João Pedro Rodrigues

Computational Structural Biology

h-Index: 12 | Publications: 26 | Citations: 824

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Education

2004 - 2008 B.Sc. Biochemistry, Universidade de Coimbra, Portugal

2008 - 2010 M.Sc. Biomolecular Sciences, Universiteit Utrecht, The Netherlands

2010 - 2014 Ph.D. Computational Structural Biology, Universiteit Utrecht, The Netherlands

Experience

2007 - 2008 Trainee at the Bioinformatics Research Group, Universidade de Aveiro, Portugal

2009 - 2010 Visiting Researcher at the Computational Structural Biology Group, Stanford University, USA

2010 Google Summer of Code Fellow at the Open Bioinformatics Foundation

2010 - 2014 Research Assistant at the NMR Spectroscopy Research Group, Universiteit Utrecht, The Netherlands

2010 - Maintainer and Core Developer of the Biopython Project

2011 Google Summer of Code Mentor at the Open Bioinformatics Foundation

2012 Visiting Researcher at the Department of Systems Biology, Harvard Medical School, USA

2015 Research Assistant at the NMR Spectroscopy Research Group, Universiteit Utrecht, The Netherlands

2016 - Postdoctoral Fellow at the Computational Structural Biology, Stanford University, USA

2017 Visiting Researcher at the Department of Structural Biology, Weizmann Institute of Science, Israel

2017 Visiting Researcher at the Laboratoire de Biochimie Théorique, Institut de Biologie Physico-Chimique, France

2018 Visiting Researcher at the Department of Structural Biology, Weizmann Institute of Science, Israel

Grants and Awards

2008 FCT Undergraduate Research Fellowship (€1.800)

2010 Google Summer of Code Fellowship ($5.000)

2016 Niels Stensen Fellowship for Postdoctoral Studies ($44.000)

2017 Stanford School of Medicine Dean's Postdoctoral Fellowship ($25.000)

2017 - 2018 France-Stanford Center for Interdisciplinary Studies Collaborative Project ($11.000)

Organizational Roles

2013 Organizer of the 1st Meeting of Young Portuguese Investigators in Computational Structural Biology (Oporto)

2015 Organizer of 5-days NMR Focus workshop (Coimbra)

2015 Organizer of the 3rd Meeting of Young Portuguese Investigators in Computational Structural Biology (Coimbra)

2016 Co-Organizer of the 1st EMBO Practical Course on Integrative Modelling of Biomolecular Interactions (Barcelona)

2018 Co-Organizer of the 2nd EMBO Practical Course on Integrative Modelling of Biomolecular Interactions (Barcelona)

Teaching

2010 - Lecturer and Teaching Assistant in several international HADDOCK workshops

2010 - 2015 Teaching Assistant in the B.Sc. Chemistry course "Molecular Modeling and Math" at Utrecht University

2010 - 2015 Teaching Assistant in the B.Sc. Chemistry course "Molecular Modeling and Math" at Utrecht University

2014 Lecturer in the M.Sc. "Molecular and Cellular Life Sciences" introductory course at Utrecht University

2014 Lecturer in the B.Sc Chemistry course "Molecular Machines" at Utrecht University

Student Supervision

2010 - 2015 Supervised 4 first-year and 6 second-year B.Sc. Chemistry students during internships at Utrecht University

2013 Co-Supervised 1 M.Sc. Thesis at Utrecht University

2016 - 2017 Supervised 4 undergraduate laboratory rotations at Stanford University

2016 Supervised visiting student under the SURF exchange program at Stanford University

Oral Presentations in Meetings

2008 “Improving Literature Searches in Gene Expression Studies” at IWPACBB, Spain

2011 “Clustering of protein structures through contact analysis” at NBIC Conference, The Netherlands

2012 “Clustering biomolecular complexes using residue contact similarity” at VIZBI, Germany

2012 “3D models of protein-protein complexes from evolutionary information” at NWO Chains, The Netherlands

2013 “Co-evolution driven HADDOCKing” at 5th EMBO Meeting, The Netherlands

2013 “Clustering biomolecular complexes using residue contact similarity” at 5th CAPRI Meeting, The Netherlands

2013 “The twilight zone of data-driven docking” at BIOMOS Meeting, Switzerland

2013 “Less is More: Coarse-Grained Models in HADDOCK” at Dutch Molecular Dynamics Day, The Netherlands

2014 “Integrative computational structural biology of biomolecular complexes” at NWO Chains, The Netherlands

2014 “Coevolution: Gains and Pitfalls when using it for structure prediction of complexes” at MMBS, The Netherlands

2015 “GPGPU use cases from the MoBrain community” at EGI Meeting, Portugal

2015 “The Biopython Project Update” at ISMB/BOSC Satellite Meeting, Ireland

2017 “Better Together: Integrative Structural Biology of Protein Interactions” at Structural Biology Retreat, USA

Invited Lectures

2014 “Integrative Modeling of Protein Interactions”, by Prof. Dean Sherry at UT Dallas

2014 “Integrative Modeling of Protein Interactions”, by Prof. Jose Rizo-Rey at UTSW in Dallas

2015 “Integrative Modeling of Protein Interactions”, by Prof. Jose Luis Oliveira at Universidade de Aveiro

2016 “Integrative Modeling of Protein Interactions”, opening lecture at 4th EJIBCE in Portugal

2017 “Better Together: Integrative Structural Biology of Protein Interactions”, by Dr. Ezgi Karaca at IBG-Izmir

2017 “Better Together: Integrative Structural Biology of Protein Interactions”, by Prof. Phillip Selenko at FMP in Berlin

2017 “Better Together: Integrative Structural Biology of Protein Interactions”, by Prof. Marc Baaden at IBPC in Paris

Scientific Outreach

2016-2017 Volunteer/Organizer at the NightLife at the California Academy of Sciences

2017 Speaker at the SF Bay Area “Taste of Science” festival

2017 Volunteer at Software Carpentry Workshop in Data Science, at Stanford University

2017 Speaker and Volunteer at the Bio-X Science/Children’s Day at Stanford University

List of Publications

Abriata, L.A., Rodrigues, J.P., Salathé, M., and Patiny, L. (2017). *Augmenting Research, Education, and Outreach with Client-Side Web Programming.* Trends in Biotechnology.

Visscher, K., Medeiros-Silva, J., Mance, D., Rodrigues, J.P., Daniëls, M., Bonvin, A.M., Baldus, M., and Weingarth, M. (2017). *Supramolecular organization and functional implications of K+ channel clusters in membranes.* Angewandte Chemie International Edition.

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

Komolov, K.E., Du, Y., Duc, N.M., Betz, R.M., Rodrigues, J.P., Leib, R.D., Patra, D., Skiniotis, G., Adams, C.M., and Dror, R.O. (2017). Structural and Functional Analysis of a β 2-Adrenergic Receptor Complex with GRK5. Cell 169, 407–421.

Kurkcuoglu, Z., Koukos, P.I., Citro, N., Trellet, M.E., Rodrigues, J., Moreira, I.S., Roel-Touris, J., Melquiond, A.S., Geng, C., and Schaarschmidt, J. (2017). Performance of HADDOCK and a simple contact-based protein–ligand binding affinity predictor in the D3R Grand Challenge 2. Journal of Computer-Aided Molecular Design 1–11.

List of Publications (continued)

Xue, L.C., Rodrigues, J.P., Dobbs, D., Honavar, V., and Bonvin, A.M. (2017). Template-based protein–protein docking exploiting pairwise interfacial residue restraints. **Briefings in Bioinformatics** 18, 458–466.

Vangone, A., Rodrigues, J., Xue, L., van Zundert, G., Geng, C., Kurkcuoglu, Z., Nellen, M., Narasimhan, S., Karaca, E., and van Dijk, M. (2017). Sense and simplicity in HADDOCK scoring: Lessons from CASP-CAPRI round 1. **Proteins: Structure, Function, and Bioinformatics** 85, 417–423.

Geng, C., Narasimhan, S., Rodrigues, J.P., and Bonvin, A.M. (2017). Information-Driven, Ensemble Flexible Peptide Docking Using HADDOCK. **Modeling Peptide-Protein Interactions: Methods and Protocols** 109–138.

Lensink, M.F., Velankar, S., Kryshtafovych, A., Huang, S., Schneidman-Duhovny, D., Sali, A., Segura, J., Fernandez-Fuentes, N., Viswanath, S., and Elber, R. (2016). Prediction of homoprotein and heteroprotein complexes by protein docking and template-based modeling: A CASP-CAPRI experiment. **Proteins: Structure, Function, and Bioinformatics** 84, 323–348.

Xue, L.C., Rodrigues, J.P., Kastritis, P.L., Bonvin, A.M., and Vangone, A. (2016). PRODIGY: a web server for predicting the binding affinity of protein–protein complexes. **Bioinformatics** 32, 3676–3678.

Liu, Y., Rodrigues, J.P., Bonvin, A.M., Zaal, E.A., Berkers, C.R., Heger, M., Gawarecka, K., Swiezewska, E., Breukink, E., and Egmond, M.R. (2016). New insight into the catalytic mechanism of bacterial MraY from enzyme kinetics and docking studies. **Journal of Biological Chemistry** 291, 15057–15068.

Rodrigues, J.P., Melquiond, A.S., and Bonvin, A.M. (2016). Molecular dynamics characterization of the conformational landscape of small peptides: A series of hands-on collaborative practical sessions for undergraduate students. **Biochemistry and Molecular Biology Education** 44, 160–167.

Van Zundert, G.*, Rodrigues, J.*, Trellet, M., Schmitz, C., Kastritis, P., Karaca, E., Melquiond, A., van Dijk, M., De Vries, S., and Bonvin, A. (2016). The HADDOCK2. 2 web server: user-friendly integrative modeling of biomolecular complexes. **Journal of Molecular Biology** 428, 720–725.

Rad-Malekshahi, M., Visscher, K.M., Rodrigues, J.P., De Vries, R., Hennink, W.E., Baldus, M., Bonvin, A.M., Mastrobattista, E., and Weingarth, M. (2015). The supramolecular organization of a peptide-based nanocarrier at high molecular detail. **Journal of the American Chemical Society** 137, 7775–7784.

Ferguson, F.M., Dias, D.M., Rodrigues, J.P., Wienk, H., Boelens, R., Bonvin, A.M., Abell, C., and Ciulli, A. (2014). Binding hotspots of BAZ2B bromodomain: Histone interaction revealed by solution NMR driven docking. **Biochemistry** 53, 6706–6716.

Hopf, T.A.*, Schärfe, C.P.*, Rodrigues, J.P*., Green, A.G., Kohlbacher, O., Sander, C., Bonvin, A.M., and Marks, D.S. (2014). Sequence co-evolution gives 3D contacts and structures of protein complexes. **Elife** 3, e03430.

Kastritis, P.L., Rodrigues, J.P., Folkers, G.E., Boelens, R., and Bonvin, A.M. (2014). Proteins feel more than they see: fine-tuning of binding affinity by properties of the non-interacting surface. **Journal of Molecular Biology** 426, 2632–2652.

Rodrigues, J.P., and Bonvin, A.M. (2014). Integrative computational modeling of protein interactions. **The FEBS Journal** 281, 1988–2003.

Kastritis, P.L., Rodrigues, J.P., and Bonvin, A.M. (2014). HADDOCK2P2I: a biophysical model for predicting the binding affinity of protein–protein interaction inhibitors. **Journal of Chemical Information and Modeling** 54, 826–836.

Rodrigues, J., Melquiond, A., Karaca, E., Trellet, M., Dijk, M., Zundert, G., Schmitz, C., Vries, S., Bordogna, A., and Bonati, L. (2013). Defining the limits of homology modeling in information-driven protein docking. **Proteins: Structure, Function, and Bioinformatics** 81, 2119–2128.

Moretti, R., Fleishman, S.J., Agius, R., Torchala, M., Bates, P.A., Kastritis, P.L., Rodrigues, J.P., Trellet, M., Bonvin, A.M., and Cui, M. (2013). Community-wide evaluation of methods for predicting the effect of mutations on protein–protein interactions. **Proteins: Structure, Function, and Bioinformatics** 81, 1980–1987.

Dias, D.M., Rodrigues, J.P., Domingues, N.S., Bonvin, A.M., and Castro, M. (2013). Unveiling the interaction of vanadium compounds with human serum albumin by using 1H STD NMR and computational docking studies. **European Journal of Inorganic Chemistry** 2013, 4619–4627.

Rodrigues, J.P., Trellet, M., Schmitz, C., Kastritis, P., Karaca, E., Melquiond, A.S., and Bonvin, A.M. (2012a). Clustering biomolecular complexes by residue contacts similarity. **Proteins: Structure, Function, and Bioinformatics** 80, 1810–1817.

Rodrigues, J.P., Levitt, M., and Chopra, G. (2012b). KoBaMIN: a knowledge-based minimization web server for protein structure refinement. **Nucleic Acids Research** 40, W323–W328.

de Vries, S.J., Melquiond, A.S., Kastritis, P.L., Karaca, E., Bordogna, A., van Dijk, M., Rodrigues, J.P., and Bonvin, A.M. (2010). Strengths and weaknesses of data-driven docking in critical assessment of prediction of interactions. **Proteins: Structure, Function, and Bioinformatics** 78, 3242–3249.

Matos, S., Arrais, J.P., Maia-Rodrigues, J., and Oliveira, J.L. (2010). Concept-based query expansion for retrieving gene related publications from MEDLINE. **BMC Bioinformatics** 11, 212.