João Rodrigues

COMPUTATIONAL STRUCTURAL BIOLOGIST

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Education

PhD in Computational Structural Biology, Universiteit Utrecht, NL 2010-2014

Msc in Biomolecular Sciences, Universiteit Utrecht, NL 2008-2010

BSc in Biochemistry, Universidade de Coimbra, PT 2004-2008

Research Experience

Principal Scientist, Schrodinger Inc, USA 2021-Present

- Product manager and team lead for density-aware structure refinement tools (GlideEM, Phenix/OPLS).
- Develop computational methods for structure prediction of protein-ligand complexes (IFD-MD).

Core Developer / Maintainer, Biopython Project 2010-Present

- Core contributor and maintainer of Bio.PDB, the structural bioinformatics module.

Postdoctoral Fellow, Dept. of Structural Biology, Stanford University, USA 2016- 2021

- Develop and apply integrative modeling to study the structure, dynamics, and interactions of GPCRs.

Postdoctoral Researcher, Bijvoet Center for Biomolecular Research, NL 2015-2015

- Create educational materials for undergraduate and graduate courses on structural bioinformatics.

Doctoral Candidate, Bijvoet Center for Biomolecular Research, NL 2010-2014

- Develop tools to predict the 3D structure of protein complexes from experimental data (HADDOCK).

Selected Publications

- Van Zundert G*, **Rodrigues JP***, Trellet M, Schmitz C, Kastritis P, Karaca E, et al. *The HADDOCK2. 2 web server: user-friendly integrative modeling of biomolecular complexes.* J Mol Biol. 2016;428: 720–725.
- Coskun D, Lihan M, **Rodrigues JP**, Vass M, Robinson D, Friesner RA, et al. *Using AlphaFold and Experimental Structures for the Prediction of the Structure and Binding Affinities of GPCR Complexes via Induced Fit Docking and Free Energy Perturbation.* J Chem Theory Comput. 2024;20: 477–489. doi:10.1021/acs.jctc.3c00839
- Abayev M, **Rodrigues JP#**, Srivastava G, Arshava B, Jaremko Ł, Jaremko M, et al. *The solution structure of monomeric CCL 5 in complex with a doubly sulfated N-terminal segment of CCR 5.* FEBS J. 2018;285: 1988–2003.
- **Rodrigues JP#**, Barrera-Vilarmau S, Teixeira JMC, Sorokina M, Seckel E, Kastritis PL, et al. *Insights on cross-species transmission of SARS-CoV-2 from structural modeling.* PLOS Comp Bio. 2020;16: e1008449. doi:10.1371/journal.pcbi.1008449
- Pataki CI, **Rodrigues JP**, Zhang L, Qian J, Efron B, Hastie T, et al. *Proteomic analysis of monolayer-integrated proteins on lipid droplets identifies amphipathic interfacial α-helical membrane anchors.* PNAS. 2018;115: E8172–E8180. doi:10.1073/pnas.1807981115
- Hopf TA, Schärfe CP*, **Rodrigues JP***, Green AG, Kohlbacher O, Sander C, et al. *Sequence co-evolution gives 3D contacts and structures of protein complexes.* eLife. 2014;3: e03430.

Full list of publications available at joaor.eu/publications

Internships & Collaborations

Visiting Researcher, Institut de Biologie Physico-Chemique, FR 11/2017 - 12/2017

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

Visiting Researcher, Dept. of Structural Biology, Weizmann Institute of Science, IL 07/2017 - 08/2017

- Helped solve the solution NMR structure of a peptide-mimic of chemokine CCL5 bound to CCR5.
- Analyzed the structure and role of post-translational tyrosine sulfation on chemokine recognition.

Visiting Researcher, Dept. of Systems Biology, Harvard Medical School, USA 06/2012 - 07/2012

- Analyzed large sequence datasets to derive spatial restraints for predicting the 3D structure of protein complexes by direct coupling analysis (co-evolution).

Visiting Researcher, Dept. of Structural Biology, Stanford University, USA 2009 - 2010

- Implemented a web server (KobaMin) for protein structure refinement using statistical potentials.

MSc Student Intern, NMR Spectroscopy Research Group, Universiteit Utrecht, NL 2008 - 2009

- Developed a pipeline for automated homology modeling and docking of E2/E3 complexes.

BSc Student Intern, Institute of Electronics and Informatics Engineering of Aveiro, PT 2007 - 2008

- Implemented and benchmarked a gene association predictor based on literature data.

Awards & Grants

Journal Cover - Cell, volume 187, issue 3 2024

The Molecular Sciences Software Institute - Seed Fellowship 2020

RCSB PDB Poster Prize - Outstanding Student Paper, ISMB/ECCB 2019

Anton2 Supercomputer Simulation Grant 2018

Journal Cover and Editor's Choice Paper - FEBS Journal, volume 285, issue 11 2018

France-Stanford Center for Interdisciplinary Studies - Collaborative Project Grant 2017

Stanford School of Medicine Dean's Postdoctoral Fellowship 2017

Best Poster Presentation - Stanford Postdoc Symposium 2016

Niels Stensen Fellowship for Postdoctoral Studies 2016

Google Summer of Code Fellowship - in support of the Open Bioinformatics Foundation 2010

Portuguese Foundation for Science and Technology - Undergraduate Research Fellowship 2008

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 Modelling Methods for Protein Interactions and Drug Design" 2015

Outreach

Guest Speaker, 2Scientists Podcast - "The protein folding biologist: Marie Kondo of the cell" 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 University, USA 2016, 2017, 2018

Volunteer, California Academy of Sciences (NightLife events) 2016, 2017

Teaching Experience

Instructor, Software Carpentry Workshops (Python, Bash, Git, Pandas) 2019 - Present

- Organized, taught, and/or assisted with multi-day workshops at several academic institutions.

Teaching Assistant, HADDOCK User Workshops 2010 - Present

- Helped organize and teach academic researchers how to use HADDOCK for protein docking.

Guest Lecturer, "Introduction to Bioinformatics", B.Sc. Biology curriculum, Utrecht, NL 2012 - 2015

- Taught theory and practical examples of homology modeling to classes of B.Sc students.

Teaching Assistant, "Molecular Modeling and Math", B.Sc. Chemistry curriculum, Utrecht, NL 2010 - 2015

- Assisted 3rd year students in preparing and running molecular dynamics simulations in an 8-week quasi-flipped classroom setting.

Invited Lecturer, Summer School "Exploring Nature's Molecular Machines", Utrecht, NL 2014

Invited Lecturer, "Molecular Machines", B.Sc. Chemistry curriculum, Utrecht, NL 2014

Invited Lecturer, M.Sc. Molecular and Cellular Life Sciences Introductory course, Utrecht, NL 2014

Journal Service

Reviewer

- Bioinformatics (ISSN: 1367-4811)
- CSBJ (ISSN: 2001-0370)
- Computers in Biology and Medicine (ISSN: 1879-0534)
- F1000Research (ISSN: 2046-1402)
- Genes (ISSN: 2073-4425)
- IJMS (ISSN: 1661-6596)
- iScience (ISSN: 2589-0042)
- Journal of Molecular Recognition (ISSN: 0952-3499)
- JCIM (ISSN: 1549-960X)
- J. Comput. Aided Mol. Des. (ISSN: 1573-4951)
- Molecules (ISSN: 1420-3049)
- Nucleic Acids Research (ISSN: 0305-1048)
- PLoS Computational Biology (ISSN: 1553-7358)
- PLoS One (ISSN: 1932-6203)
- Proteins (ISSN: 1097-0134)
- SoftwareX (ISSN: 2352-7110)
- The Journal of Physical Chemistry A (ISSN: 1520-5207)