Stanford

Joao Pedro Garcia Lopes Maia Rodrigues

Postdoctoral Research Fellow, Structural Biology

Curriculum Vitae available Online

Bio

HONORS AND AWARDS

- Seed Fellowship, The Molecular Sciences Software Institute (2019)
- Dean’s Postdoctoral Fellowship, Stanford School of Medicine (2017)
- Niels Stensen Fellowship for Postdoctoral Studies, Niels Stensen Foundation (2016)
- Google Summer of Code Fellowship, Google & Open Bioinformatics Foundation (2010)

PROFESSIONAL EDUCATION

- Bachelor of Science, Universidade De Coimbra (2008)
- Master of Science, Utrecht University (2010)
- Doctor of Philosophy, Utrecht University (2014)

STANFORD ADVISORS

- Michael Levitt, Postdoctoral Faculty Sponsor

LINKS

- Personal Site: http://unstructuredbio.com/

Research & Scholarship

CURRENT RESEARCH AND SCHOLARLY INTERESTS

I am interested in the structure of protein complexes and understanding how it relates to their biological function. Throughout my career, I have developed and applied computational methods to integrate crystallography, NMR, FRET, Cryo-EM, and mutagenesis data to build high-resolution (atomic) models of proteins and protein interactions. I am also interested in education and outreach, and in how computational tools can help the public understand science better.

LAB AFFILIATIONS

- Michael Levitt, Levitt Lab (1/1/2016)

Publications

PUBLICATIONS

- **Insights on cross-species transmission of SARS-CoV-2 from structural modeling.** *bioRxiv : the preprint server for biology*
  Rodrigues, J. P., Barrera-Vilarmau, S. n., Teixeira, J. M., Seckel, E. n., Kastritis, P. n., Levitt, M. n.
  2020

- **The HADDOCK2.2 Web Server: User-Friendly Integrative Modeling of Biomolecular Complexes** *JOURNAL OF MOLECULAR BIOLOGY*
  van Zundert, G. C., Rodrigues, J. P., Trellet, M., Schmitz, C., Kastritis, P. L., Karaca, E., Melquiond, A. S., Van Dijk, M., de Vries, S. J., Bonvin, A. M.
  2016; 428 (4): 720-725

- **Integrative computational modeling of protein interactions** *FEBS JOURNAL*
  Rodrigues, J. P., Bonvin, A. M.
  2014; 281 (8): 1988-2003

- **PDB-tools web: A user-friendly interface for the manipulation of PDB files.** *Proteins*
  Jimenez-Garcia, B., Teixeira, J. M., Trellet, M., Rodrigues, J. P., Bonvin, A. M.
  2020

- **Interfacea: Open-Source Library for Protein Interface Analysis**
  Rodrigues, J., Levitt, M.
  CELL PRESS.2020: 516A

- **Insights on cross-species transmission of SARS-CoV-2 from structural modeling** *bioRxiv*
  Rodrigues, J. P., Barrera-Vilarmau, S., Teixeira, J. M., Seckel, E., Kastritis, P., Levitt, M.
  2020

- **Structural models of human ACE2 variants with SARS-CoV-2 Spike protein for structure-based drug design.** *Scientific data*
  Sorokina, M., M C Teixeira, J., Barrera-Vilarmau, S., Paschke, R., Papasotiriou, I., Rodrigues, J. P., Kastritis, P. L.
  2020; 7 (1): 309

- **Bacterial flagellar motor PL-ring disassembly subcomplexes are widespread and ancient.** *Proceedings of the National Academy of Sciences of the United States of America*
  Kaplan, M. n., Sweredoski, M. J., Rodrigues, J. P., Tocheva, E. I., Chang, Y. W., Ortega, D. R., Beeby, M. n., Jensen, G. J.
  2020

- **Less Is More: Coarse-Grained Integrative Modeling of Large Biomolecular Assemblies with HADDOCK.** *Journal of chemical theory and computation*
  Roel-Touris, J. n., Don, C. G., V Honorato, R. n., Rodrigues, J. P., Bonvin, A. M.
  2019

- **Publisher Correction: Structural insights into binding specificity, efficacy and bias of a beta2AR partial agonist.** *Nature chemical biology*
  Masureel, M., Zou, Y., Picard, L., van der Westhuizen, E., Mahoney, J. P., Rodrigues, J. P., Mildorf, T. J., Dror, R. O., Shaw, D. E., Bouvier, M., Pardon, E., Steyaert, J., Sunahara, et al
  2018

- **Structural insights into binding specificity, efficacy and bias of a beta2AR partial agonist.** *Nature chemical biology*
  Masureel, M., Zou, Y., Picard, L., van der Westhuizen, E., Mahoney, J. P., Rodrigues, J. P., Mildorf, T. J., Dror, R. O., Shaw, D. E., Bouvier, M., Pardon, E., Steyaert, J., Sunahara, et al
  2018; 14 (11): 1059–66

- **Proteomic analysis of monolayer-integrated proteins on lipid droplets identifies amphipathic interfacial alpha-helical membrane anchors.** *Proceedings of the National Academy of Sciences of the United States of America*
  Pataki, C. I., Rodrigues, J., Zhang, L., Qian, J., Efron, B., Hastie, T., Elias, J. E., Levitt, M., Kopito, R. R.
  2018

- **Defining distance restraints in HADDOCK.** *Nature protocols*
  Bonvin, A. M., Karaca, E., Kastritis, P. L., Rodrigues, J. P.
  2018

- **The solution structure of monomeric CCL5 in complex with a doubly sulfated N-terminal segment of CCR5** *FEBS JOURNAL*
  Abayev, M., Rodrigues, J. M., Srivastava, G., Arshava, B., Jaremko, L., Jaremko, M., Naider, F., Levitt, M., Anglister, J.
  2018; 285 (11): 1988–2003

- **SILAC-based phosphoproteomics reveals new PP2A-Cdc55-regulated processes in budding** *GIGASCIENCE*
  Baro, B., Jativa, S., Calabria, I., Vinaixa, J., Bech-Serra, J., de LaTorre, C., Rodrigues, J., Luisa Hernaez, M., Gil, C., Barcelo-Batllori, S., Larsen, M. R., Queralt, E.
  2018; 7 (5)

- **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*
  Kurkcuoglu, Z. n., Koukos, P. I., Citro, N. n., Trellet, M. E., Rodrigues, J. P., Moreira, I. S., Roel-Touris, J. n., Melquiond, A. S., Geng, C. n., Schaarschmidt, J. n., Xue, L. C., Vangone, A. n., Bonvin, et al
  2018; 32 (1): 175–85

- **pdb-tools: a swiss army knife for molecular structures.** *F1000Research*
  Rodrigues, J. P., Teixeira, J. M., Trellet, M., Bonvin, A. M.
  2018; 7: 1961

- **Template-based protein-protein docking exploiting pairwise interfacial residue restraints.** *Briefings in bioinformatics*
  Xue, L. C., Rodrigues, J. P., Dobbs, D., Honavar, V., Bonvin, A. M.
  2017; 18 (3): 458-466

- **Structural and Functional Analysis of a beta(2)-Adrenergic Receptor Complex with GRK5** *Cell*
  Komolov, K. E., Du, Y., Duc, N. M., Betz, R. M., Rodrigues, J. P., Leib, R. D., Patra, D., Skiniotis, G., Adams, C. M., Dror, R. O., Chung, K. Y., Kobilka, B. K., Benovic, et al
  2017; 169 (3): 407-421 e16

- **Structural and Functional Analysis of a beta(2)-Adrenergic Receptor Complex with GRK5** *CELL*
  Komolov, K. E., Du, Y., Nguyen Minh Duc, N. M., Betz, R. M., Rodrigues, J. P., Leib, R. D., Patra, D., Skiniotis, G., Adams, C. M., Dror, R. O., Chung, K. Y., Kobilka, B. K., Benovic, et al
  2017; 169 (3): 407-?

- **Sense and Simplicity in HADDOCK Scoring: Lessons from CASP-CAPRI (page 418).** *Proteins*
  Vangone, A. n., Rodrigues, J. P., Xue, L. C., van Zundert, G. C., Geng, C. n., Kurkcuoglu, Z. n., Nellen, M. n., Narasimhan, S. n., Karaca, E. n., van Dijk, M. n., Melquiond, A. S., Visscher, K. M., Trellet, et al
  2017; 85 (8): 1589–90

- **M3: an integrative framework for structure determination of molecular machines.** *Nature methods*
  Karaca, E. n., Rodrigues, J. P., Graziadei, A. n., Bonvin, A. M., Carlomagno, T. n.
  2017; 14 (9): 897–902

- **Supramolecular Organization and Functional Implications of K+ Channel Clusters in Membranes.** *Angewandte Chemie (International ed. in English)*
  Visscher, K. M., Medeiros-Silva, J. n., Mance, D. n., Rodrigues, J. P., Daniëls, M. n., Bonvin, A. M., Baldus, M. n., Weingarth, M. n.
  2017; 56 (43): 13222–27

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

- **Information-Driven, Ensemble Flexible Peptide Docking Using HADDOCK.** *Methods in molecular biology (Clifton, N.J.)*
  Geng, C., Narasimhan, S., Rodrigues, J. P., Bonvin, A. M.
  2017; 1561: 109-138

- **PRODIGY: a web server for predicting the binding affinity of protein-protein complexes** *BIOINFORMATICS*
  Xue, L. C., Rodrigues, J. P., Kastritis, P. L., Bonvin, A. M., Vangone, A.
  2016; 32 (23): 3676-3678

- **Prediction of homoprotein and heteroprotein complexes by protein docking and template-based modeling: A CASP-CAPRI experiment** *PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS*
  Lensink, M. F., Velankar, S., Kryshtafovych, A., Huang, S., Schneidman-Duhovny, D., Sali, A., Segura, J., Fernandez-Fuentes, N., Viswanath, S., Elber, R., Grudinin, S., Popov, P., Neveu, et al
  2016; 84: 323-348

- **New Insight into the Catalytic Mechanism of Bacterial MraY from Enzyme Kinetics and Docking Studies** *JOURNAL OF BIOLOGICAL CHEMISTRY*
  Liu, Y., Rodrigues, J. P., Bonvin, A. M., Zaal, E. A., Berkers, C. R., Heger, M., Gawarecka, K., Swiezewska, E., Breukink, E., Egmond, M. R.
  2016; 291 (29): 15057-15068

- **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*

Rodrigues, J. P., Melquiond, A. S., Bonvin, A. M.
2016; 44 (2): 160-167

- **The Supramolecular Organization of a Peptide-Based Nanocarrier at High Molecular Detail** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Rad-Malekshahi, M., Visscher, K. M., Rodrigues, J. P., de Vries, R., Hennink, W. E., Baldus, M., Bonvin, A. M., Mastrobattista, E., Weingarth, M.
  2015; 137 (24): 7775-7784

- **Information-driven structural modelling of protein-protein interactions.** *Methods in molecular biology (Clifton, N.J.)*
  Rodrigues, J. P., Karaca, E., Bonvin, A. M.
  2015; 1215: 399-424

- **Binding Hotspots of BAZ2B Bromodomain: Histone Interaction Revealed by Solution NMR Driven Docking** *BIOCHEMISTRY*
  Ferguson, F. M., Dias, D. M., Rodrigues, J. P., Wienk, H., Boelens, R., Bonvin, A. M., Abell, C., Ciulli, A.
  2014; 53 (42): 6706-6716

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

- **Proteins Feel More Than They See: Fine-Tuning of Binding Affinity by Properties of the Non-Interacting Surface** *JOURNAL OF MOLECULAR BIOLOGY*
  Kastritis, P. L., Rodrigues, J. P., Folkers, G. E., Boelens, R., Bonvin, A. M.
  2014; 426 (14): 2632-2652

- **HADDOCK(2P2I): A Biophysical Model for Predicting the Binding Affinity of Protein-Protein Interaction Inhibitors** *JOURNAL OF CHEMICAL INFORMATION AND MODELING*
  Kastritis, P. L., Rodrigues, J. P., Bonvin, A. M.
  2014; 54 (3): 826-836

- **Defining the limits of homology modeling in information-driven protein docking** *PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS*
  Rodrigues, J. P., Melquiond, A. S., Karaca, E., Trellet, M., Van Dijk, M., van Zundert, G. C., Schmitz, C., de Vries, S. J., Bordogna, A., Bonati, L., Kastritis, P. L., Bonvin, A. M.
  2013; 81 (12): 2119-2128

- **Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions** *PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS*
  Moretti, R., Fleishman, S. J., Agius, R., Torchala, M., Bates, P. A., Kastritis, P. L., Rodrigues, J. P., Trellet, M., Bonvin, A. M., Cui, M., Rooman, M., Gillis, D., Dehouck, et al
  2013; 81 (11): 1980-1987

- **Unveiling the Interaction of Vanadium Compounds with Human Serum Albumin by Using H-1 STD NMR and Computational Docking Studies** *EUROPEAN JOURNAL OF INORGANIC CHEMISTRY*
  Dias, D. M., Rodrigues, J. P., Domingues, N. S., Bonvin, A. M., Castro, M. M.
  2013; 2013 (26): 4619-4627

- **KoBaMIN: a knowledge-based minimization web server for protein structure refinement** *NUCLEIC ACIDS RESEARCH*
  Rodrigues, J. P., Levitt, M., Chopra, G.
  2012; 40 (W1): W323-W328

- **KoBaMIN: a knowledge-based minimization web server for protein structure refinement.** *Nucleic acids research*
  Rodrigues, J. P., Levitt, M., Chopra, G.
  2012; 40 (Web Server issue): W323-8

- **Clustering biomolecular complexes by residue contacts similarity** *PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS*
  Rodrigues, J. P., Trellet, M., Schmitz, C., Kastritis, P., Karaca, E., Melquiond, A. S., Bonvin, A. M.
  2012; 80 (7): 1810-1817

- **Strengths and weaknesses of data-driven docking in critical assessment of prediction of interactions** *PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS*
  de Vries, S. J., Melquiond, A. S., Kastritis, P. L., Karaca, E., Bordogna, A., van Dijk, M., Rodrigues, J. P., Bonvin, A. M.
  2010; 78 (15): 3242-3249