João Rodrigues

j.p.g.l.m.rodrigues@gmail.com

Education

Ph.D. in Computational Structural Biology 2010 - 2014
Bonvin Lab, Universiteit Utrecht, The Netherlands
Thesis: Computational Structural Biology of Macromolecular Interactions

M.Sc. in Biomolecular Sciences 2008- 2010
Universiteit Utrecht, The Netherlands
Thesis: Predicting the Specifity of E2/E3 Complexes in the Ubiquitination Pathway

B.Sc. in Biochemistry 2004 - 2008
Universidade de Coimbra, Portugal
Thesis: Concept-based Query Expansion for Gene Association Prediction from Literature Data

Research Experience

Schrödinger, NY, USA

Senior Principal Scientist 01.2026 - Present
Principal Scientist II 06.2024 - 12.2025

- Scientific lead for several key products in the Schrödinger suite (e.g. Protein Preparation)
- Led development of cryo-EM refinement and macrocycle modeling technologies.
- Daily supervision of a team of 5 scientists and software engineers.
- Co-authored 5 publications (3 as corresponding author).

Principal Scientist I 01.2023 - 06.2024
Senior Scientist II 01.2022 - 12.2022
Senior Scientist I 01.2021 - 12.2021

- Led the development of a new method to find homologous ligand-bound structures.
- Implemented novel algorithms improving the performance of flexible docking (IFD-MD).
- Developed a method to model flexible linkers between protein domains.
- Developed a protocol for flexible ligand docking for membrane protein targets.
- Co-authored 2 publications (1 featured as cover of the journal Cell, vol 187, issue 3).

Stanford University, CA, USA

Postdoctoral Scholar, *with Michael Levitt* 01.2016 - 12.2020

- Applied integrative modeling methods to study structure and pharmacology of GPCRs.
- Co-authored 15 peer-reviewed publications (2 as corresponding author)

Universiteit Utrecht, The Netherlands

Postdoctoral Scholar, *with Alexandre Bonvin* 04.2015 - 09.2015

- Created and led the development of pdb-tools, a popular toolkit for structure manipulation.
- Developed methods to predict the structure and affinity of protein-protein interactions.
- Created materials for undergraduate and graduate courses on structural bioinformatics.
- Co-authored 13 peer-reviewed publications.

Doctoral Candidate, *with Alexandre Bonvin* 10.2010 - 03.2015

- Developed tools to predict the 3D structure of protein complexes from experimental data.
- Contributed to the development of HADDOCK, a widely-used protein docking software.
- Participated in several rounds of the CAPRI community challenge.
- Co-authored 10 peer-reviewed publications.

Visiting Appointments

Institut de Biologie Physico-Chemique, Paris, France 11.2017 - 12.2017
- Contributed to the development of VR-assisted methods for protein docking.
- Acquired funding from the France-Stanford Center for Interdisciplinary Studies.

Department of Structural Biology, Weizmann Institute of Science, Israel 07.2017 - 08.2017
- Helped solve the NMR structure of a peptide-mimic of chemokine CCL5 bound to CCR5.
- Studied the role of post-translational tyrosine sulfation on chemokine recognition.

Department of Systems Biology, Harvard Medical School, MA, 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).

Department of Structural Biology, Stanford University, CA, USA 10.2009 - 06.2010
- Implemented a web server for protein structure refinement using statistical potentials.

Awards & Grants

The Molecular Sciences Software Institute - Seed Fellowship ($25,000) 2020
ISMB/ECCB - RCSB PDB Poster Prize - Outstanding Student Paper 2019
Niels-Stensen Fellowship for Postdoctoral Studies ($44,000) 2016
Stanford School of Medicine - Dean's Postdoctoral Fellowship ($25,000) 2016
Google Summer of Code Fellowship, Open Bioinformatics Foundation ($5,000) 2010

Community Engagement

Invited Panelist, Sustainability Committee, Biophysical Society Meeting 2026
Invited Keynote, MICROBIOTEC'25, Azores (declined) 2025
Invited Panelist, Careers in Comp Chem, New York Area Group for Informatics and Modeling 2024
Co-Organizer, 3rd EMBO Practical Course on "Integrative Modeling of Biomolecular Interactions" 2020
Guest, 2Scientists Podcast 2019
Scientific Committee, HIBIT Conference 2019-2025
Presenter, STEAM Festival Redwood City 2018-2019
Co-organizer, 2nd EMBO Practical Course on "Integrative Modeling of Biomolecular Interactions" 2018
Speaker, Taste of Science Festival - San Francisco Bay Area 2017-2018
Co-organizer, 1st EMBO Practical Course on "Integrative Modeling of Biomolecular Interactions" 2016
Presenter, NightLife, California Academy of Sciences 2016-2017
Volunteer, Bio-X Science Children's Day - Stanford University 2016-2018
Co-organizer, 3rd Meeting of Young Portuguese Researchers in Structural Biology (EJIBCE) 2015
Co-organizer, NMR Focus Workshop - "Methods for Protein Interactions and Drug Design" 2015
Invited Lecturer, Summer School "Exploring Nature's Molecular Machines", at Uni. Utrecht 2014
Invited Lecturer, "Molecular Machines", B.Sc. Chemistry curriculum at Uni. Utrecht 2014
Invited Lecturer, M.Sc. Molecular and Cellular Life Sciences Introductory course at Uni. Utrecht 2014
Co-organizer, 1st Meeting of Young Portuguese Researchers in Structural Biology (EJIBCE) 2013

Teaching

Instructor, Python and Machine Learning Virtual Classes 2024
Instructor, Software Carpentry 2019-Present
Teaching Assistant, HADDOCK User Workshops 2010 - 2021
Guest Lecturer, "Introduction to Bioinformatics", B.Sc. Biology curriculum, Utrecht 2018-2019
Teaching Assistant, "Molecular Modeling and Math", B.Sc. Chemistry curriculum, Utrecht 2018

Journal Service

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)
JCTC (ISSN: 1549-9618)
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)

Publications

# indicates corresponding author, * indicates co-first author

46. Zhang, L, Friesner, RA, Miller, EB, and **Rodrigues, JP#** (2026). *Generalization and Usability of Co-Folded GPCR–Ligand Complexes: A Physics-Guided Assessment.* Preprint
45. Robson-Tull, J, and **Rodrigues, JP#** (2026). *Accurate Physics-Based Flexible Docking of Macrocyclic Ligands.* J. Med. Chem.
44. Boyaci Selcuk, H, Reggiano, G, Robson-Tull, J, Zhang, L, and **Rodrigues, JP#** (2025). *Towards better structural models from cryo-electron microscopy data with physics-based methods.* FEBS Letters.
43. Miller, EB, Hwang, H, Shelley, M, Placzek, A, **Rodrigues, JP**, et al. (2024). *Enabling structure-based drug discovery utilizing predicted models.* Cell.
42. Honorato, RV, Trellet, ME, Jiménez-García, B, Schaarschmidt, JJ, Giulini, M, et al. (2024). *The HADDOCK2.4 web server for integrative modeling of biomolecular complexes.* Nat Protoc.
41. Eastman, P, Galvelis, R, Peláez, RP, Abreu, CRA, Farr, SE, et al. (2024). *OpenMM 8: Molecular Dynamics Simulation with Machine Learning Potentials.* J. Phys. Chem. B.
40. Coskun, D*, Lihan, M*, **Rodrigues, JP***, Vass, M, Robinson, D, et al. (2024). *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.
39. Sorokina, M, Belapure, J, Tüting, C, Paschke, R, Papasotiriou, I, et al. (2022). *An Electrostatically-steered Conformational Selection Mechanism Promotes SARS-CoV-2 Spike Protein Variation.* Journal of Molecular Biology.
38. Karakulak, T, Rifaioglu, AS, **Rodrigues, JP**, and Karaca, E (2021). *Predicting the Specificity- Determining Positions of Receptor Tyrosine Kinase Axl.* Front. Mol. Biosci.
37. Jiménez-García, B, Teixeira, JMC, Trellet, M, **Rodrigues, JP**, and Bonvin, AMJJ (2021). *PDB-tools web: A user-friendly interface for the manipulation of PDB files.* Proteins.
36. Fischhoff, IR, Castellanos, AA, **Rodrigues, JP**, Varsani, A, and Han, BA (2021). *Predicting the zoonotic capacity of mammals to transmit SARS-CoV-2.* Proceedings of the Royal Society B: Biological Sciences.
35. Sorokina, M, M. C. Teixeira, J, Barrera-Vilarmau, S, Paschke, R, Papasotiriou, I, et al. (2020). *Structural models of human ACE2 variants with SARS-CoV-2 Spike protein for structure-based drug design.* Sci Data.
34. **Rodrigues, JP#**, Barrera-Vilarmau, S, M. C. Teixeira, J, Sorokina, M, Seckel, E, et al. (2020). *Insights on cross-species transmission of SARS-CoV-2 from structural modeling.* PLoS Comput Biol.
33. Kaplan, M, Sweredoski, MJ, **Rodrigues, JP**, Tocheva, EI, Chang, Y-W, et al. (2020). *Bacterial flagellar motor PL-ring disassembly subcomplexes are widespread and ancient.* Proc. Natl. Acad. Sci. U.S.A.
32. Roel-Touris, J, Don, CG, V. Honorato, R, **Rodrigues, JP**, and Bonvin, AMJJ (2019). *Less Is More: Coarse-Grained Integrative Modeling of Large Biomolecular Assemblies with HADDOCK.* J. Chem. Theory Comput.
31. **Rodrigues, JP#**, Teixeira, JMC, Trellet, M, and Bonvin, AMJJ (2018). *pdb-tools: a swiss army knife for molecular structures.* F1000Res.
30. Pataki, CI, **Rodrigues, JP**, Zhang, L, Qian, J, Efron, B, et al. (2018). *Proteomic analysis of monolayer-integrated proteins on lipid droplets identifies amphipathic interfacial α-helical membrane anchors.* Proc. Natl. Acad. Sci. U.S.A.
29. Masureel, M, Zou, Y, Picard, L-P, Van Der Westhuizen, E, Mahoney, JP, et al. (2018). *Structural insights into binding specificity, efficacy and bias of a β2AR partial agonist.* Nat Chem Biol.
28. Kurkcuoglu, Z, Koukos, PI, Citro, N, Trellet, ME, **Rodrigues, JP**, et al. (2018). Performance of HADDOCK and a simple contact-based protein–ligand binding affinity predictor in the D3R Grand Challenge 2. J Comput Aided Mol Des.

Publications (continued)

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27. Bonvin, AMJJ, Karaca, E, Kastritis, PL, and **Rodrigues, JP** (2018). *Defining distance restraints in HADDOCK*. Nat Protoc.
26. Baro, B, Játiva, S, Calabria, I, Vinaixa, J, Bech-Serra, J-J, et al. (2018). *SILAC-based phosphoproteomics reveals new PP2A-Cdc55-regulated processes in budding yeast.* GigaScience.
25. Abriata, LA, **Rodrigues, JP**, Salathé, M, and Patiny, L (2018). *Augmenting Research, Education, and Outreach with Client-Side Web Programming.* Trends in Biotechnology.
24. Abayev, M, **Rodrigues, JP**#, Srivastava, G, Arshava, B, Jaremko, Ł, et al. (2018). *The solution structure of monomeric CCL5 in complex with a doubly sulfated N-terminal segment of CCR5*. The FEBS Journal.
23. Visscher, KM, Medeiros-Silva, J, Mance, D, **Rodrigues, JP**, Daniëls, M, et al. (2017). *Supramolecular Organization and Functional Implications of K+ Channel Clusters in Membranes.* Angew Chem Int Ed.
22. Vangone, A, **Rodrigues, JP**, Xue, LC, Van Zundert, GCP, Geng, C, et al. (2017). *Sense and simplicity in HADDOCK scoring: Lessons from CASP-CAPRI round 1.* Proteins.
21. Komolov, KE, Du, Y, Duc, NM, Betz, RM, **Rodrigues, JP**, et al. (2017). *Structural and Functional Analysis of a β2-Adrenergic Receptor Complex with GRK5*. Cell.
20. Karaca, E, **Rodrigues, JP**, Graziadei, A, Bonvin, AMJJ, and Carlomagno, T (2017). *M3: an integrative framework for structure determination of molecular machines.* Nat Methods.
19. Xue, LC, **Rodrigues, JP**, Kastritis, PL, Bonvin, AM, and Vangone, A (2016). *PRODIGY: a web server for predicting the binding affinity of protein–protein complexes.* Bioinformatics.
18. Xue, LC, **Rodrigues, JP**, Dobbs, D, Honavar, V, and Bonvin, AMJJ (2016). *Template-based protein–protein docking exploiting pairwise interfacial residue restraints*. Brief Bioinform.
17. Van Zundert, GCP, **Rodrigues, JP***, Trellet, M, Schmitz, C, Kastritis, PL, et al. (2016). *The HADDOCK2.2 Web Server: User-Friendly Integrative Modeling of Biomolecular Complexes.* Journal of Molecular Biology.
16. **Rodrigues, JP**, Melquiond, ASJ, and Bonvin, AMJJ (2016). *Molecular dynamics characterization of the conformational landscape of small peptides: A series of hands-on collaborative practical sessions for undergraduate students.* Biochem Molecular Bio Educ.
15. Liu, Y, **Rodrigues, JP**, Bonvin, AMJJ, Zaal, EA, et al. (2016). *New Insight into the Catalytic Mechanism of Bacterial MraY from Enzyme Kinetics and Docking Studies*. Journal of Biological Chemistry.
14. Lensink, MF, Velankar, S, Kryshtafovych, A, Huang, S, Schneidman-Duhovny, D, et al. (2016). *Prediction of homoprotein and heteroprotein complexes by protein docking and template-based modeling: A CASP-CAPRI experiment*. Proteins.
13. Rad-Malekshahi, M, Visscher, KM, **Rodrigues, JP**, De Vries, R, Hennink, WE, et al. (2015). *The Supramolecular Organization of a Peptide-Based Nanocarrier at High Molecular Detail.* J. Am. Chem. Soc.
12. **Rodrigues, JP**, and Bonvin, AMJJ (2014). *Integrative computational modeling of protein interactions*. The FEBS Journal.
11. Kastritis, PL, **Rodrigues, JP**, Folkers, GE, Boelens, R, and Bonvin, AMJJ (2014). *Proteins Feel More Than They See: Fine-Tuning of Binding Affinity by Properties of the Non-Interacting Surface.* Journal of Molecular Biology.
10. Kastritis, PL, **Rodrigues, JP**, and Bonvin, AMJJ (2014). *HADDOCK2P2I : A Biophysical Model for Predicting the Binding Affinity of Protein–Protein Interaction Inhibitors.* J. Chem. Inf. Model.
9. Hopf, TA, Schärfe, CPI, **Rodrigues, JP***, Green, AG, Kohlbacher, O, et al. (2014). *Sequence co-evolution gives 3D contacts and structures of protein complexes*. eLife.
8. Ferguson, FM, Dias, DM, **Rodrigues, JP**, Wienk, H, Boelens, R, et al. (2014). *Binding Hotspots of BAZ2B Bromodomain: Histone Interaction Revealed by Solution NMR Driven Docking.* Biochemistry.
7. **Rodrigues, JP**, Melquiond, ASJ, Karaca, E, Trellet, M, Van Dijk, M, et al. (2013). *Defining the limits of homology modeling in information-driven protein docking.* Proteins.
6. Moretti, R, Fleishman, SJ, Agius, R, Torchala, M, Bates, PA, et al. (2013). *Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions: Evaluation of Interaction Mutation Prediction.* Proteins.
5. Dias, DM, **Rodrigues, JP**, Domingues, NS, Bonvin, AMJJ, and Castro, MMCA (2013). *Unveiling the Interaction of Vanadium Compounds with Human Serum Albumin by Using1 H STD NMR and Computational Docking Studies.* Eur J Inorg Chem.
4. **Rodrigues, JP**, Trellet, M, Schmitz, C, Kastritis, P, Karaca, E, et al. (2012). *Clustering biomolecular complexes by residue contacts similarity.* Proteins.
3. **Rodrigues, JP**, Levitt, M, and Chopra, G (2012). *KoBaMIN: a knowledge-based minimization web server for protein structure refinement.* Nucleic Acids Research.

Publications (continued)

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2. De Vries, SJ, Melquiond, ASJ, Kastritis, PL, Karaca, E, Bordogna, A, et al. (2010). *Strengths and weaknesses of data-driven docking in critical assessment of prediction of interactions.* Proteins.
1. Matos, S, Arrais, JP, **Rodrigues, JP**, and Oliveira, JL (2010). *Concept-based query expansion for retrieving gene related publications from MEDLINE.* BMC Bioinformatics.

Book Chapters

2. Geng, C, Narasimhan, S, **Rodrigues, JP**, and Bonvin, AMJJ (2017). *Information-Driven, Ensemble Flexible Peptide Docking Using HADDOCK.* In Modeling Peptide-Protein Interactions: Methods and Protocols, O. Schueler-Furman and N. London, eds. (Springer).
1. **Rodrigues, JP**, Karaca, E, and Bonvin, AMJJ (2015). *Information-Driven Structural Modelling of Protein–Protein Interactions.* In Molecular Modeling of Proteins Methods in Molecular Biology., A. Kukol, ed. (Springer New York).

Links

Github	github.com/joaorodrigues
Google Scholar	scholar.google.com/citations?user=UeXRdzQAAAAJ
LinkedIn	linkedin.com/in/jpglmrodrigues
ORCID	orcid.org/0000-0001-9796-3193
Personal	joaor.eu

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