# Jitao David Zhang

A Computational Biologist in Drug Discovery

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## Key facts

- Interdisciplinary researcher with 10+ years' experience in drug discovery.
- O 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

- Senior Principal 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 and the Small-molecule PAthway Research Kit (SPARK) library.
- Lecturer, University of Basel, Basel, Switzerland, I teach 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 at the Department of Mathematics and Informatics.

#### 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	<b>Dr.rer.nat. Bioinformatics</b> , 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, LATeX

#### Personal information

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

Marital status Married, father of two daughters

Languages English, German, Chinese