

# Günter Klambauer

## Curriculum Vitae

Dr. Mag. Günter Klambauer  
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### Education

- Since 2019 **Assistant Professor for “Artificial Intelligence in Life Sciences”**, *LIT AI Lab & Institute for Machine Learning, Johannes Kepler University Linz.*
- 2017–2019 **Group Leader “Artificial Intelligence in Drug Discovery”**, *LIT AI Lab & Institute for Machine Learning, Johannes Kepler University Linz.*
- 2014–2017 **Postdoc Researcher**, *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.
- 2010-2014 **PhD Study Bioinformatics**, *Johannes Kepler University Linz*, Supervisor: Sepp Hochreiter.
- 2007-2010 **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, Conformal Mappings and Residue-Theory*, Supervisor: Maria Hoffmann-Ostenhof. Passed with distinction.
- 09/2006-02/2007 **Studies Abroad**, *Università degli Studi Padova.*
- 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 & Honors

- 2020 **Member of the ELLIS society**, *Society for excellent machine learners in Europe*, <https://ellis.eu/members>.
- 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:

- 2019 **Accurate Prediction of Biological Assays with High-Throughput Microscopy Images and Convolutional Networks**, Markus Hofmarcher, Elisabeth Rumetshofer, Djork-Arne Clevert, Sepp Hochreiter, Günter Klambauer, *Journal of chemical information and modeling*.
- 2018 **Frechet Chemnet Distance: a Metric for Generative Models for Molecules in Drug Discovery**, Kristina Preuer, Philipp Renz, Thomas Unterthiner, Sepp Hochreiter, Günter Klambauer, *Journal of chemical information and modeling*: 58(9), 1736–1741.
- 2017 **Self-normalizing neural networks**, Günter Klambauer, Andreas Mayr, Thomas Unterthiner, and Sepp Hochreiter, *Advances in Neural Information Processing Systems* 30: 972–981.
- 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> .
- 2016 **Deeptox: Toxicity prediction using Deep Learning**, Günter Klambauer, Andreas Mayr, Thomas Unterthiner, and Sepp Hochreiter, *Frontiers in Environmental Science* (2016): 3, 80.
- 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 **Using Transcriptomics to Guide Lead Optimization in Drug Discovery Projects: Lessons Learned from the QSTAR Project**, Günter Klambauer, *The QSTAR Constortium*, and Sepp Hochreiter, *Drug Discovery Today* (2015): 20(5), [doi:10.1016/j.drudis.2014.12.014](https://doi.org/10.1016/j.drudis.2014.12.014).
- 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)*.
- 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](https://doi.org/10.1093/nar/gkt834).
- 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-Arne Clevert, Andreas Miterecker, Ulrich Bodenhofer and Sepp Hochreiter, *Nucleic Acids Research* (2012): 40(9), e69-e69, [doi:10.1093/nar/gks003](https://doi.org/10.1093/nar/gks003).

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## Projects

- 3/2018 - **DeepToxGen: Deep Learning for in-silico toxicogenetics testing**, *Project*  
8/2020 *funded by LIT (Linz Institute of Technology).*
- 10/2019 - **AI-SNN: Self-normalizing neural networks as enablers of functional mod-**  
9/2021 **ularity in large AI systems**, *Project funded by LIT (Linz Institute of Technology).*
- 9/2019 - **MadeSMART: Deep Learning for in-silico toxicogenetics testing**, *Project*  
8/2021 *funded by Janssen Pharmaceuticals.*
- 10/2019 - **UCBnet: Driving drug design with deep multimodal and multi-task learn-**  
9/2021 **ing**, *Project funded by UCB Biopharma.*
- 11/2019 - **Merck: Drug target prediction**, *Project funded by Merck.*  
10/2022

Vienna, June 12, 2020

*Klambauer Günter*