Jitao David Zhang

A Computational Biologist in Drug Discovery

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Key facts

- Interdisciplinary researcher with 10+ years' experience in drug discovery.
- Supporting drug discovery projects between target identification and Phase I.
- Proponent of multiscale modeling and causal inference of drug mechanism and safety.
- Open-source software developer and open-access author (40+ publications, *h*-index 25).

Research and teaching

2011– **Expert Computational Biologist**, *F. Hoffmann-La Roche AG*, Basel, Switzerland.
I develop algorithms and software to mine, interpret, model and integrate heterogeneous data, and apply mathematical and computational tools to support preclinical drug discovery projects. I am responsible for target assessment and validation, multiscale modeling and causal inference of drug mechanism and safety, and MoA characterisation and de-risking of drug candidates. With colleagues I co-develop novel platforms and resources to support drug discovery, for instance the molecular phenotyping platform, the Pathway-Annotated Chemical Ensemble (PACE) library, and new methods for computational toxicology and safety assessment.

2018– **Lecturer**, *Department of Mathematics and Computer Science, University of Basel.*
Teaching the lecture series *Introduction to **A**pplied **M**athematics and **I**nformatics In **D**rug **D**iscovery* (http://AMIDD.ch) in autumn semesters, and ***M**athematical and **C**omputational **B**iology in **D**rug **D**iscovery* (http://MCBDD.ch) in spring semesters.

Training, mentoring, and academic commitment

2022– Co-organizer of Roche PMDA (Predictive Modeling and Data Analytics) Summer School for PhD students.

2021– Certified *Lehrmeister* for informatics vocational apprenticeship.

2020– Certified Software and Data Carpentry instructor, hosting company internal carpentries.

2018– Participation in the lecture series *From Novel Targets To Novel Therapeutic Modalities*, Master Programme Drug Sciences, University of Basel.

2016– Supervising master students in bioinformatics and computational biology, and co-supervise PostDocs in collaboration with academic and industrial collaboration partners.

2012– Reviewing research proposals for funding agencies and manuscripts for journals including *Bioinformatics*, *PLOS Comp. Biol.*, *NAR Genom. and Bioinform.*, *etc.*

2012– Leading courses, seminars and workshops about programming, bioinformatics, and computational biology in drug discovery.

Education

2008–2011 **Dr.rer.nat. Bioinformatics**, *German Cancer Research Center/ Universität Heidelberg*.
Computational and statistical approaches to study gene networks, supervised by Dr. Stefan Wiemann

2007-2007 **Marie-Curie Fellow**, *Huber Group, European Institute of Bioinformatics*, Cambridge, UK.

2006–2008 **M.Sc. Bioinformatics**, *Universität Heidelberg*, Germany.

2002–2006 **B.Sc. Biology, hon.**, *Peking University*, Beijing, China.

Selected peer-reviewed publications

Optimization of the teratox assay for preclinical teratogenicity assessment. *Toxicological Sciences*, 2022.

Besca, a single-cell transcriptomics analysis toolkit to accelerate translational research. *NAR Genomics and Bioinformatics*, 2021.

Inducers of the endothelial cell barrier identified through chemogenomic screening in genome-edited hPSC-endothelial cells. *PNAS*, 2020.

Multiscale modelling of drug mechanism and safety. *Drug Discovery Today*, 2020.

Assessment of network module identification across complex diseases. *Nature Methods*, 2019.

Comprehensive evaluation of transcriptome-based cell-type quantification methods for immuno-oncology. *Bioinformatics*, 2019.

→ See the full, manually curated list at Google Scholar (http://goo.gl/CoeJu7).

Selected invited talks

2021 *Optimization of the TeraTox assay for preclinical teratogenicity assessment*, co-presentation with Manuela Jaklin, OpenTox Virtual Conference, 2021

2019 *Bioinformatics and exploratory data analysis in drug discovery: an industrial perspective*, ISMB/ECCB, 2019, Basel, Switzerland

2018 *Mathematics in drug discovery: a practitioner's view*, Perlen-Kolloquium, University of Basel, Basel, Switzerland

Selected open-source software

BESCA Single-cell omics data analysis pipeline, built together with BEDA colleagues.

BioQC Detecting tissue heterogeneity in high-throughput expression data.

KEGGgraph Data mining and network analysis of biological pathways as graphs in R and Bioconductor.

Computer skills

Programming R/Bioconductor, C/C++, Java, Python

Scripting Python, Bash, Erlang

OS Debian Linux, Windows

Database PostgreSQL, SQLite, MongoDB

Web HTML, CSS, JavaScript, Flask, FastAPI

Others d3js, OpenCV, ImageMagick, LaTeX

Personal information

Date of Birth Sept. 28^{th}, 1983 in Tianjin, China

Marital status Married, father of two daughters

Languages English, German, Chinese