

Julian Zaugg

Curriculum Vitae

Contact details

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Education

Jul 2013 - Jan 2018 (expected)	<p>PhD candidate in Bioinformatics - School of Chemistry and Molecular Biosciences, University of Queensland, Brisbane, Australia.</p> <p>Thesis : <i>Computational Modelling of Enzymes – Methods to Understand the Origin of Function and Predict Beneficial Mutations</i></p> <p>The thesis investigated how experimental data produced from protein engineering studies could be complemented by computational and statistical methods to predict beneficial mutations and understand protein function. Sequence, structural and biochemical data for the epoxide hydrolase from the fungus <i>Aspergillus niger</i> was used as a model system. The ability of contrasting machine learning methods, i.e. <i>generative</i> vs <i>discriminative</i>, to predict selectivity-enhancing mutations was evaluated. Molecular modelling methods such as docking, molecular dynamics and free energy calculations were used to understand the origin of enantioselectivity.</p> <p>Primary supervisor : Assoc. Prof. Dr. Mikael Bodén</p>
2009–2012	<p>Bachelor of Biomedical Science - Honours First Class, School of Chemistry and Molecular Biosciences, University of Queensland, Brisbane, Australia</p> <p>Thesis : <i>Predicting the fold status of a hybrid protein – an in-silico study of cytochrome P450 enzymes</i></p> <p>The Honours thesis focused on the development of a generalised tool/model framework for the prediction protein fold status. This involved the identification of highly co-evolved residues within the Cytochrome P450 super family and their use as variables within predictive models.</p> <p>Primary supervisor : Assoc. Prof. Dr. Mikael Bodén</p>

Scholarship supported research

**Apr 2014 -
Jan 2017**

Australian Postgraduate Award (APA) for PhD, University of Queensland, Brisbane, Australia

“APA scholarships are awarded to students of exceptional research potential undertaking a higher research degree in Australia”. This scholarship was used to support a PhD candidacy at the University of Queensland. From 1st of January 2017, APA scholarships are now referred to as Research Training Program (RTP) scholarships.

**Dec 2011 -
Feb 2012**

Undergraduate Research Scholar, School of Chemistry and Molecular Biosciences, University of Queensland, Brisbane, Australia

The project involved the design and development of a code package for constructing Bayesian networks. This package was to be used for the modelling of biological systems, e.g. for motif discovery, protein abundance prediction, etc. Work was primarily performed in Python with optimisation with Cython, converting from an existing Java implementation.

Primary supervisor : Assoc. Prof. Dr. Mikael Bodén

Professional/Teaching experience

**Feb 2017 -
Jun 2017**

Tutor, University of Queensland, Brisbane, Australia

Tutored in and developed material for ‘Introduction to Bioinformatics’ course (SCIE2100). Helped students with programming and data analysis tasks during practical sessions.

**Mar 2016 -
Jun 2016**

Access Assistant, University of Queensland, Brisbane, Australia

Access Assistants are casual staff employed to carry out tasks required by a student with a disability. In this case, assistance was provided to a student for the ‘Introduction to Bioinformatics’ course (SCIE2100).

Research publications

**Manuscripts available on request*

Book chapter

- **Zaugg J.**, Gumulya Y., Gillam E. M. J. and Bodén M., *Computational tools for directed evolution: a comparison of prospective and retrospective strategies*. *Methods in Molecular Biology*, 2014, 1179, 315-333.

Peer reviewed journals

- **Zaugg J.**, Gumulya Y., Malde A. K. and Bodén M., *Learning epistatic interactions from sequence-activity data to predict enantioselectivity*, 2017, doi:10.1007/s10822-017-0090-x
- **Zaugg J.**, Gumulya Y., Bodén M., Mark A. E. and Malde A. K., *The effect of binding on the enantioselectivity of an epoxide hydrolase*, 2017 [Under revision]

Research and Technical skills

■ **Computational biology and structural modelling**

Extensive knowledge of computational and statistical methods for library and sequence design for protein engineering. Good knowledge of and experience in performing evolutionary analysis, e.g. ancestral sequence reconstruction, phylogenetics and multiple sequence alignment. Experienced in protein-ligand docking, conformer analysis and the development of virtual screening pipelines for the discovery of enzyme inhibitors. Also experienced in the use of molecular dynamics simulations, energy minimisation, free-energy calculations and 3-dimensional structure alignments to understand enzyme properties.

■ **Machine learning and statistics**

Experienced in applying Bayesian, specifically Bayesian networks, and support vector machine methods to model complex biological systems. Working knowledge of alternative machine learning and various statistical methods used for data analysis.

■ **High performance computing**

Experienced user of high performance computing clusters (HPCCs) 'Euramoo' and 'Tinaroo', provided by the University of Queensland and the Queensland Cyber Infrastructure Foundation (QCIF). Also user of HPCC 'Raijin' serviced by the National Computational Infrastructure (NCI), which is supported by the Australian government.

■ **Version control**

Experience in using version control, e.g. Subversion and Git (GitHub and GitLab), for reproducible research and collaborative development of code projects.

■ **Programming/Other languages**

Python (strong knowledge, preferred and primary language)
LaTeX (strong knowledge)
Java, R, Bash (good knowledge)

■ **Open-source software setup on UNIX systems**

Experienced in the installation and setup of open-sourced software used on UNIX operating systems (Linux/MacOS), e.g. for scientific research. Regular user of software management tools such as Home/LinuxBrew, Pip, Fink and Macports. Familiar with compiling software from source.

■ **Graphic design and data visualisation**

Experienced in the use of graphic design software, i.e. Adobe Illustrator/Photoshop and Inkscape, for development of high-quality technical illustrations. Also experienced in the use of data visualisation packages, e.g. matplotlib (Python) and ggplot (R) for data analysis and presentation. Familiar with javascript visualisation packages, e.g. D3.

Conferences and Workshops

Oral presentations

- **Zaugg J.**, Gumulya Y., Mark A.E., Bodén M. and Malde A. K., *Understanding the enantioselectivity of enzymes using computational methods*, Centre for Theoretical and Computational Molecular Science (CTCMS) Symposium on Computational Methods and Applications, University of Queensland, Brisbane, Australia, November 4th, [2016](#)
- **Zaugg J.**, Gumulya Y., Bodén M., Malde A. K., *Guiding protein design using higher-order evolutionary model based kernel functions*, School of Chemistry and Molecular Biosciences (SCMB) Structural Theme Meeting, April 26th, [2016](#)

- **Zaugg J.**, Gumulya Y., Bodén M., *Computational methods to explore evolutionary pathways – utilising family-specific features to design fitter enzymes*, School of Chemistry and Molecular Biosciences (SCMB) Research Students Symposium, University of Queensland, Brisbane, Australia, November 26th, 2014

Poster presentations

- **Zaugg J.**, Gumulya Y., Malde A. K., and Bodén M., *Learning epistatic interactions from sequence-activity data to predict enantioselectivity*, Australian Bioinformatics and Computational Biology Society (ABACBS) National Conference, Adelaide, Australia, November 13th-15th, 2017
- **Zaugg J.**, Gumulya Y., Mark A.E., Bodén M. and Malde A. K., *The effect of binding on the enantioselectivity of an epoxide hydrolase*, Australian Bioinformatics and Computational Biology Society (ABACBS) National Conference, Adelaide, Australia, November 13th-15th, 2017
- **Zaugg J.**, Gumulya Y., Mark A.E., Bodén M. and Malde A. K., *Using modelling to complement experiment: understanding the origin of enantioselectivity of epoxide hydrolase*, The 21st Annual International Conference on Research in Computational Molecular Biology (RECOMB2017), Hong Kong, May 3rd-7th, 2017
- **Zaugg J.**, Gumulya Y., Bodén M., *Guiding walks across fitness landscapes–modelling epistatic interactions with probabilistic evolutionary kernel functions*, School of Chemistry and Molecular Biosciences (SCMB) Research Students Symposium, University of Queensland, Brisbane, Australia, November 26th, 2015
- **Zaugg J.**, Gumulya Y., Bodén M., *probabilistic evolutionary kernel function for analysis of protein sequence-function relationships*, The Australian Bioinformatics and Computational Biology Society (ABACBS) conference, Sydney, Australia, November 10th, 2015

Professional membership

- The Australian Bioinformatics and Computational Biology Society (ABACBS)

References

On request.