Günter Klambauer
Curriculum Vitae

Dr. Mag. Günter Klambauer
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Education

since 2014 **Postdoc Researcher**, *LIT AI LAB & Institute of Bioinformatics, Johannes Kepler University Linz*.

04/2014 **Dr. rer. nat. (PhD) degree**, *Johannes Kepler University Linz*, Thesis: *Machine Learning Techniques for the Analysis of High-Throughput DNA and RNA Sequencing Data*, Supervisor: Sepp Hochreiter. Passed with distinction.

2011-2014 **PhD Study Bioinformatics**, *Johannes Kepler University Linz*, Supervisor: Sepp Hochreiter.

2007-2011 **Master Study Bioinformatics**, *Johannes Kepler University Linz*.

2007-2009 **Secondary School Teacher**, *BORG Linz and BORG Bad Leonfelden*.

07/2007 **Mag. rer. nat. (MSc) Degree**, *University of Vienna*, Thesis: *Topics in Complex Analysis: Laurent-Series, Comformal Mappings and Residue-Theory*, Supervisor: Maria Hoffmann-Ostenhof. Passed with distinction.

09/2006- **Studies Abroad**, *Universitá degli Studi Padova*.
02/2007

2001-2007 **Mathematics and Biology Diploma-Studies**, *University of Vienna*.

Scientific Challenges

2014 **Tox21 Data Challenge**, *Winner of the Grand Challenge, Nuclear Receptor Panel, Stress Response Panel, and six of twelve subchallenges*, `https://tripod.nih.gov/tox21/challenge/leaderboard.jsp` (Team "Bioinf@JKU").

2013 **NIEHS-NCATS-UNC DREAM Toxicogenetics Challenge**, *Best performing method at the prediction of average cytotoxicity*, `https://www.synapse.org/#!Synapse:syn1761567/wiki/60840` (Team "Austria").

Awards

2014 **Award of Excellence 2014**, *Award given by the Austrian Ministry of Science*, `http://www.jku.at/content/e213/e63/e43?apath=e32681/e225072/e261074/e261376`.

2012 **Austrian Life Science Award 2012**, *http://www.chemiereport.at/alsa-2012-wissenschaftspreis-wien-vergeben*.

Selected Publications

2017 **Self-normalizing neural networks**, *Günter Klambauer, Andreas Mayr, Thomas Unterthiner, and Sepp Hochreiter*, Advances in Neural Information Processing Systems 30: 972–981.

2016 **Deeptox: Toxicity prediction using Deep Learning**, *Günter Klambauer, Andreas Mayr, Thomas Unterthiner, and Sepp Hochreiter*, Frontiers in Environmental Science (2016): 3, 80.

2014 **Deep Learning as an Opportunity in Virtual Screening**, *Thomas Unterthiner, Andreas Mayr, Günter Klambauer, Marvin Steijart, Jörg Wegner, Hugo Ceulemans, and Sepp Hochreiter*, Deep Learning and Representation Learning Workshop (NIPS 2014).

2014 **Deep Learning for Drug Target Prediction**, *Thomas Unterthiner, Andreas Mayr, Günter Klambauer, Marvin Steijart, Jörg Wegner, Hugo Ceulemans, and Sepp Hochreiter*, Workshop on Representation and Learning Methods for Complex Outputs (NIPS2014).

2015 **ELU-Networks - Fast and Accurate CNN Learning on ImageNet**, *Martin Heusel, Djork-Arne Clevert , Günter Klambauer, Andreas Mayr, Karin Schwarzbauer, Thomas Unterthiner, Sepp Hochreiter*, International Conference on Computer Vision 2015.

2017 **Repurposed high-throughput images enable biological activity prediction for drug discovery**, *Guenter Klambauer, Jaak Simm, Adam Arany, Marvin Steijaert, Jörg Kurt Wegner, Emmanuel Gustin, Vladimir Chupakhin, Yolanda T. Chong, Jorge Vialard, Peter Buijnsters, Ingrid Velter, Alexander Vapirev, Shantanu Singh, Anne Carpenter, Roel Wuyts, Sepp Hochreiter, Yves Moreau, Hugo Ceulemans*, bioRxiv (2017): 108399, `https://doi.org/10.1101/108399` .

2015 **Prediction of human population responses to toxic compounds by a collaborative competition**, *Federica Eduati, Lara M Mangravite, Tao Wang, ... , Sepp Hochreiter, Günter Klambauer, Andreas Mayr, ..., Ivan Rusyn, Fred A Wright, Gustavo Stolovitzky, Yang Xie, and Julio Saez-Rodriguez*, Nature Biotechnology (2015), `http://doi:10.1038/nbt.3299` .

2015 **Rchemcpp: a web service for structural analoging in ChEMBL, Drugbank and the Connectivity Map**, *Günter Klambauer, Martin Wischenbart, Michael Mahr, Thomas Unterthiner, Andreas Mayr, and Sepp Hochreiter*, Bioinformatics (2015), `doi: 10.1093/bioinformatics/btv373` .

2015 **Using Transcriptomics to Guide Lead Optimization in Drug Discovery Projects: Lessons Learned from the QSTAR Project**, *Günter Klambauer, The QSTAR Consortium, and Sepp Hochreiter*, Drug Discovery Today (2015): 20(5), `doi:10.1016/j.drudis.2014.12.014`.

2013 **DEXUS: identifying differential expression in RNA-Seq studies with unknown conditions**, *Günter Klambauer,Thomas Unterthiner and Sepp Hochreiter*, Nucleic Acids Research (2013): 41(21), e198-e98, `doi:10.1093/nar/gkt834`.

2013 **Increasing the discovery power of -omics studies**, *Djork-Arné Clevert, Andreas Mayr, Andreas Mitterecker, Günter Klambauer, Armand Valsesia, Karl Forner, Marianne Tuefferd, Willem Talloen, Jérôme Wojcik, Hinrich Göhlmann and Sepp Hochreiter*, Systems Biomedicine (2013): 1(2), 0-9.

2012 **Exploiting the Japanese toxicogenomics project for predictive modelling of drug toxicity**, *Djork-Arné Clevert, Martin Heusel, Andreas Mitterecker, Willem Talloen, Hinrich Göhlmann, Jörg Wegner, Andreas Mayr, Günter Klambauer, Sepp Hochreiter*, CAMDA (2012).

2012 **cn.MOPS: mixture of Poissons for discovering copy number variations in next generation sequencing data with a low false discovery rate**, *Günter Klambauer, Karin Schwarzbauer, Andreas Mayr, Djork-Arné Clevert, Andreas Mitterecker, Ulrich Bodenhofer and Sepp Hochreiter*, Nucleic Acids Research (2012): 40(9), e69-e69, `doi:10.1093/nar/gks003`.

2011 **cn.FARMS: a latent variable model to detect copy number variations in microarray data with a low false discovery rate**, *Djork-Arné Clevert, Andreas Mitterecker, Andreas Mayr, Marianne Tuefferd, An De Bondt, Willem Talloen, Hinrich W.H. Göhlmann and Sepp Hochreiter*, Nucleic Acids Research (2011): 39(12), e79-e79, `doi:10.1093/nar/gkr197` .

Selected Research Projects

4/2016 - 4/2018 **Exaptation – Scalable solutions for image-based and across-partner compound activity prediction and application to compound selection**, *Project founded by JANSSEN RESEARCH & DEVELOPMENT, a division of JANSSEN PHARMACEUTICA N.V.*, Project supported by Belgium government., Research Partners: University of Leuven (ESAT), Belgium; Johannes Kepler University, Institute of Bioinformatics, Austria.

7/2014 - 6/2016 **ChemBioBridge – Bridging chemistry and biology for pharma industry through kernel-based large-scale data fusion**, *Project founded by JANSSEN RESEARCH & DEVELOPMENT, a division of JANSSEN PHARMACEUTICA N.V.*, Project supported by Belgium government., Research Partners: University of Leuven (ESAT), Belgium; Johannes Kepler University, Institute of Bioinformatics, Austria.

10/2011 - 2/2014 **QSTAR — Gene expression assisted compound chemistry**, *Project funded by Johnson & Johnson Pharmacedutical Research and Development, Divisie Van Janssen Pharmaceutica N.V.*, Project supported by Belgium government., Research Partners: Hasselt University, Center for Statistics, Belgium; Johannes Kepler University, Institute of Bioinformatics, Austria .

1/2009 - 12/2010 **Cell line based compound prioritization and response prediction**, *Project funded by Johnson & Johnson Pharmacedutical Research and Development, Divisie Van Janssen Pharmaceutica N.V.*, Project supported by Belgium government through project no. IWT 80536, Research Partners: Hasselt University, Center for Statistics, Belgium; Johannes Kepler University, Institute of Bioinformatics, Austria.

Conference Talks

2017 **Self-normalizing neural networks**, Thirty-first Annual Conference on Neural Information Processing Systems, Long Beach, USA, December 4-9 2017.

2016 **DeepTox: Deep Learning for Toxicity Prediction**, 55th Annual Meeting of the Society of Toxicology, New Orleans, USA, March 13-17 2016.

2015 **Deep Learning for Toxicity Prediction**, German Conference on Chemoinformatics 2015, Fulda, Germany, Nov 8-11 2015.

2015 **Machine Learning Techniques for the Analysis of High-Throughput DNA- and RNA-Sequencing Data**, Dagstuhl Seminar 15202: Kolloquium zum GI Dissertationspreis 2014, Dagstuhl, Germany, May 10-23 2015.

2013 **Detecting differentially expressed genes in RNA-Seq drug design studies**, Dagstuhl Seminar 13212: Computational Methods Aiding Early-Stage Drug Design, Dagstuhl, Germany, May 19-24 2013.

2012 **CNV detection from exome sequencing data using a generative probabilistic model**, 13th International Meeting on Human Genome Variation and Complex Genome Analysis (HGV 2012), Shanghai, China, Sept 6-8 2012.

2012 **cn.MOPS: mixture of Poissons for discovering copy number variations in next generation sequencing data with a low false discovery rate**, 20th Annual International Conference on Intelligent Systems for Molecular Biology (ISMB), Long Beach, CA USA, July 15-17 2012.

Posters

2017 **Self-normalizing neural networks**, Thirty-first Annual Conference on Neural Information Processing Systems, Long Beach, USA, December 4-9 2017.

2014 **Detection of Copy Number Variations in Cancer Genomes from High Throughput Sequencing Data**, Annual Meeting of the American Society of Human Genetics (ASHG2014), San Diego, USA, October 18-22, 2014.

2013 **Detecting differentially expressed genes in RNA-Seq data with unknown conditions**, Annual Meeting of the American Society of Human Genetics (ASHG2013), Boston, USA, October 22-26, 2013.

2011 **Accurate detection of copy number variations in next generation sequencing data by a latent variable model**, 12th International Congress of Human Genetics and the American Society of Human Genetics (ICHG/ASHG 2011), Montreal, Canada, Oct 11-15 2011.

2011 **cn.MOPS: mixture of Poissons for discovering copy number variations in next generation sequencing data**, International Meeting on Human Genome Variation and Complex Genome Analysis (HGV 2011), San Francisco,CA USA, Sept 8-10 2011.

2011 **cn.MOPS: mixture of Poissons for discovering copy number variations in next generation sequencing data**, 19th Annual International Conference on Intelligent Systems for Molecular Biology (ISMB), Vienna, Austria, July 17-19 2011.

2010 **A normalization technique for next generation sequencing experiments**, 18th Annual International Conference on Intelligent Systems for Molecular Biology (ISMB), Boston, MA USA, July 11-13 2010, `doi:10.1038/npre.2010.4710.1`.

2010 **Identifying copy number variations based on next generation sequencing data by a mixture of Poisson model**, 18th Annual International Conference on Intelligent Systems for Molecular Biology (ISMB), Boston, MA USA, July 11-13 2010, `doi:10.1038/npre.2010.4716.1`.

Supervised master theses

2017 **Backward dynamics of self-normalizing networks**, *Pieter-Jan Hoedt*.

2017 **Generative RNN models for molecular strings with biological activity profiles**, *Philipp Renz*, ongoing.

2017 **Generative adversarial networks for molecular strings**, *Isaac Lazzeri*, ongoing.

2017 **Improving image-based compound activity prediction with convolutional neural networks**, *Katrin Strasser*, ongoing.

2016 **Deep Learning for Drug Combination Synergy Prediction**, *Kristina Preuer*.

2015 **The Maximum Common Subgraph Kernel For Predicting Kinase Inhibitors**, *Sabine Schwandegger*.

2015 **Panelcn.MOPS reaches clinical standards as a copy number variation detection tool for targeted panel sequencing**, *Verena Haunschmid*.

2015 **Accurate detection of tumor copy number variations in high-throughput sequencing data**, *Patrick Praher*.

2014 **Detecting CNVs in the 1000 Genomes Project Data Using cn.MOPS and Relating the Results to Transcriptome Sequencing Data**, *Anna Langmüller*.

Teaching Experience

2017 **Special Topics on Bioinformatics: Population genetics**, *Lecturer*, Johannes Kepler University, Linz, Austria.

2016 **Special Topics on Bioinformatics: Population genetics**, *Lecturer*, Johannes Kepler University, Linz, Austria.

2014 **Special Topics on Bioinformatics: Population genetics**, *Lecturer*, Johannes Kepler University, Linz, Austria.

2013/2014 **Sequence Analysis and Phylogenetics**, *Lecturer*, Johannes Kepler University, Linz, Austria.

2013 **Special Topics on Bioinformatics: Population genetics**, *Lecturer*, Johannes Kepler University, Linz, Austria.

2012/2013 **Sequence Analysis and Phylogenetics**, *Lecturer*, Johannes Kepler University, Linz, Austria.

2012 **Special Topics on Bioinformatics: Population genetics**, *Lecturer*, Johannes Kepler University, Linz, Austria.

2011/2012 **Exercises in Bioinformatics I: Sequence Analysis and Phylogenetics**, *Lecturer*, Johannes Kepler University, Linz, Austria.

2011	**Special Topics on Bioinformatics: Population genetics**, *Lecturer*, Johannes Kepler University, Linz, Austria.
2010/2011	**Exercises in Bioinformatics I: Sequence Analysis and Phylogenetics**, *Lecturer*, Johannes Kepler University, Linz, Austria.
2010	**Special Topics on Bioinformatics: Population genetics**, *Lecturer*, Johannes Kepler University, Linz, Austria.
2009/2010	**Exercises in Bioinformatics I: Sequence Analysis and Phylogenetics**, *Lecturer*, Johannes Kepler University, Linz, Austria.
2008-2009	**Mathematics and Biology**, *Secondary School Teacher*, Bundesoberstufenrealgymnasium BORG Linz, Linz, Austria.
2007-2008	**Mathematics and Biology**, *Secondary School Teacher*, Bundesoberstufenrealgymnasium Bad Leonfelden, Bad Leonfelden, Austria.

Linz, December 18, 2017

Klambauer Günter