João Pedro Rodrigues

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Summary

I am a computational biologist interested in highly collaborative and interdisciplinary projects bridging chemistry and biology to study protein structure and dynamics in the context of human health. My work has resulted in 31 peer-reviewed publications as well as several scientific software packages, collectively cited more than 1000 times. I have a successful track record of acquiring competitive funding and resources. I am also enthusiastic about teaching and mentoring, having taught and worked together with students at the undergraduate and graduate levels, and organized multiple courses and workshops for the scientific community and the general public.

Education

Ph.D. in Computational Structural Biology, Universiteit Utrecht, The Netherlands	2010 - 2014
M.Sc. in Biomolecular Sciences (Prestige Programme), Universiteit Utrecht, The Netherlands	2008 - 2010
B.Sc. in Biochemistry, Universidade de Coimbra, Portugal	2004 - 2008

Awards and Grants

The Molecular Sciences Software Institute – Seed Fellowship ($25.000)	2020
RCSB PDB Poster Prize – Outstanding Student Paper, ISMB/ECCB 2019	2019
Award for simulation time on Anton2 Supercomputer (460,000 simulation units)	2018
Journal Cover and Editor's Choice Paper for FEBS Journal, volume 285, issue 11	2018
France-Stanford Center for Interdisciplinary Studies – Collaborative Project Grant ($11.000)	2017
Stanford School of Medicine Dean's Postdoctoral Fellowship ($25.000)	2017
Best Poster Presentation, Stanford Postdoc Symposium	2016
Niels Stensen Fellowship for Postdoctoral Studies ($44.000)	2016
Google Summer of Code Fellowship ($5.000)	2010
Portuguese Foundation for Science and Technology, Undergraduate Research Fellowship (1.800€)	2008

Research Experience

Postdoctoral Fellow, Dept. of Structural Biology, Stanford University **2016 - Present**

Developed and applied integrative modeling methods to study the structure, dynamics, and interactions of GPCRs.

Core Software Developer, Open Bioinformatics Foundation – Biopython Project 2010 - Present

Long-term code contributor and maintainer of structural bioinformatics module (Bio.PDB).

Visiting Researcher, Institut de Biologie Physico-Chimique Nov – Dec 2017

Acquired funding and contributed to the development of virtual reality-assisted methods for protein docking.

Visiting Researcher, Dept. of Structural Biology, Weizmann Institute of Science August 2017

Helped solve the NMR structure of chemokine CCR5 bound to a peptide-mimic of receptor CCL5 and interpret the role of post-translational tyrosine sulfation in chemokine recognition.

Postdoctoral Researcher, NMR Spectroscopy Research Group, Universiteit Utrecht Mar – Sep 2015

Created undergraduate course materials for homology modeling, molecular dynamics, and protein docking.

Visiting Researcher, Department of Systems Biology, Harvard Medical School June 2012

Analyzed large sequence datasets to derive spatial restraints to accurately model the 3D structure of protein complexes.

Doctoral Candidate, NMR Spectroscopy Research Group, Universiteit Utrecht 2010 - 2014

Developed and applied several integrative modeling methods to study the 3D structure of protein complexes.

Visiting Researcher, Department of Structural Biology, Stanford University 2009 – 2010

Implemented bioinformatics pipeline for robust protein structure refinement protocols using statistical potentials.

M.Sc. Intern, NMR Spectroscopy Research Group, Universiteit Utrecht 2008 - 2009

Applied homology modeling and protein docking to study the specificity of E2/E3 complexes in the ubiquitination pathway.

Selected Publications

Abayev, M., Rodrigues, J.P.G.L.M., Srivastava, G., Arshava, B., Jaremko, Ł., Jaremko, M., Naider, F., Levitt, M., and Anglister, J. (2018). The solution structure of monomeric CCL5 in complex with a doubly sulfated N-terminal segment of CCR5. FEBS J. *285*, 1988–2003.

Karaca, E., Rodrigues, J.P.G.L.M., Graziadei, A., Bonvin, A.M.J.J., and Carlomagno, T. (2017). M3: an integrative framework for structure determination of molecular machines. Nature Methods *14*, 897–902.

van Zundert, G.C.P.*, Rodrigues, J.P.G.L.M.*, Trellet, M., Schmitz, C., Kastritis, P.L., Karaca, E., Melquiond, A.S.J., van Dijk, M., de Vries, S.J., and Bonvin, A.M.J.J. (2016). The HADDOCK2.2 Web Server: User-Friendly Integrative Modeling of Biomolecular Complexes. Journal of Molecular Biology *428*, 720–725.

Full list available at: orcid.org/0000-0001-9796-3193

Conference Organization

EMBO Practical Course on "Integrative Modeling of Biomolecular Interactions"	2016, 2018, 2020
Meeting of Young Portuguese Researchers in Structural Biology (EJIBCE)	2013, 2015
NMR Focus Workshop: "NMR and Modeling Methods for Protein Interactions and Drug Design"	2015

Teaching Experience

Instructor, Software Carpentry Workshops (Python, Bash, Git)	2019 – Present
Assistant in several international workshops on integrative modeling with HADDOCK	2010 – Present
Guest Lecturer, B.Sc. Biology course "Introduction to Bioinformatics", Utrecht, NL	2012 – 2015
Teaching Assistant, B.Sc. Chemistry course "Molecular Modelling and Math", Utrecht, NL	2010 – 2015
Guest Lecturer, Summer School "Exploring Nature's Molecular Machines", Utrecht, NL	2014
Guest Lecturer, B.Sc. Chemistry course "Molecular Machines", Utrecht, NL	2014
Guest Lecturer, M.Sc. Molecular and Cellular Life Sciences introductory course, Utrecht, NL	2014

Mentoring Experience

Supervised 2 undergraduate students during independent research semesters	2017 – 2018
Supervised 3 undergraduate lab rotation students (3 months), Stanford, USA	2016 – 2017
Co-mentored Summer Undergraduate Research Fellow, Stanford, USA	2016
Supervised 4 first-year (3 weeks) and 8 second-year (6 weeks) chemistry students, Utrecht, NL	2012 - 2015
Daily supervisor, M.Sc. thesis project (9 months), Utrecht, NL	2012, 2015
Google Summer of Code Mentor, Open Bioinformatics Foundation – Biopython Project	2011

Scientific Communication and Outreach

Guest Speaker, 2Scientists Podcast ("The protein folding biologist: Marie Kondo of the cell")	Feb 2019
Volunteer, "STEAM Festival", Redwood City, USA	2018, 2019
Speaker, "Taste of Science" festival, SF Bay Area, USA	2017, 2018
Volunteer, Bio-X Science/Children's Day, Stanford, USA	2016, 2017, 2018
Volunteer, California Academy of Sciences (NightLife events)	2016, 2017

Journal Service

Reviewer for *Computers in Biology and Medicine*, *SoftwareX*, *PLoS Computational Biology*, *Molecules*, *Nucleic Acids Research*, *Journal of Computer-Aided Drug Design*, *International Journal of Molecular Sciences* and *Journal of Molecular Recognition*.

References

Prof. Alexandre Bonvin, Ph.D. advisor

Prof. Michael Levitt, postdoctoral research advisor