Fábio Madeira

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EXPERIENCE

Since 2016 Postdoctoral Research Assistant in Bioinformatics

Geoff Barton's Group, Division of Computational Biology, University of Dundee, UK. Currently Working on the Dundee Resources, "Tier-1" by the ELIXIR-UK Network (Protein Structure and Function), and developing new approaches to analyse structural and genomic data.

2012-2016 Wellcome Trust PhD in Computational Biology

Geoff Barton's Group, Division of Computational Biology, University of Dundee, UK. My work focused on the analysis of genetic variation in protein structure interaction surfaces. The project was heavy on software development, data analysis and visualisation, development/benchmarking of machine learning classifiers, and web development.

2010-2012 Research Studentship in Bioinformatics and Artificial Intelligence Ludwig Krippahl's Group, Department of Computer Science, Universidade Nova de Lisboa, Portugal. The project involved software development and benchmarking of coevolution methods as constraints for protein docking, and development of new approaches to generate multiple sequence alignments.

EDUCATION

2012-2016 PhD in Computational Biology, University of Dundee

Supervisor: Prof Geoff J. Barton; Internal Examiner: Prof Helen Walden (University of Dundee); external Examiner: Prof David T. Jones (University College London). PhD Thesis: "Analysis of variation in protein domain families and interfaces". Viva voce passed with minor corrections.

2008-2010 MSc in Molecular Genetics, Universidade Nova de Lisboa

Supervisiors: Prof. Maria João Romão's and Prof. Ana Paula Leandro. Master Thesis: "Estudos estruturais e funcionais da fenilalanina hidroxilase humana" (Written in Portuguese). Santander-NOVA Merit Scholarship Award.

2004-2008 BSc in Biochemistry, Universidade Nova de Lisboa

ECTN Chemistry Eurobachelor Degree. Ranked 2nd in class.

PUBLICATIONS

Fábio Madeira, Thiago Britto-Borges, Stuart MacGowan and Geoffrey J. Barton (2017) **ProteoFAV: fast structural data integration with Pandas**. About to be submitted to Bioinformatics.

Peter V. Troshin, Alexander Sherstnev, James B. Procter, Daniel L. Barton, Fábio Madeira and Geoffrey J. Barton (2017) **JABAWS 2.2 Distributed Web Services** for Bioinformatics: Protein Disorder, Conservation and RNA Secondary Structure. About to be submitted to Bioinformatics.

Peter Troshin, Agnieszka Golicz, David Martin, Fábio Madeira, James B. Procter and Geoffrey J. Barton (2017) **AACon: A Fast Amino Acid Conservation Calculation Service**. About to be submitted to Bioinformatics.

Stuart A MacGowan, Fábio Madeira, Thiago Britto Borges, Melanie S Schmittner, Christian Cole, Geoffrey J. Barton (2017) Human Missense Variation is Constrained by Domain Structure and Highlights Functional and Pathogenic Residues. bioRxiv doi:10.1101/127050. Submitted to Nature Genetics.

Fábio Madeira, Michele Tinti, Gavuthami Murugesan, Emily Berrett, Margaret Stafford, Rachel Toth, Christian Cole, Carol MacKintosh and Geoffrey J. Barton (2015) **14-3-3-Pred: Improved methods to predict 14-3-3-binding phosphopeptides**. Bioinformatics (Oxford) 2015 Mar 3; doi:10.1093/bioinformatics/btv133

Michele Tinti, Fábio Madeira, Gavuthami Murugesan, Gerta Hoxhaj, Rachel Toth and Carol MacKintosh (2014) **ANIA** - **ANnotation and Integrated Analysis of the 14-3-3-interactome**. Database (Oxford) 2014 Feb 5; doi:10.1093/database/bat085

Ludwig Krippahl and Fábio Madeira (2014) Improving Protein Docking with Constraining Programming and Coevolution Data. bioRxiv doi:10.1101/002329

Ludwig Krippahl, Fábio Madeira and Pedro Barahona (2013) Constraining Protein Docking with Coevolution Data for Medical Research. Proceedings of the 14th Conference on Artificial Intelligence in Medicine pp 110-114. doi:10.1007/978-3-642-38326-7

Fábio Madeira and Ludwig Krippahl (2012) **PYCOEVOL - A Python Workflow to Study Protein-protein Coevolution**. Proceedings of the International Conference on Bioinformatics Models, Methods and Algorithms pp 143-149. doi:10.5220/0003737901430149

Marco Correia, Fábio Madeira, Pedro Barahona and Ludwig Krippahl (2011) Improving Multiple Sequence Alignments with Constraint Programming and Local Search. Prooceedings of the Workshop on Constraint Based Methods for Bioinformatics pp 37-44. www.dmi.unipg.it/WCB11/wcb11proc.pdf

POSTERS

Fábio Madeira and Geoffrey J. Barton (2015) **Analysis of protein domain interactions and genetic variation**. SLS PhD Poster Session at University of Dundee, Oct. 9. doi:10.6084/m9.figshare.1584880. <u>Selected as Poster Prize Winner</u>.

Fábio Madeira and Geoffrey J. Barton (2015) **Protein interactions and genetic variation**. ISMB/ECCB 2015 (23rd Annual International Conference on Intelligent Systems for Molecular Biology - 14th European Conference on Computational Biology) Dublin, Jul. 10-14. doi:10.6084/m9.figshare.1485641. Selected for Oral Poster Presentation and Travel Fellowship.

Fábio Madeira, Michele Tinti, Gerta Hoxhaj, Geoffrey J. Barton and Carol MacKintosh (2015) **Predicting and mapping the human 14-3-3 interactome to test a new signalling paradigm**. Wellcome Trust Retreat in Firbush, University of Dundee, May 23. doi:10.6084/m9.figshare.923439

Michele Tinti, Fábio Madeira, Catherine Johnson, Margaret Malcolm and Carol MacKintosh (2012) **Evolution of 14-3-3-binding sites and 2R-Ohnologue families**. PTMs in Cell Signaling, Copenhagen Denmark, Dec. 2-5. doi:10.6084/m9.figshare.923438

Paulo Roque Lino, Fábio Madeira, Isabel Tavares de Almeida and Paula Leandro (2010) Alternative Answers to Everlasting Problems: Protein Engineering Towards New Approaches for Phenylketonuria Treatment. SPDM Annual Symposium Albufeira, Portugal, Nov. 4-5.

Catarina Coelho, Fábio Madeira, Paulo Roque Lino, Isabel Tavares de Almeida, Paula Leandro and Maria João Romão (2010) Crystallization of a Stable Form of Human Phenylalanine Hydroxylase: Towards the 3D Structure Determination. UK-Portuguese Teams Meeting Protein-protein interaction and Protein folding. FCT-UNL, Mar. 29-31. doi:10.6084/m9.figshare.923437

INITIATIVES

2015 TEDx University of Dundee

Organization and development/design of the event's website and ticket sale.

• http://tedxuod.github.io

2014 PiCLS Annual Symposium

Organization and development/design of the event's website.

• http://picls-symposium.org/2014

2013 Biotechnology YES

Participated with a team project "IntelliGene: Empower your future" in the Biotechnology Young Entrepreneurs Scheme Competition.

SOFTWARE DEVELOPMENT

2017 **JABAWS**

JABAWS 2.2: Distributed Web Services for Bioinformatics.

• http://www.compbio.dundee.ac.uk/jabaws

2017 **AACon**

AACon 1.1: A Fast Amino Acid Conservation Calculation Service.

• http://www.compbio.dundee.ac.uk/aacon

2017 BioDownloader

A Command Line Tool for downloading protein structures, protein sequences and multiple sequence alignments. \bullet biomadeira/BioDownloader

2015 **pvPDBeREST**

A python wrapper for the PDBe REST API powered by Requests.

• biomadeira/pyPDBeREST

Since 2013 **ProIntVar**

Python package for analysis of protein structures and genetic variants, developed in the Barton Group. Extensive use of the *Pandas* data structures and analysis tools. Source code available for review upon request.

2013-2015 **14-3-3-Pred**

A webserver to predict 14-3-3-binding sites in proteins. Built with *Flask*, and related technologies.

• http://www.compbio.dundee.ac.uk/1433pred

2011-2012 **Pycoevol**

A Python workflow to study protein-protein coevolution and interaction.

Ω biomadeira/pycoevol

2012 **BibYAML**

A webserver for converting BibTeX bibliographies to YAML, deployed with Google App Engine. • bibayaml

2012 Pubmed2Rss

Pubmed Rss ID Generator, deployed with Google App Engine.

O biomadeira/gae pubmed2rss

2015 **Jasper**

Full-featured clone of Ghost's default theme 'Casper' for GitHub pages powered by Jekyll. \bigcirc biomadeira/jasper

2015 Sustain

A personal blog theme developed with Bootstrap for GitHub pages powered by Jekyll. \bigcirc biomadeira/sustain

Vitae

A personal resume theme developed with *Skeleton* for GitHub pages powered by *Jekyll*. • biomadeira/vitae

TECHNICAL SKILLS

Software Development

Adopter of Test-driven development practices. OOP Python 2 and 3 (Numpy, SciPy, IPython, Click, Unittests, Nose, Mock, etc.), Version control (Git/Github) and Continuous Integration (Travis-CI, Coveralls, Landscape.io, Virtualenv, Tox, etc.).

Web Development

Python (Flask, webapp2, requests, jinja2, GAE, etc.), Java Servlet (Apache Tomcat), HTML/CSS frameworks (Bootstrap and Skeleton), JavaScript (jQuery) and static-site generators (Jekyll, liquid).

Data Analysis and Visualisation

Python (pandas and matplotlib), Jupyter Notebooks, R/RStudio (ggplot2, ROCR, etc.), Plotly, Microsoft Excel, etc.

Machine Learning

Feature selection and training/testing of Support-Vector Machines, Neural Networks, Random Forests, Naive Bayes, and other classification models, with Python (scikit-learn, PyML and TensorFlow) and R (RSNNS).

Databases

Relational (MySQL and SQLite3) with Python SQLAlchemy and non-relational (MongoDB) with PyMongo. Data mangling with JSON and tabular data formats.

Documentation

ETFX, (R)Markdown, reStructuredText, Sphinx, ReadTheDocs, R Bookdown, etc.

Others

Scripting/coding (Bash, Java, C and Perl), Build and distribution (Docker, Makefile, Common Workflow Language, Apache Ant, Maven, etc.), Linux/MacOS Systems (Sun Grid Engine, TurnKey linux, CentOS, etc.).

Bioinformatics

UCSF Chimera, PyMOL, Jalview, Biopython, HHMER, etc.

SOFT-SKILLS

Technical Writing

Wrote two dissertations, a few journal/conference papers and research reports. ORCID: 0000-0001-9892-9368

Communication

Presented my research (oral/poster presentation) in several conferences and public meetings. Some of my talks are available online in *figshare*. Additionally, I have been an helper in Coding Courses, such as Software Carpentry, at the University of Dundee.

Interpersonal

Problem solver, collaborative, supportive and respectful.

WORKSHOPS ATTENDED

Apr. 2017 3rd BiVi Annual Meeting

Biological Visualisation Community Meeting, Edinburgh Napier University.

Mar. 2016 Error Statistics Analysis

Lecture Series on Error Analysis, Statistical Tests and P-values, by Marek Gierliński, University of Dundee.

Nov. 2014 PDBe API Workshop

PDBe Workshop for Programmers on Programmatic Access to Molecular Structure Information, EMBL-EBI Hinxton.

Sept. 2014 Data Visualisation and Infographics Design

Workshop on data visualisation by Andy Kirk, the curator of "Visualizing Data" (www.visualisingdata.com). University of Dundee.

May 2011 Bioinformatics using Python for Biologists

Gulbenkian Training Programme in Bioinformatics with Allegra Via and Fabrizio Ferrè (Sapienza Università di Roma). Instituto Gulbenkian de Ciência.

Feb. 2010 Advanced Course in Protein Crystallography

Macromolecular Crystallography Laboratory, REQUIMTE-UNL.

LANGUAGES

Portuguese (native) and English (proficient)

HOBBIES AND INTERESTS

Music, Piano, Reading, Movies, Gaming, Running, Cycling, Swimming...

REFERENCES

Professor Geoff J. Barton

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Professor Carol MacKintosh

Division of Cell and Developmental Biology School of Life Sciences University of Dundee ☑ c.mackintosh@dundee.ac.uk • +44 (0) 1382-385766, ext. 85766