in Goslar, Germany
Journal of Cheminformatics (2010), 2 (Suppl 1): P14
(online)

2008 **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 on Chemoinformatics" from November 9 to 11, 2008, in Goslar, Germany
Chemistry Central Journal (2009), 3 (Suppl 1): P42
(online)

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

2007 **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 on Chemoinformatics" from November 11 to 13, 2007, in Goslar, Germany,
Chemistry Central Journal (2008), 2 (Suppl 1): P27
(online)

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 on Chemoinformatics" from November 12 to 14, 2006, in Goslar, Germany

2005 **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 on Chemoinformatics" from November 13 to 15, 2005, in Goslar, Germany

2005 **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 on 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, Nîmes, 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

Iterated Rank based Methods for Clustering
S.W. Perrey, H. Brinck, A. Zielesny
Proceedings of the CSB 2003: IEEE Computer Society Bioinformatics Conference (2003, Stanford), 478-479

2002 **Neural-Network based IT Methods for Job-Man Matching – the personalized Internet Labour Portal** (in German)
H. M. Stindt, A. Zielesny
Workshop „Modern Services for the Labour Market“ of the „Hartz-Committee” of the German Government, May 17, 2002, in Berlin

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
Proc. Int. Chem. Inf. Conf. (1998), 112-119 (Proceedings of the „1998 International Chemical Information Conference & Exhibition (ICIC)“, Nîmes, France)

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**
A. Zielesny, M.Becker, A. Köhler, J. Sendelbach, C. Zirz, W. T. Donner
Proc. Int. Chem. Inf. Conf. (1996), 125-129 (Proceedings of the „1996 International Chemical Information Conference & Exhibition (ICIC)“, Nîmes, France)

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

Scientific Education

Cooperative Dissertation

- **Development of deep learning applications for the automated extraction of chemical information from scientific literature**

  Student: Henning Otto Brinkhaus
  Year: 2023

- **Development and implementation of *in silico* molecule fragmentation algorithms for the cheminformatics analysis of natural product spaces**

  Student: Jonas Schaub
  Year: 2023

- **DARLING: Deep leARning for chemicaL Information processING**

  Student: Kohulan Rajan
  Year: 2021

- **Development of an Open Biomolecular Mesoscopic Simulation Environment for the Study of Cyclotide/Membrane Interactions**

  Student: Karina van den Broek
  Year: 2021

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

  Student: Andreas Truszkowski
  Year: 2015

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

  Student: Thomas Kuhn
  Year: 2009

Master Thesis

- **Standardizing the Natural Product Chemical Space**

  Student: Samuel Behr
  Year: 2023

- **Exploring the natural product space with fragment fingerprinting and clustering**

  Student: Betül Sevindik
  Year: 2023

- **Implementation of Molecular Scaffold Tree Functionality in the Chemistry Development Kit (CDK)**

  Student: Julian Zander
  Year: 2022

- **Machine learning models for biomolecular interaction parameters**

  Student: Lisa Sophie Kersten
  Year: 2021

- **Evaluation of machine learning approaches to support biomolecular simulation**

  Student: Ann-Kathrin Brüggemann
  Year: 2021

- **Molecule Set Comparator – A Cheminformatics Tool for the Evaluation of Machine Learning based Biomolecule Recognition**

  Student: Jan-Mathis Hein
  Year: 2020

- **Design of a computational Information and Analysis Platform for Lead Discovery**

  Student: Jonas Schaub
  Year: 2019

- **Decision Support for Acute Lymphoblastic Leukemia (ALL) Diagnostics**

  Student: Felix Bänsch
  Year: 2018

- **Implementation of an algorithm for the identification of functional groups in organic molecules for the Chemistry development Kit (CDK)**

  Student: Sebastian Fritsch
  Year: 2018

- **Investigation of the Interaction between the Cyclotide Cycloviolacin O2 and Phospholipid Bilayers on the basis of Mutation Studies with Molecular Fragment Dynamics (MFD)**

  Student: Sarah Albert
  Year: 2017

- **Molecular Fragment Dynamics Study of Biological Membranes and Zinc Ricinoleate Layers for Enzyme Purification**

  Student: Karina van den Broek
  Year: 2014

- **Enabling molecular Biosciences: Re-engineering, reaction enumeration and machine learning enhancements for the open workflow platform CDK-Taverna**

  Student: Andreas Truszkowski
  Year: 2011

Bachelor Thesis

- **Successive algorithmic fragmentation of alkyl and cycloalkyl groups in natural products**

  Student: Maximilian Rottmann
  Year: 2023

- **Development of a Rich-Client Graphical User Interface (GUI) for Force Field based Biomolecular Mesoscopic Parameter Estimation**

  Student: Veit Hucke
  Year: 2021

- **Extension of the Molecular Fragmentation Framework MORTAR**

  Student: Samuel Behr
  Year: 2021

- **Development of a Rich-Client Graphical User Interface (GUI) for Machine Learning based Biomolecular Mesoscopic Parameter Estimation**

  Student: Jana Wilms
  Year: 2021

- **Molecular Fragmentation Heuristics for Natural Products**

  Student: Betül Sevindik
  Year: 2021

- **Automated molecular fragmentation for mesoscopic simulation based on functional groups**

  Student: Julian Zander
  Year: 2019

- **Design and Generation of Animated Property Diagrams for Biomolecular Simulation**

  Student: Jan-Mathis Hein
  Year: 2018

- **Simulation of realistic biomolecular Membrane Models with Dissipative Particle Dynamics**

  Student: Lisa Sophie Kersten
  Year: 2018

- **Flexible Design of Protein Fragmentation Patterns for Biomolecular Simulation**

  Student: Katrin Tietz
  Year: 2018

- **Development of an Open Software Component for Validation and Visualization of Fragment-Based Topologic Representation of complex Biomolecular Structures (Particle SMILES)**

  Student: Jonas Schaub
  Year: 2017

- **Descriptor calculation for structural Bioinformatics based on the Chemistry Development Kit (CDK)**

  Student: Felix Jonathan Bänsch
  Year: 2016

- **Investigation of the Interaction between Peptides/Proteins and Phospholipid Bilayers with Molecular Fragment Dynamics (MFD)**

  Student: Sarah Albert
  Year: 2015

- **Development of parallelized machine learning algorithms for biological data analysis with Mathematica**

  Student: Kolja Berger
  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
  Year: 2013

- **Design and development of a rich client application for compound selection based on the Chemistry Development Kit (CDK)**

  Student: Hendrik Göddeke
  Year: 2013

- **Programming a neural Hopfield-Network for pattern recognition**

  Student: Carina Goretzky
  Year: 2012

- **Dependency structures in protein expression data of invasive breast cancer**

  Student: Florian Boecker
  Year: 2012

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

  Student: Julian Jorzik
  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
  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
  Year: 2010

- **Alignment of molecular structures represented by Gaussian functions**

  Student: Christian Geiger
  Year: 2008

- **Molecular Fragment Dynamics Simulations for the Aggregation of Phospholipids at solid Surfaces**

  Student: Christoph Engels
  Year: 2007

- **Quantum-chemical Investigations on Cucurbit[6]uril and α-Cyclodextrin Complexes**

  Student: Jan-Niklas Schäfer
  Year: 2006

- **Software Design Aspects of an electronic Notebook for Materials Sciences**

  Student: Holger Schulte
  Year: 2006

- **Development and implementation of algorithms and software components for the comparison and representation of biological sequences**

  Student: Thomas Kuhn
  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**

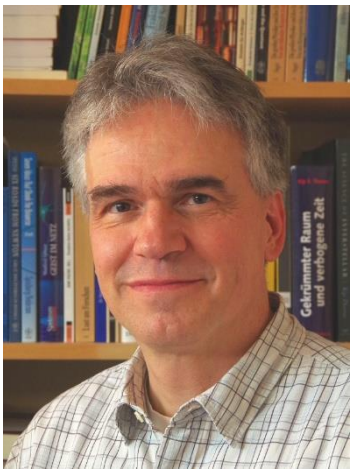
  Student: Stefan Neuman
  Year: 2004

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

  Student: Emrah Ergörül
  Year: 2004

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

  Student: Sandra Bittner
  Year: 2003



Prof. Dr. Achim Zielesny

Westphalian University of Applied Sciences
Institute for Bioinformatics and Chemoinformatics (IBCI)

August-Schmidt-Ring 10
D-45665 Recklinghausen, Germany

Phone +49-2361-915530
E-Mail achim.zielesny@w-hs.de

Day and place of Birth	1964/08/26 in Düsseldorf, Germany

School, Job Training and Military Service

1984	German Abitur and degree as a biological technical assistant
1984/1985	Laboratory assistant in chemical analytics at the Medical Services Research Institute of the German Federal Armed Forces

Academic Education

1986 – 1993	Study of chemistry at the University of Cologne, diploma and doctoral thesis at the Institute of Physical Chemistry (Prof. Dr. D. Woermann) of the University of Cologne Scholarship holder of the German National Academic Foundation (1989 – 1991), Final-Degree Award of the German Chemical Industry Association (1993)

Job

1991 – 1994	Scientific assistant at the University of Cologne
1994 – 2001	Employee of the Bayer AG, Leverkusen (project and group manager in the central research, the computer science and the managerial human resources division)
Since 2001	Professor of Chemistry, Chemoinformatics and Bioinformatics at the Westphalian University of Applied Sciences

Miscellaneous

2004	Founder of the GNWI, a company for scientific computing solutions, Dortmund, Germany
Since 2005	Founder and chairman of the Institute for Bio- and Chemoinformatics at the Westphalian University of Applied Sciences
2005 – 2012	Board member of the Computers in Chemistry (CIC) section of the German Chemical Society (GDCh)
2005 – 2012	Member of the Scientific Advisory Board of the German Conference on Chemoinformatics (GCC)
2007 – 2020	Personal tutor of the German National Academic Foundation (Studienstiftung des deutschen Volkes)
Since 2012	Board member of the Westphalian Institute of Health (WIGE) and person in charge of the research focus Biomedical Modelling and Simulation
2016 – 2021	Founding member of the Life Sciences section of the Graduate Institute for Applied Research at Universities of Applied Sciences in North Rhine-Westphalia (Graduierteninstitut NRW)
Since 2017	Member of the selection committee for the Gmelin-Beilstein-Denkmuenze award of the German Chemical Society (GDCh)
2018	Scientific coordinator of the 32nd Molecular Modelling Workshop (MMWS) 2018 in Erlangen, Germany
2019	Research stay at the Friedrich Schiller University Jena
Since 2021	Associated member of section Life Sciences and Health Technologies of the Doctoral Studies Program in North Rhine-Westphalia (Promotionskolleg NRW)
Since 2021	Member of the Advisory Board *Industry* of the Chemistry Consortium (NFDI4Chem) in the NFDI (Nationale Forschungsdateninfrastruktur)
Since 2021	Member of the organizational committee of the International Workshop on Open Molecular Informatics (IWOMI)
2023	Research stay at the Friedrich Schiller University Jena