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EDUCATION

2002 **Spec.** **Bioinformatics for Tropical Diseases Research**, WHO-TDR, University of São Paulo (USP).

1994 **Ph.D.** **Computational Molecular Biophysics**, Department of Crystallography - Birkbeck College, University of London, London, England. Advisor: Professor Julia M. Goodfellow.

1990 **M.Sc.** **Computer Modeling of Molecular and Biological Processes**, Department of Crystallography - Birkbeck College, University of London, England. Advisor: Professor Julia M. Goodfellow.

1988 **Spec.** **Graduate Course of Specialization in Modern Biotechnology,** Center for Biotechnology - Universidade Federal do Rio Grande do Sul (UFRGS), Porto Alegre, RS, Brazil.

1987 **B.Sc.** **Physics**, Department of Physics - Universidade Federal de Minas Gerais (UFMG), Belo Horizonte, MG, Brazil.

PROFESSIONAL EXPERIENCE

2002 – Present **M.Sc. and Ph.D. Advisor**
Graduate Program in Computer Science (Faculty of Informatics, PUCRS); Graduate Program in Molecular and Cellular Biology (Faculty of Biosciences, PUCRS), and Graduate Program in Pharmaceutical Biotechnology (Faculty of Pharmacy, PUCRS).

2002 – Present **Associate Professor (Reader) of Bioinformatics and Computational Molecular Biophysics**
Faculty of Informatics – Pontifical Catholic University of Rio Grande do Sul (PUCRS), Porto Alegre, RS, Brasil. Head of the Laboratory for Bioinformatics, Modelling and Simulation of Biosystems (LABIO). Research focused on the sequence-structure-dynamics-function relationship of enzymes from the Fatty Acid Synthase II (FAS II) and the Shikimate Pathways from *Mycobacterium tuberculosis* (MTB), *Plasmodium spp.*, DNA-protein interaction in eukaryotic transcription, *Ab initio* protein structure prediction, and computer-aided drug design.

2001 – 2002 **FAPERGS Visiting Scientist**
Faculty of Informatics - Pontifical Catholic University of Rio Grande do Sul (PUCRS), Porto Alegre, RS, Brasil.

1999 – 2001 **FAPESP Young Investigator and Group Leader – Molecular Modeling and Simulation**
Center for Structural Molecular Biology – Laboratório Nacional de Luz Síncrotron (LNLS), Campinas, São Paulo, Brazil.

1995 - 1998 **Postdoctoral Scientist - Modeling and Simulation of DNA and Enzymes Complexes**
Theory, Modeling & Simulation Group - Environmental Molecular Sciences Laboratory (EMSL), Pacific Northwest National Laboratory (PNNL-DOE, USA). Advisor: Rick L. Ornstein. Research on structure-dynamics-function relationships of the detoxification enzymes Glutathione S-Transferase and Phosphotriesterase. The initial focus of the research was in the conformation and flexibility of DNA sequences containing a TATA-Box motif.

1990 - 1994 **Graduate Research Assistant - Molecular Dynamics Studies of DNA Intrinsic Curvature**
Department of Crystallography - Birkbeck College, University of London, London, England. Research focused on the use of molecular dynamics simulations to bridge the knowledge gap between X-ray crystallography and gel-electrophoresis analysis of DNA sequence-dependent conformation.

1986 - 1988 **Undergraduate Research Assistant**
Department of Physics - Universidade Federal de Minas Gerais (UFMG), Belo Horizonte, MG, Brazil.
1987-1988 Design, preparation, and testing of high-temperature ceramic superconductors.
1986-1987 Investigations of the electrical properties of fuel alcohol-water mixtures.

TEACHING EXPERIENCE

2001 – Present **Associate Professor (Reader) of Bioinformatics and Computational Molecular Biophysics**
Faculty of Informatics, Faculty of Biosciences, and Faculty of Pharmacy. Pontifical Catholic University of Rio Grande do Sul (PUCRS). Lecturing bioinformatics, computational molecular biophysics, information technology, and scientific methodology for computer science and biological sciences at both undergraduate and graduate levels.

1990 - 1992 **Teaching Assistant**
Department of Crystallography - Birkbeck College, University of London, London, England. Statistical Techniques in Molecular and Biological Structure. M.Sc. Course in Computer Modeling of Molecular and Biological Processes.

1985 - 1987 **Demonstrator/Teaching Assistant**
Department of Physics - Universidade Federal de Minas Gerais, MG, Brazil. Courses in Electricity & Magnetism.

ACADEMIC/SCHOLASTIC HONORS

- Research Fellow of the Brazilian National Research Council-CNPq, 2013-2016.
- Elected Chair of the CEBioComp (The Special Interest Group on Computational Biology) of the Brazilian Computer Society, August 2011, for the period 2011-2012.
- Research Fellow of the Brazilian National Research Council-CNPq, 2010-2013.
- Elected Member of the CEBioComp of the Brazilian Computer Society, since August 2008.
- Third Best Full Paper of the III Brazilian Symposium on Bioinformatics (BSB2008), August 2008.
- ICGEB Grant for Junior Scientists, International Centre for Genetic Engineering & Biotechnology, ICGEB/LNCC, May 2007.
- Best Poster Award, X-Meeting, AB^{3}C 3rd International Conference, November 2007.
- Research Fellow of the Brazilian National Research Council-CNPq, 2007-2010.
- Elected Member for the Brazilian Association for Bioinformatics and Computational Biology (AB^{3}C) directorship, July 2006, for the period 2007-2008.
- Honorable Mention for work on Flexible Ligand-Flexible Enzyme Interactions in the 5th Ibero-American Congress of Biophysics, Rio de Janeiro, Brazil, October 2003.
- Special Award for outstanding research on *ab initio* protein structure prediction in the Research-Training Congress from the Universidade Federal do Rio Grande do Sul (UFRGS), RS, Brazil, September 2002.
- *Ad-hoc* reviewer for Biophysical Journal, CABIOS (now Bioinformatics), and several other international journals.
- AWU and DOE Post-doctoral Fellowship, 1995-1998.
- President-elect of the Lillian Penson Hall Residents Union, 1991 to 1992, Lillian Penson Hall, London, England. Lillian Penson Hall housed approximately 550 postgraduate students from over 80 countries.
- Ph.D. CNPq-RAHE Fellowship, 1990-1994; M. Sc. CNPq-RAHE Scholarship, 1989-1990.
- Class representative for the M.Sc. course in Computer Modeling of Molecular and Biological Processes, Department of Crystallography, Birkbeck College, University of London, London, England, 1989-1990.
- CNPq-RHAE Scholarship, 1988-1989.
- Co-winner of the Santos Dumont Silver Medal of Science and Technology for contribution to research on High-temperature Ceramic Superconductors, Belo Horizonte, MG, Brazil, April 1988.
- Demonstrator, Teaching Assistant, and Research-Training CNPq and FAPEMIG Scholarships, 1984-1987.

LIST OF ACCEPTED PUBLICATIONS

1. Winck, A. T.; Machado, K. S.; Norberto de Souza, O.; Ruiz, D. D. Context-based data preprocessing of molecular docking data. **BMC Genomics**, 2013.

2. Wink, P. L.; Quitian, Z. A. S.; Rosado, L. A.; Rodrigues Junior, V. S.; Petersen, G. O.; Lorenzini, D. M.; Lipinski-Paes, T.; Timmers, L. F. S. M.; Norberto de Souza, O.; Basso, L. A.; Santos, D. S. Biochemical characterization of recombinant nucleoside hydrolase from Mycobacterium tuberculosis H37Rv. **Archives of Biochemistry and Biophysics** (Print), D.O.I: 10.1016/j.abb.2013.08.011, 2013.

LIST OF MAJOR PUBLICATIONS

Periodicals

1. Pauli, I.; Santos, R. N.; Rostirolla, D. C.; Martinelli, L. K. ; Ducati, R. G.; Timmers, L. F. S. M.; Basso, L. A.; Santos, D. S.; Guido, R. V. C.; Andricopulo, A. D.; Norberto de Souza, O. Discovery of New Inhibitors of Mycobacterium tuberculosis InhA Enzyme using Virtual Screening and a 3D-Pharmacophore-Based Approach. **Journal of Chemical Information and Modeling**, Vol. 53, pp. DOI: 10.1021/ci400202t, 2013.

2. Dall'Agno, K. C. M.; Norberto de Souza, O. An expert protein loop refinement protocol by molecular dynamics simulations with restraints. **Expert Systems with Applications**, Vol. 40, pp. 2568-2574, 2013.

3. De Paris, R.; Frantz, F. A.; Norberto de Souza, O.; Ruiz, D. D. wFReDoW: a cloud-based web environment to handle molecular docking simulations of a fully-flexible receptor model. **Journal of Biomedicine and Biotechnology**, Vol. 2013, p. 1-12, 2013.

4. Jaskulsky, L.; Rosado, L. A.; Rostirolla, D. C.; Timmers, L. F. S. M.; Norberto de Souza, O.; Santos, D. S.; Basso, L. A. Kinetic mechanism and energetics of binding of phosphoryl group acceptors to Mycobacterium tuberculosis Cytidine Monophosphate Kinase. **Archives of Biochemistry and Biophysics**, Vol. 536, pp. 53-63, 2013.

5. Dorn, M.; Norberto de Souza, O. An interval-based algorithm to represent conformational states of experimentally determined polypeptide templates and fast prediction of approximated 3D protein structures. **International Journal of Bioinformatics Research and Applications**, Vol. 9, pp. 462-486, 2013.

6. Costa, A. L. P., Pauli, I., Dorn, M., Schroeder, E. K., Zhan, C.-G., Norberto de Souza, O. Conformational changes in 2-trans-enoyl-ACP (CoA) Reductase (InhA) from M. tuberculosis induced by an inorganic complex: a molecular dynamics simulation study. **Journal of Molecular Modeling**, Vol. 18, pp. 1779-1790, 2012.

7. Barros, R. C.; Winck, A. T.; Machado, K. S.; Basgalupp, M.P.; Carvalho, A. C. P. L. F.; Ruiz, D. D.; Norberto de Souza, O. Automatic design of decision-tree induction algorithms tailored to flexible-receptor docking data. BMC Bioinformatics, Vol. 13, pp. 310, 2012.

8. Winck, A. T., Quevedo, C. V., Machado, K. S., Norberto de Souza, O., Ruiz, D. D. A Comparative Analysis of Public Ligand Databases Based on Molecular Descriptors. **Lecture Notes in Computer Science**, Vol. 7409, pp. 156-167, 2012.

9. Machado, K. S., Winck, A. T., Ruiz, D. D., Norberto de Souza, O. Mining flexible-receptor molecular docking data. **Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery**, Vol. 1, Issue 6, pp. 532-541, 2011.

10. Machado, K. S., Schroeder, E. K., Ruiz, D. D., Cohen, E. M. L., Norberto de Souza, O. FReDoWS: a method to automate molecular docking simulations with explicit receptor flexibility and snapshots selection. **BMC Genomics**, Vol. 12, pp. S6, 2011.

11. Cohen, E. M. L., Machado, K. S., Cohen, M., Norberto de Souza, O. Effect of the explicit flexibility of the InhA enzyme from Mycobacterium tuberculosis in molecular docking simulations. **BMC Genomics,** Vol. 12, pp. S7, 2011.

12. De Paris, R., Frantz, F. A., Ruiz, D. D., Norberto de Souza, O. A Conceptual Many Tasks Computing Architecture to Execute Molecular Docking Simulations of a Fully-Flexible Receptor Model. **Lecture Notes in Computer Science**, Vol. 6832, pp. 75-78, 2011.

13. Machado, K. S., Winck, A. T., Ruiz, D. D., Norberto de Souza, O. Mining flexible-receptor docking experiments to select promising protein receptor snapshots. **BMC Genomics**, Vol. 11, (Suppl. 5):S6, 2010.

14. Machado, K. S., Winck, A. T., Ruiz, D. D.A., Norberto de Souza, O. Discretization of Flexible-Receptor Docking Data. **Lecture Notes in Computer Science**, Vol. 6368, pp. 75-79, 2010.

15. Dorn, M., Norberto de Souza, O. A3N: an Artificial Neural Network N-gram-based method to approximate 3-D polypeptides structure prediction. **Expert Systems with Applications**, Vol. 37, Issue 12, pp. 7497-7508, 2010.

16. Dorn, M., Norberto de Souza, O. Mining the Protein Data Bank with CReF to predict approximate 3-D structures of polypeptides. **International Journal of Data Mining and Bioinformatics**, Vol. 4, Issue 3, pp. 281-299, 2010.

17. Thompson, C. E., Fernandes, C. L., Norberto de Souza, O., Freitas, L. B., Salzano, F. M. Evaluation of the impact of functional diversification on Poaceae, Brassicaceae, Fabaceae, and Pinaceae alcohol dehydrogenase enzymes**. Journal of Molecular Modeling**, Vol. 16, pp. 919-928, 2010.

18. Winck, A. T., Machado, K. S., Norberto de Souza, O., Ruiz, D. D. FReDD: supporting mining strategies though a flexible-receptor docking database. **Lecture Notes in Computer Science**, Vol. 5676, pp. 143-146, 2009.

19. Machado, K. S., Schroeder, E. K., Ruiz, D. D. A., Wink, A., Norberto de Souza, O. Extracting Information from Flexible Receptor-Flexible Ligand Docking Experiments. **Lecture Notes in Computer Science**, Vol. 5167, pp. 104-114, 2008.

20. Dorn, M., Breda, A., Norberto de Souza, O. A Hybrid Method for the Protein Structure Prediction Problem. **Lecture Notes in Computer Science**, Vol. 5167, pp. 47-56, 2008.

21. Breda A., Santos, D. S., Basso, L. A., Norberto de Souza, O. *Ab initio* 3-D structure prediction of an artificially designed three-α-helix bundle via all-atom molecular dynamics simulations. **Genetics and Molecular Research**, Vol. 6, Issue 3, pp. 901-910, 2007.

22. Thompson, C. E., Freitas, L. B., Salzano, F. M., Norberto de Souza, O**.** Sequence and structural aspects of the functional diversification of plant alcohol dehydrogenases. **Gene (Amsterdan)**, Vol. 396, Issue 1, pp. 108-115, 2007.

23. Machado, K. S., Schroeder, E. K., Ruiz, D. D. A., Norberto de Souza, O. Automating molecular docking with explicit receptor flexibility using scientific workflows. **Lecture Notes in Computer Science**, Vol. 4643, pp. 1-11, 2007.

24. Fonseca, I. O., Silva, R. G., Fernandes, C. L., Norberto de Souza, O., Basso, L. A., Santos, D. S. Shikimate dehydrogenase from *Mycobacterium tuberculosis* H37Rv: Kinetic and Chemical Mechanisms. **Archives of Biochemistry and Biophysics**, Vol. 457, Issue 2, 15 January 2007, pp. 123-133.

25. Fernandes, C. L., Breda, A., Santos, D. S., Basso, L. A., Norberto de Souza, O. A structural model for chorismate synthase from Mycobacterium tuberculosis in complex with coenzyme and substrate. **Computers in Biology and Medicine**, Vol. 37, Issue 2, pp. 149-158, 2007.

26. Czekster, R. M. & Norberto de Souza, O. SimVIZ - A desktop virtual environment for visualization and analysis of protein multiple simulation trajectories. **Lecture Notes in Computer Science**, Vol. 3980, pp. 202-211, 2006.

27. Oliveira, J. S., Souza, E. H., Norberto de Souza, O., Moreira, I. S., Santos, D. S., Basso, L. A. Slow onset inhibition of wild-type and isoniazid-resistant 2-trans-Enoyl-ACP (CoA) reductase from Mycobacterium tuberculosis. **Current Pharmaceutical Design**, Vol. 12, Issue 19, 2409-2424, 2006.

28. Thompson, C. E., Fernandes, C. L., Norberto de Souza, O., Salzano, F. M., Bonatto, S. L., Freitas, L. B. Molecular modelling of pathogenesis-related proteins of family 5. **Cell Biochemistry and Biophysics**, Vol. 44, pp. 385-394, 2006.

29. Oliveira, J. S., Pereira, J. H., Canduri, F., Norberto de Souza, O., Azevedo-Junior, W. F., Basso, L. A., Santos, D. S. Crystallographic and pre-steady state kinetics studies on binding of NADH to wild-type and isoniazid-resistant enoyl-ACP (CoA) reductase enzymes from Mycobacterium tuberculosis. **Journal of Molecular Biology**, Vol. 359, pp. 646-666, 2006.

30. Schroeder, E. K., Santos, D. S., Basso, L. A., Norberto de Souza, O. Molecular dynamics simulation studies of the wild-type, I21V and I16T mutants of isoniazid resistant Mycobacterium tuberculosis enoyl reductase (InhA) in complex with NADH: Towards the understanding of NADH-InhA different affinities, **Biophysical Journal**, Vol. 89, pp. 876-884, 2005.

31. Fernandes, C. L., Santos, D. S., Basso, L. A., Norberto de Souza, O. Structure prediction and docking studies of chorismate synthase from Mycobacterium tuberculosis. **Lecture Notes in Computer Science**, Vol. 3594, pp. 118-127, 2005.

32. Czekster, R. M., & Norberto de Souza, O. VIZ - A graphical open-source architecture for use in structural bioinformatics. **Lecture Notes in Computer Science**, Vol. 3594, pp. 226-229, 2005.

33. Benedetti, C. E., Kobarg, J., Pertinhez, T. A., Gatti, R. M., Norberto de Souza, O., Spisni, A., Meneghini, R. Plasmodium falciparum histidine-rich protein II binds to actin, phosphatidylinositol 4,5-bisphosphate and erythrocyte ghosts in a pH-dependent manner and undergoes coil-to-helix transitions in anionic micelles. **Molecular and Biochemical Parasitology**, Vol. 128, pp. 157-166, 2003.

34. Schroeder, E. K., Norberto de Souza, O., Santos, D. S., Blanchard, J. S., Basso, L. A. Drugs that inhibit mycolic acid biosynthesis in Mycobacterium tuberculosis. **Current Pharmaceutical Biotechnology**, Vol. 3, pp. 197-225, 2002.

35. Norberto de Souza, O. & Ornstein, R. L. Molecular dynamics simulations of a protein-protein dimer: Particle-Mesh Ewald electrostatic model yields far superior results to standard cutoff model, **Journal of Biomolecular Structure and Dynamics,** Vol. 16, pp. 1205-1211, 1999.

36. Zhan, C.-G., Norberto de Souza, O., Rittenhouse, R., Ornstein, R. L. Determination of two structural forms of catalytic bridging ligand in zinc phosphotriesterase by molecular dynamics simulation and quantum chemical calculation, **Journal of the American Chemical Society**, Vol. 121, pp. 7279 -7282, 1999.

37. Norberto de Souza, O. & Ornstein, R. L. Inherent DNA curvature and flexibility correlate with TATA-Box functionality, **Biopolymers,** Vol. 46, pp. 403-415, 1998.

38. Norberto de Souza, O. & Ornstein, R. L. Effect of warm up protocol and sampling time on convergence of molecular dynamics simulations of a DNA dodecamer using AMBER 4.1 and particle-mesh Ewald method, **Journal of Biomolecular Structure and Dynamics**, Vol. 14, pp. 607-611, 1998.

39. Norberto de Souza, O. & Ornstein, R. L. Effect of periodic box size on aqueous molecular dynamics simulation of a DNA dodecamer with particle-mesh Ewald method, **Biophysical Journal,** Vol. 72, pp. 2395-2397, 1997.

40. Norberto de Souza, O & Goodfellow, J. M. Molecular dynamics simulations of oligonucleotides in solution: Visualization of intrinsic curvature, **Journal of Computer-Aided Molecular Design**, Vol. 8, pp. 307-322, 1994.

Conferences

41. Winck, A. T., Machado, K. S., Norberto de Souza, O., Ruiz, D. D. Supporting Intermolecular Interaction Analyses of Flexible-Receptor Docking Simulations. In: IADIS International Conference Applied Computing, Timisoara, Romania. **Proceedings of the IADIS International Conference Applied Computing**, pp. 183-190, 2010.

42. Machado, K. S., Winck, A. T., Ruiz, D. D., Norberto de Souza, O. Comparison of Discretization Methods of Flexible-Receptor Docking Data for Analyses by Decision Trees. In: IADIS International Conference Applied Computing, Timisoara, Romania. **Proceedings of the IADIS International Conference on Applied Computing**, pp. 225-229, 2010.

43. Dorn, M., Norberto de Souza, O. CReF: A central-residue-fragment-based method for predicting approximate 3-D polypeptides structures. In: **Proceedings of the 23th ACM Symposium on Applied Computing**, Fortaleza/CE. New York: ACM, Inc., Vol. 2, pp.1261-1267, 2008.

44. Netto, M. A. S., Breda, A., Norberto de Souza, O. Scheduling Complex Computer Simulations on Heterogeneous Non-dedicated Machines: A case study in structural bioinformatics. In: **Proceedings of the 5th IEEE International Symposium on Cluster Computing and the Grid**, Cardiff-UK. **CCGRID2005**, Vol. 2, pp. 768-775, 2005.

45. Silva, A. O. & Norberto de Souza, O. A Framework for result handling in bioinformatics: An application to computer-assisted drug design. In: **Proceedings of the 20th ACM Symposium on Applied Computing**, Santa Fe- USA. **SAC2005**, pp. 128-132, 2005.

Published or Edited Books

46. Norberto de Souza, O., Telles, G. P., Palakal, M. J. (Orgs.). Advances in Bioinformatics and Computational Biology - 6th Brazilian Symposium on Bioinformatics, BSB 2011, **Lecture Notes in Computer Science**, Vol. 6832. 1. Ed. Berlin: Springer, 2011. 83 pp.

47. Norberto de Souza, O., Telles, G. P., Palakal, M. J. (Orgs.). Digital Proceedings of the 6th Brazilian Symposium on Bioinformatics. Porto Alegre: Sociedade Brasileira de Computação (SBC), 2011.

Book Chapters

48. Winck, A. T., Machado, K. S., Ruiz, D. D., Norberto de Souza, O. Processo de KDD aplicado a Bioinformática. In: Adriano C. Machado Pereira; Gisele Lobo Pappa. Marco Winckler; Roberta Lima Gomes. (Org.). Tópicos em sistemas colaborativos, multimídia, web e banco de dados. Porto Alegre: Sociedade Brasileira de Computação, 2010, Vol. 1, pp. 159-180.

49. Breda, A., Valadares, N. F., Norberto de Souza, O., Garratt, R. C. Protein Structure, Modelling and Applications. In: Arthur Gruber; Alan M. Durham; Chuong Huynh; Hernando A. del Portillo. (Org.). Bioinformatics for Tropical Disease Research: A Practical and Case-Study Approach. Maryland: NIH/NCBI, 2008, http://www.ncbi.nlm.nih.gov/books/NBK6824/.

50. Goodfellow, J. M., Norberto de Souza, O., Parker, K., Cruzeiro-Hansson, L. Simulations of biomolecular systems, in **Simulation of Biomolecular Systems: Theoretical and Experimental Applications**, Vol. 2, Eds. Wilfred F. van Gunsteren, Paul K. Weiner, & Anthony J. Wilkinson, Escom, Holland, pp. 483-495, 1993.

SOCIETY MEMBERSHIP

- American Computer Machinery (ACM) – USA
- Associação Brasileira de Bioinformática e Biologia Computacional (AB^{3}C)
- Biophysical Society – USA
- International Society for Computational Biology (ISCB) – USA
- Sociedade Brasileira de Biofísica (SBBf)
- Sociedade Brasileira de Computação (SBC)

PERSONAL DETAILS

Date of Birth: 14th January
Marital Status: Single
Driving License: Full clean

DETAILED CV IN PORTUGUESE

Please, see the following page:
http://buscatextual.cnpq.br/buscatextual/visualizacv.do?metodo=apresentar&id=K4781658Z2