Jitao David Zhang

A Computational Biologist in Drug Discovery

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Key facts

- Interdisciplinary researcher with more than ten years' experience in drug discovery.
- Supporting 30+ projects per year by algorithm development and data modelling.
- Open-source software developer and open-access author (40+ publications, *h*-index 24).
- Proponent of multiscale modelling of drug mechanism and safety.

Research career

2011– **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 modelling 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.

Teaching, mentoring, and academic commitment

2018– Teaching lecture series *Introduction to **A**pplied **M**athematics and **I**nformatics In **D**rug **D**iscovery* (http://AMIDD.ch) and *Mathematical and **C**omputational **B**iology in **D**rug **D**iscovery* (http://MCBDD.ch), Department of Mathematics and Informatics, University of Basel.

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. Certificated as a Carpentury Instructor in 2021.

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

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.

A novel orally available small molecule that inhibits hepatitis B virus expression. *Journal of Hepatology*, 2018.

Detect tissue heterogeneity in gene expression data with BioQC. *BMC Genomics*, 2017.

Molecular phenotyping combines molecular information, biological relevance, and patient data to improve productivity of early drug discovery. *Cell Chemical Biology*, 2017.

Genomic analysis of the molecular neuropathology of tuberous sclerosis using a human stem cell model. *Genome Medicine*, 2016.

14-3-3ζ turns TGF-β's function from tumor suppressor to metastasis promoter in breast cancer by contextual changes of smad partners from p53 to Gli2. *Cancer Cell*, 2015.

White-to-brown metabolic conversion of human adipocytes by JAK inhibition. *Nature Cell Biology*, 2015.

Data mining reveals a network of early-response genes as a consensus signature of drug-induced *in vitro* and *in vivo* toxicity. *The Pharmacogenomics Journal*, 2013.

KEGGgraph: a graph approach to KEGG PATHWAY in R and Bioconductor. *Bioinformatics*, 2009.

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

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
Hobbies	Family, run & bike, reading, mathematics, programming, music
Languages	English, German, Chinese