

# 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 Applied Mathematics and Informatics In Drug Discovery* (<http://AMIDD.ch>) in autumn semesters, and *Mathematical and Computational Biology in Drug Discovery* (<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	Database	PostgreSQL, SQLite, MongoDB
Scripting	Python, Bash, Erlang	Web	HTML, CSS, JavaScript, Flask, FastAPI
OS	Debian Linux, Windows	Others	d3js, OpenCV, ImageMagick, L <sup>A</sup> T <sub>E</sub> X

## Personal information

- Date of Birth Sept. 28<sup>th</sup>, 1983 in Tianjin, China
- Marital status Married, father of two daughters
- Languages English, German, Chinese