

Prof. Thereza Amélia Soares**BioMaterial Modeling Group**

Department of Fundamental Chemistry
Federal University of Pernambuco
Av. Prof. Luiz Freire S/N
Cidade Universitária 50740-540
Recife, PE, Brazil

Phone +55.81.2126.8440

Email thereza.soares@ufpe.br

Personal Information

Citizenship - Brazilian

Languages - Portuguese (native)

- English (fluent)

- French (intermediate)

webpage - dqfnet.ufpe.br/biomat

ResearcherID: G-1065-2010

Brief Research Statement

My major research interest is in the application of computational chemistry methodologies to understanding molecular processes and to interpret experimental observations. My current research work deals with the development, validation and application of molecular models of bacterial outer membranes and the development of computational tools to investigate the polymorphism induced by external agents (cation type, ionic strength, antimicrobials) and chemotypes on lipopolysaccharide membranes. Recently, I have also initiated research in the field of molecular brushes where we aim to develop molecular models to investigate the mechanism by which conformational changes induced by ionic strength, salt type, pH modulates the swollen/salt-in/salt-out phenomena in these materials. The ultimate goal is to probe structure-dependent behavior of the interface between bacterial outer membranes (including outer membranes) and molecular brushes of biomedical interest.

Professional Experience

2010-Present **Tenured Professor**, Federal University of Pernambuco, Recife, Brazil.

2016 **Invited Professor**, University of Umeå, Sweden (6 months)

2013 **Professeur Invité**, École Polytechnique Fédérale de Lausanne, Switzerland
(3 months)

2005-2009 **Senior Research Scientist**, Pacific Northwest National Laboratory; Richland,
WA, USA

2001-2003 **Postdoctoral Fellow**, Swiss Federal Institute of Technology, Zürich, Switzerland,

2004-2005 **Postdoctoral Fellow**, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Education

Chemistry, Ph.D. - Federal University of Pernambuco, Brazil - 06/1996-01/2001.

Research visiting fellow, the Scripps Research Institute, La Jolla, CA, USA, 06/1997 - 10/1998
Research visiting fellow, University of Houston, TX, USA, 11/1998 - 01/2000
Research visiting fellow, Pacific Northwest National Laboratory, Richland, WA, USA, 02 - 11/2000

Enology, Extension Program - Washington State University, USA - 03/2006-12/2008.

Chemistry, M.Sc. - Federal University of Pernambuco, Brazil - 08/1994-04/1996.

Biology, B.Sc. - Federal University of Pernambuco, Brazil - 03/1989-06/1994.

Funded Grants

Title: Computational Simulations of Polymer Brushes.

Funding Organization: Newton Fund, UK.

Role: Principal Foreigner Investigator

Period: 2015-2017

Title: Development of Computational Tools for Biomedical Research: From Molecular Modeling to Translational Research.

Funding Organization: Coordination for the Improvement of Higher Education (CAPES).

Role: Co-Investigator

Period: 2014-2019

Title: Molecular Basis of Infectious Diseases: Bacterial Resistance em Gram-Negative Bacteria and Engineering of Immune-reactive epitopes.

Funding Organization: Research Funding Agency from Pernambuco State (FACEPE).

Role: Principal Investigator

Period: 2015-2018

Title: Interactions and Binding of Drug Molecules to Organic Metal Frameworks for Controlled Drug Release.

Funding Organization: Brazilian Council for Scientific Research and Development (CNPq).

Role: Principal Investigator

Period: 2013-2015

Title: Computational Simulations of Bacterial Membranes and Outer Membrane Proteins.

Funding Organization: Brazilian Council for Scientific Research and Development (CNPq).

Role: Principal Investigator

Period: 2013-2015

Title: Computational Simulations of Antimicrobial Peptides in Bacterial Membranes.

Funding Organization: Research Funding Agency from Pernambuco State (FACEPE).

Role: Principal Investigator

Period: 2012-2015

Title: The Effect of Cationic Antimicrobial Peptides on the Structure and Dynamics of Lipopolysaccharide Chemotype Membranes of *Pseudomonas aeruginosa*.

Funding Organization: Brazilian Council for Scientific Research and Development (CNPq).

Role: Principal Investigator

Period: 2012-2015

Title: Hybrid Platform Cluster: The Neumann II Multiuser Cluster

Funding Organization: Research Funding Agency from Pernambuco State (FACEPE).

Role: Co-Investigator

Period: 2012-2014

Title: Understanding the Biocompatibility of Polymeric Biomaterial Surfaces.

Funding Organization: Swedish Foundation for International Cooperation in Research and Higher-Education (STINT).

Role: Principal Foreign Investigator

Period: 2011-2013, 2013-2017

Title: Characterization of the Interface Biomolecule-Nanomaterials via Computational Simulations.

Funding Organization: Brazilian Council of Scientific and Technological Development (CNPq).

Role: Co-Investigator

Period: 2009-2012

Title: Enhanced sensing of threat agents through engineered multivalent binding scaffolds.

Funding Organization: U.S. Department of Defense.

Role: Co-Investigator

Period: 2009-2012

Title: Protein renaturation in a nanofunctionalized configuration.

Funding Organization: National Institutes of Health.

Role: Co-Investigator

Period: 2008-2011

Title: *Pseudomonas aeruginosa* outer membrane modeling.

Client Organization: National Institutes of Health.

Role: Key-Investigator

Period: 2005-2010

Computer Time Allocations through Peer-Reviewed Proposals (last 4 years)

Pacific Northwest National Laboratory (MSCF-PNNL), USA; Argonne National Laboratory (ACLF-ANL), USA; Swiss SuperComputer Center (CSCS), Switzerland; High Performance Computer Center North (HPC2N), Sweden.

Invited Talks (Last 6 yrs)

University of Umeå (Sweden, 2016), Advanced Mini-Workshop on Cell Adhesion and Biocompatibility of Polymeric Surfaces (Recife, Brazil, 2015), V STINT Workshop (Olinda, Brazil, 2015), Advanced School of Computational Simulations (Recife, Brazil, 2015) University of Oslo (Oslo, Norway, 2015), IV STINT Workshop (Umeå, Sweden, 2015), University of Bern (Switzerland, 2013) III STINT Workshop (Oxford, UK, 2013), University of Bern (Switzerland, 2013), EPFL (Switzerland, 2013), Queen Mary University of London (London, UK, 2013), II Brazilian School of Molecular Modeling (Santo André, Brazil, 2013), XLII Annual Meeting of the Brazilian Society of Biochemistry and Molecular Biology (Foz do Iguaçu, Brazil, 2013), II USP Conference on Nanotechnology (São Carlos, Brazil, 2012), II STINT Workshop (Recife, Brazil, 2012), University of São Paulo (Brazil, 2013), STINT Workshop (Umeå, Sweden, 2011), XVI Brazilian Symposium of Theoretical Chemistry (Ouro Preto, Brazil, 2011), I Brazilian School of Molecular Modeling (Santo André, Brazil, 2011), I Workshop of Applied Nanotechnology of the Amazon (Belém, Brazil, 2011), Molecular Simulation (São Paulo, Brazil, 2010), V School of Molecular Modeling of Biological Systems (Petrópolis, Brazil, 2010).

Student Supervisions

Ongoing 03 Postdoctoral fellows, 03 Ph.D. students, 01 master student and 04 undergraduate students.

Concluded 02 Postdoctoral fellows, 03 Ph.D. students, 01 M.Sc. student, and 05 undergraduate students.

Acting Member in a Total of 25 thesis committees in Brazil and Abroad

Lectures

Post-Graduate Level

Computational Simulations of BioMaterials. Lecturer. 4 hours/week/6mo, Federal University of Pernambuco, Brazil (1st semester 2016).

Biological Chemistry: Structure and Function of Biomolecules. Lecturer. 4 hours/week/6mo, Federal University of Pernambuco, Brazil (2nd semester 2010-Present).

How to Prepare and Present Scientific Talks. Lecturer. 4 hours/week/6mo, Federal University of Pernambuco, Brazil (2nd semester 2012-Present)

Graduate Level

Chemistry of Biological Processes. Lecturer. 4 hours/week/6mo, Federal University of Pernambuco, Brazil (2010-Present).

Electrochemistry and Chemical Kinetics (Theoretical course). Lecturer. 4 hours/week/6mo, Federal University of Pernambuco, Brazil (2010-2011)

Electrochemistry and Chemical Kinetics (Experimental course). Lecturer. 4 hours/week/6mo, Federal University of Pernambuco, Brazil (2010-Present)

Course on preparation and writing of academic reports. Lecturer. 4 hours/week/6mo, Federal University of Pernambuco, Brazil (2012-present)

Computer Simulation in Chemistry and Physics: Assistant. 4 hours/week/4mo, ETH-Zürich, Switzerland (winter semester 2001 - 2003).

Introduction to C++ for Biologists: Assistant. 2 hours/week/4mo, ETH-Zurich, Switzerland (winter semester 2001 - 2003).

Institutional Responsibilities

Coordinator of the Graduate Program in Chemistry (UFPE). 2015-Present.

Vice-Coordinator of the Graduate Program in Chemistry (UFPE). 2013-2015.

Member of the Chemistry Graduate Commission (UFPE), 2010-Present

Member of the Chemistry Undergraduate Collegiate (UFPE), 2010-Present

Commissions of Trust

Referee Assistance for Scientific Journals

ACS Applied Materials & Interfaces USA, Journal of the American Chemical Society, Soft Matter UK, RSC Advance UK, Journal of Chemical Theory and Computation USA, Journal of Physical Chemistry USA, PLoS ONE USA, Physical Chemistry Chemical Physics UK, Biochemistry USA, Protein Engineering, Design & Selection (USA), Journal of Molecular Recognition USA, Journal of Biomolecular Structure & Dynamics USA, International Journal of Quantum Chemistry USA, International of Molecular Sciences Switzerland, Journal of Biomolecular Structure and Dynamics USA, Journal of the Brazilian Chemical Society Brazil (*Invited Editor for special issue*)

Reviewer Assistance for Funding Agencies and Panels

European Research Council (ERC), The Brazilian National Council for Scientific and Technological Development (CNPq), São Paulo Research Foundation (FAPESP), Pernambuco Research Foundation (FACEPE), Partnership for Advanced Computing in Europe (PRACE), The Swiss National Supercomputing Centre (CSCS).

Organization of Scientific Meetings and Schools

V STINT Workshop on Understanding Biocompatibility of Polymeric Biomaterial Surfaces, Recife, 2015. Advanced School on Biomolecular Simulation, Recife, Brazil, 2015. III School of Chemistry Prof. Ricardo Ferreira, Recife, 2014. XVII Brazilian Symposium of Theoretical Chemistry, Angra dos Reis, 2013. II STINT Workshop on Understanding Biocompatibility of Polymeric Biomaterial Surfaces, Recife, 2012. I School of Chemistry Prof. Ricardo Ferreira, Recife, 2012.

Publications

[53] Membrane Negative Curvature Induced by a Hybrid Peptide from Pediocin PA-1 and Plantaricin 149 as Revealed by Atomistic Molecular Dynamic Simulations. G.A. da Hora, N.L. Archilha, J.L.S Lopes, D. Mueller, K. Coutinho, R. Itri, T.A. Soares. *Soft Matter*, 2016. *Just accepted for publication*. DOI:10.1039/C6SM01714B

[52] Impact of the Molecular Environment on the Thiol-Ene Coupling for Bio-Functionalisation and Conjugation. B. Colak, J.C.S. da Silva, T.A. Soares and J.E. Gautrot. *Bioconjugate Chemistry*. 2016. 27, 2111–2123

[51] Single-Amino Acid Modifications Reveal Additional Controls on the Proton Pathway of [FeFe]-Hydrogenase. A.J. Cornish, B. Ginovska, A. Thelen, J.C.S. da Silva, T.A. Soares, S. Raugei, M. Dupuis, W.J. Shaw, E.L. Hegg. *Biochemistry*. 2016, 55, 3165-3173.

[50] Effect of dimerization on the mechanism of action of aurein 1.2. E.N. Lorenzón, K.A. Riske, G.F.A Troiano, G.C.A. da Hora, T.A. Soares, E.M Cilli. *BBA-Biomembrane*. 2016, 1858, 1129-1138.

- [49] The Role of the Conformational Dynamics of Glutathione S-Transferase Epsilon Class on Insecticide Resistance in *Anopheles gambiae*. F.J.S. Pontes, R.T. Maia, M.C.P. Lima, C.F. J. Ayres, T.A. Soares. *J. Braz. Chem. Soc.* 2016, 26, 1602-1615.
- [48] J. Liu, X.F. Li, C.Y. Gu, J.C.S. da Silva, A.L. Barros, S. Alves-Jr., B.H. Li, F. Ren, S.R. Batten, T.A. Soares. Combined experimental and simulation study of large nanocage-based metal-organic frameworks for drug delivery. *Dalton Trans.* 2015, 44, 19370-19382.
- [47] R.D. Dias, G.C.A. da Hora, M. Ramstedt, T.A. Soares. Outer membrane remodeling: The structural dynamics and electrostatics of rough lipopolysaccharide chemotypes. *J. Chem. Theor. Comp.* 2014, 10, 2488-2497.
- [46] R.D. Dias, L. Li, T.A. Soares, E. Alexov. Modeling the electrostatic potential of asymmetric lipopolysaccharide membranes: The MEMPOT algorithm implemented in DelPhi. *J. Comp. Chem.* 2014, 35, 1418-1429.
- [45] J. Liu, J. Wu, Z. Jia, H. Chen, C. Daignebonne, O. Guillou, H. Sakiyamad; T. A. Soares, F. Ren, S.W. Ng, Q. Li. Two isoreticular metal-organic frameworks with CdSO₄-like topology: selective gas sorption and drug delivery. *Dalton Trans.* 2014, 43, 17265-17273.
- [44] A. R. Mota, P.H.P.R. Carvalho, B. C. Guido, H. C. de Oliveira, T. A. Soares, J. R. Correa, B. A. Neto. Bioimaging, cellular uptake and dynamics in living cells of a lipophilic fluorescent benzothiadiazole at low temperature (4 °C). *Chem. Sci.* 2014, 5, 3995-4003.
- [43] P.H.P.R. Carvalho, J. R. Correa, B. C. Guido, C.C. Gatto, H. C. de Oliveira, T.A. Soares, B. A. Neto. Designed Benzothiadiazole Fluorophores for Selective Mitochondrial Imaging and Dynamics. *Chemistry - A European Journal*, 2014, 20, 15360-15374.
- [42] A. Nascimento, F.J.S. Pontes, R.D. Lins; T.A. Soares. Hydration, ionic valence and cross-linking propensities of cations determine the stability of lipopolysaccharide membranes. *Chem. Comm.* 2013, 50, 231-233.
- [41] H.K. Ravi, M. Stach, T.A. Soares, T. Darbis, J.-L. Raymond, M. Cascella. Electrostatics and flexibility drive membrane recognition and early penetration by antimicrobial peptide dendrimer bH1. *Chem. Comm.* 2013, 49, 8821-8823.
- [40] I.F.T. Viana, T.A. Soares, L.F.O. Lima ; E.T.A. Marques, M. Krieger, R. Dhalia, R.D. Lins. De novo design of immunoreactive conformation-specific HIV-1 epitopes based on Top7 Scaffold. *RSC Advances.* 2013, 3, 11790-11800.
- [39] V.S. Oliveira, C. Pimenteira, D.C.B. da Silva-Alves, L.L.L. Leal, R.A.W. Neves-Filho, D.M.A.F. Navarro, G.K.N. Santos; K.A. Dutra; J.V. dos Anjos, T.A. Soares. The enzyme 3-hydroxykynurenine transaminase as potential target for 1,2,4-oxadiazoles with larvicide activity against the dengue vector *Aedes aegypti*. *Bioorg. Med. Chem.* 2013, 21, 6996-7003.
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- [34] F.J.S. Pontes, V.H. Rusu, T.A. Soares, R.D. Lins. The effect of the temperature, cations and number of acyl chains on the lamellar to non-lamellar transition in LipidA membranes: A microscopic view. *J. Chem. Theory Comp.* 2012, 8, 3830-3838.
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- [24] T.A. Soares, T.P. Straatsma, R.D. Lins. Influence of the B-band O-antigen chain in the structure and electrostatics of the lipopolysaccharide membrane of *Pseudomonas aeruginosa*. Invited (peer-reviewed) contribution. 2008, *J. Braz. Chem. Soc.* 2, 312-320.
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- [22] E.S. Peterson, L. Williams, E.G. Stephan, S. Rose, A. Corrigan, C. Lai, R.D. Lins, T. Critchlow, T.P. Straatsma, T.A. Soares, R. Scarberry. Northwest Trajectory Analysis Capability: A Platform for Enhancing Computational Biophysics Analysis. 2008. *Proceedings of Bioinformatics and Computational Biology (BIOCOMP'08)*. Conference paper.
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- [20] T.A. Soares, M. Osman, T.P. Straatsma. Molecular dynamics of the organophosphorous hydrolase bound to the nerve agent soman. 2007, *J. Chem. Theory and Comp.*, 3, 1569-1579.
- [19.] C. Oostenbrink, T.A. Soares, Nico F.A. van der Vegt, W. F. van Gunsteren. Validation of the 53A6 GROMOS force field. 2005, *Eur. Bioph. J.*, 34, 273-284.
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- [7.] R.D. Lins, T.A Soares, R. Ferreira. Unusual kinetic pathway for the prebiotic oligomerization of ribonucleic acids explains the monochirality of the polyribotides. 1998, *An. Bras. Acad. Ci.*, 70: 423-428.
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- [5.] R.D. Lins, T.A. Soares and R. Ferreira. Plural Origins of Homochirality in our biota. 1996, *Zeit. Naturf.* 51c: 71-74.

Book:

- [4.] T.A. Soares. 1996. Introduction to the study of the ribozymes. Brazilian Society of Genetics Publisher. São Paulo, Brazil. 200 p.

Scientific Politics and Education:

- [3.] T.A. Soares and R. Ferreira. 2004. Applications of the Poisson-Boltzmann equation to the calculations of pH-dependent properties. *Quím. Nova*, 27: 640-647.
- [2.] T.A. Soares. 2001. Women in science and technology: Restricted success. *Quím. Nova*, 24: 281-285.
- [1.] T.A. Soares, R.D. Lins. 1995. Ribozymes – not every enzyme is a protein. *Quím. Nova*, 18: 375-378.