Thereza A. Soares
Professor Titular

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Institute of Physics (IFUSP)
BioMaterial Modeling Group
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1. Personal Information

Citizenship - Brazilian
Languages - Portuguese (native), English (fluent), French (intermediate)
webpage - www.biomatsite.net
ResearcherID: G-1065-2010
ORCID: 0000-0002-5891-6906
Google Scholar: https://scholar.google.com.br/citations?user=lcsOOXQAAAAJ&hl=en
CV Lattes: http://lattes.cnpq.br/7252959688681950

CNPq research productivity Fellow - PQ-B

2. Brief Research Statement

My research focuses on leveraging computational chemistry methodologies to elucidate molecular processes and provide mechanistic insights that complement and interpret experimental observations. Currently, my work centers on the development, validation, and application of molecular models of bacterial outer membranes, with particular emphasis on understanding how external agents—such as cation type, ionic strength, and antimicrobials—and variations in lipopolysaccharide chemotypes drive membrane polymorphism. In recent years, I have extended these efforts to the study of molecular brushes, developing and applying molecular models to uncover how environmental factors (ionic strength, salt type, pH) govern conformational transitions and modulate the complex swollen/salt-in/salt-out behaviors observed in these materials. A central aim of this research is to probe the structure-dependent dynamics at the interface between bacterial outer membranes and molecular brushes, advancing our understanding of their potential biomedical applications. My group also leads the development of *SuAVE* (Surface Assessment via Grid Evaluation), an open-source software platform designed to analyze curvature-dependent properties of chemical interfaces. By employing differential geometry techniques to represent chemical surfaces as fully differentiable, *SuAVE* enables highly accurate calculations of structural and mechanical properties across a broad range of systems—including biological membranes, micelles, vesicles, and crystalline porous materials. Its ability to handle both open and closed surfaces, irrespective of chemical composition, asymmetry, or resolution, makes it a powerful and versatile tool for investigating complex interfacial phenomena.

3. Professional Experience

3.1. Employment

2022-present. **Full Professor (Professor Titular)**
Universidade de São Paulo (USP), Brazil

2021-2025. **Professor II** (Visiting Professor)

Hylleraas Centre for Quantum Molecular Sciences, University of Oslo (UiO), Norway.

2010-2021. **Full Professor**
Dept. of Chemistry, Universidade Federal de Pernambuco (UFPE), Recife, Brazil.

2005-2009. **Senior Research Scientist L-III**
Computational Sciences and Mathematics Division, Pacific Northwest National Laboratory (PNNL), USA

3.2 Post-doctoral Training

2004-2005. **Postdoctoral Fellow**, École Polytechnique Fédérale de Lausanne, Switzerland
2001-2003. **Postdoctoral Fellow**, Swiss Federal Institute of Technology, Zürich, Switzerland

4. Awards and Professorships

2021 **Theodore von Kármán Fellowship,** RWTH Aachen University, Germany
2020 **Invited Researcher,** Hylleraas Centre for Quantum Molecular Sciences, University of Oslo, Norway (2 months)
2019 **JSPS Invitational Fellowship for Research**, National Institute of Infectious Diseases, Tokyo, Japan (2 months)
2016 **UCMR Linnaeus Visiting Professor**, University of Umeå, Sweden (9 months)
2013 **SNSF Professeur Invité**, École Polytechnique Fédérale de Lausanne, Switzerland (3 months)

5. Education

Chemistry, Ph.D. Federal University of Pernambuco, Brazil - 06/1996-01/2001 with at least 1-yr stays at:

Research fellow, the Scripps Research Institute, La Jolla, CA, USA, 06/1997 - 10/1998
Research fellow, University of Houston, TX, USA, 11/1998 - 01/2000
Research 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.

6. External Funding

6.1. Principal-Investigator

FAPESP Post-Doctoral Fellowship. Dra. Mariana Yoshinaga, USP
Title: Uma Investigação Comparativa da Permeabilidade de Pequenas Moléculas e Peptídeos Antimicrobianos em Membranas Fosfolipídicas e Lipopolissacarídicas.
Funding Organization: FAPESP, Brazil.
Grant Number: 2025/03260-0
Role: Coordinator/Supervisor
Period: 01/17/2025 to 30/06/2028
Total: 475,200,00 BRL

FAPESP Post-Doctoral Fellowship. Dr. Anderson A. Do Espírito Santo, USP

Title: Combinando Modelagem Generativa e Algoritmo Evolutivo para a Previsão de Novas Sequências de Peptídeos Antimicrobianos
Funding Organization: FAPESP, Brazil.
Grant Number: 2024/19541-6
Role: Coordinator/Supervisor
Period: 01/02/2026 a 31/01/2029
Total: 475,200,00 BRL

FAPESP Professorship for Foreigner Scholars. Prof. Wilfred van Gunsteren, ETHZ, Switzerland
Title: Development and Applications of Computational Methods to treat Soft-Matter
Funding Organization: FAPESP, Brazil.
Grant Number: 2023/03748-8
Role: Coordinator/PI.
Period: 05/10/2023 to 07/11/2023
Total: 19,000,00 BRL

FAPESP Technical Training (TT-5) Fellowship. Dr. Anderson A. o Espírito Santo
Title: Implementation of a Numerical Methodology for Integrating Data Obtained from Molecular Dynamics Simulations and SAXS/SANS in Biological Membranes
Funding Organization: FAPESP, Brazil.
Grant Number: 2024/09991-4
Role: Supervisor.
Period: 01/08/2024 a 31/07/2025
Total: 111.840 BRL

FAPESP Post-Doctoral Fellowship. Dr. Eduardo R. Almeida, USP
Title: Computational Simulations of the Interface between Polymeric Brushes and Bacterial Outer Membranes
Funding Organization: FAPESP, Brazil.
Grant Number: 2023/02556-8
Role: Coordinator/Supervisor
Period: 01/11/2023 to 31/10/2025
Total: 239,000,00 BRL

FAPESP BEPE Fellowship. Diane Lima, PPG-Química, USP
Title: Investigating the Lipid Composition Effect on the Biogenesis of External Vesicles: A Molecular perspective.
Funding Organization: FAPESP, Brazil.
Grant Number: 2023/03184-7
Role: Coordinator/Supervisor.
Period: 22/01/2024 to 21/01/2025
Total: 28.000,00 BRL + 34.000,00 USD

FAPESP Doctorate Fellowship. Diane Lima, PPG-Química, USP
Title: Investigação do Papel da Composição de Lipídeo-A na Formação de Vesículas de Membrana Externa via Espalhamento de Raios X a Baixo Ângulo (SAXS).
Funding Organization: FAPESP, Brazil.
Grant Number: 2021/12285-6
Role: Coordinator/Supervisor.
Period: 01/06/2022 to 31/03/2025
Total: 163,000,00 BRL

FAPESP Technical Training (TT-5) Fellowship. Dr. Daniel Zago Caetano
Title: Implementation of Numerical Methodologies in the SuAVE Software for the Calculation of Mechanical Properties in Soft Matter.
Funding Organization: FAPESP, Brazil.
Grant Number: 2022/13855-3
Role: Coordinator/Supervisor.
Period: 01/11/2022 a 31/10/2023
Total: 103.446,00 BRL

FAPESP Regular Grant 2021 Call
Title: A Multi-Resolution Approach to Cation-induced Polymorphism of Lipopolysaccharide Aggregates.
Funding Organization: FAPESP, Brazil.
Grant Number: 2021/04283-3
Role: Coordinator/PI.
Period: 01/09/2021 to 31/08/2023
Total: 160,000,00 BRL

CNPq/SNSF 2018 Call
Title: Tailoring Antimicrobial Peptide – Phospholipid Interactions for Fighting Bacteria.
Funding Organization: CNPq, Brazil and SNSF, Switzerland.
Grant Number: 402681/2019-3
Role: Principal investigator together with Stefan Salentinig, UniFribourg, Switzerland.
Period: 01/04/2019 to 31/03/2022
Total: 20,000,00 BRL

STINT Call
Title: Understanding the Biocompatibility of Polymeric Biomaterial Surfaces.
Funding Organization: STINT, Sweden
Grant Number: IG2011-2048
Role: Principal investigator together with Madeleine Ramstedt, UmU, Sweden.
Period: 01/06/2011 to 31/05/2013 with extensions until 2019
Total: 880,000,00 SEK

Edital Programa de Apoio a Núcleos Emergentes - PRONEM - 08/2014
Title: Molecular Basis of Infectious Diseases: Drug Resistance in Gram-Negative Bacteria and Engineering of Immune-reactive epitopes.
Funding Organization: FACEPE, Brazil
Grant number: APQ-0732-1.06/14
Role: Coordinator/Principal Investigator
Period: 2015-2019
Total: 198,000.00 BRL

Royal Society International Exchange Scheme
Title: Computational Simulations of Polymer Brushes
Funding Organization: Newton Fund/Royal Society, UK
Grant number: NI140090
Role: Principal Investigator together with Julien Gautrot, QMUL, UK
Period: 01/03/2015 to 28/02/2017
Total: 11,560.00 GBP

Chamada 71/2012 L2 (Ciência sem Fronteiras)
Title: Interactions and Binding of Drug Molecules to Organic Metal Frameworks for Controlled Drug Release.
Funding Organization: CNPq, Brazil
Grant number: 400193/2013-2
Role: Coordinator/PI.
Period: 2013-2015
Total: 427,133.57 BRL

Chamada Pública MCTI/FINEP/CT-INFRA 01/2013
Title: Desenvolvimento de uma Química Biológica de Fronteira na Região Nordeste: Resolução Estrutural de Macromoléculas e Bio-imagem.
Funding Organization: FINEP, Brazil
Grant number: 0648/13
Role: Coordinator/PI.
Period: 2013-2015
Total: 2,593,663.00 BRL

Edital Auxílio a Projetos de Pesquisa - APQ-FACEPE - 15/2012
Title: Computational Simulations of Antimicrobial Peptides in Bacterial Membranes. Funding **Organization:** FACEPE, Brazil.
Role: Coordinator/PI.
Grant number: APQ-1013-1.06/12
Period: 2012-2015
Total: 55,000.00 BRL

Chamada Pública MCT/CNPq Nº 14/2012 - Universal 14/2012
Title: The Effect of Cationic Antimicrobial Peptides on the Structure and Dynamics of Lipopolysaccharide Chemotype Membranes of Pseudomonas aeruginosa.
Funding Organization: CNPq, Brazil
Grant number: 470232/2012-9
Role: Coordinator/PI.
Period: 2012-2014
Total: 24,000.00 BRL

Computer Time Allocations via Peer-Reviewed Proposals

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, Santos Dumont SuperComputer Center (LNCC), Brazil.

6.2. Co-Investigator

FAPESP Temático
Title: Plasticity and Functional Modulation of Intrinsically Disordered Proteins
Funding Organization: FAPESP, Brazil.
Grant Number: 2022/07231-7
Role: Principal investigator.
Coordinator: Vitor B. Leite, UNESP, Brazil
Period: 01/03/2024 to 28/02/2029
Total: ca. 1.700,000,00 BRL

Seed Money for Bilateral Research Collaboration with Brazil and the Latin American Region
Title: Tailoring Antimicrobial Peptide - Phospholipid Interactions for Fighting Bacteria
Funding Organization: Swiss State Secretariat for Education, Research and Innovation, Switzerland
PI: Stefan Salentinig
Period: 2018
Total: 25,000.00 CHF

Chamada INCT - MCTI/CNPq/CAPES/FAPs nº 16/2014
Title: National Institute of Science and Technology in Complex Fluids - INCT-FCx
Funding Organization: CNPq, Brazil
Grant number: 465259/2014-6.
PI: Antônio Martins Figueiredo Neto
Period: 2017-2023
Total: 3,525,132.64

Edital CAPES Biologia Computacional 51/2013
Title: Development of Computational Tools for Biomedical Research: From Molecular Modeling to Translational Research.
Funding Organization: CAPES, Brazil
Grant number: 23038.004630/2014-35
PI: Kaline Coutinho and Roberto D. Lins
Period: 2014-2019
Total: 2,580,368.80 BRL

Edital Multiusuário FACEPE 16/2012
Title: Hybrid Platform Cluster: The Neumann II Multiuser Cluster
Funding Organization: FACEPE, Brazil
Grant number: 186410612
PI: Ricardo Longo
Period: 2012-2014
Total: 470,000.00 BRL

Title: Enhanced Sensing of Threat Agents Through Engineered Multivalent Binding Scaffolds.
Funding Organization: U.S. Department of Defense.
PI: Thomas Squire
Period: 2009-2012
Total: ca. 300,000.00 USD

Title: Protein renaturation in a nanofunctionalized configuration.
Funding Organization: National Institutes of Health.
PI: Chenghong Lei
Period: 2008-2011
Total: ca. 400,000.00 USD

Title: *Pseudomonas aeruginosa* Outer Membrane Modeling.
Client Organization: National Institutes of Health.
PI: Tjerk Straatsma
Period: 2005-2010
Total: ca. 350,000.00 USD

7. Student Supervisions (since hiring at UFPE)

7.1. Ongoing

04 post-doctoral researchers.

7.2. Concluded

08 Postdoctoral fellows, 09 Ph.D. students, 08 M.Sc. student, and 10 undergraduate students with the the Brazilian scientific initiation program.

Acting Member in more than 35 graduate evaluation committees

Acting Member in more than 10 faculty hiring/promotion advisory committees

8. Lectures

8.1. Post-Graduate Level

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

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)

8.2. Graduate Level

General Chemistry. Lecturer (Experimental Course). 4 hours/week/12mo, University of São Paulo, Brazil (2022-Present).

Chemistry of Biological Processes. Lecturer. 4 hours/week/6mo, Federal University of Pernambuco, Brazil (2010-2021).

Electrochemistry and Chemical Kinetics (Theoretical course). Lecturer. 4 hours/week/6mo, Federal University of Pernambuco, Brazil (2010-2013)

Electrochemistry and Chemical Kinetics (Experimental course). Lecturer. 4 hours/week/6mo, Federal University of Pernambuco, Brazil (2010-2021)

Course on preparation and writing of scientific texts. Lecturer. 4 hours/week/6mo, Federal University of Pernambuco, Brazil (2012-2021)

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).

9. Institutional Responsibilities (since 2010)

Coordinator of the Graduate Program in Chemistry (UFPE). 2015-2018.

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

Member of the Chemistry Graduate Commission (UFPE), 2010-2022

Member of the Chemistry Undergraduate Collegiate (UFPE), 2010-2022

Member Titular in the Council of the Department of Chemistry (USP). 2022-2025

Member Titular in the Commission of Research and Innovation (USP). 2023-2025

10. Commissions of Trust (since 2010)

10.1. Editorships

2023-Present. **Executive Editor.** Journal of Computational Information and Modeling (American Chemical Society)

2020-2022. **Associate Editor.** Journal of Computational Information and Modeling (American Chemical Society)

10.2. Member of Editorial Boards of Scientific Journals

2026-Present. Journal of Physical Chemistry A/B/C (American Chemical Society).

2013-2024. Computational Structure and Biotechnology Journal (Elsevier).

2019. Journal of Computational Information and Modeling (American Chemical Society).

2008. Journal of the Brazilian Chemical Society (*Invited Editor for special issue*).

10.2. Regular Referee Assistance for Scientific Journals (since 2010)

ACS Central Science, ACS Applied Materials & Interfaces, ACS Applied Nano Materials, Small, Journal of the American Chemical Society, Soft Matter, RSC Advance, Chemical Communications, Journal of Chemical Information and Modeling, Journal of Chemical Theory and Computation, Journal of Physical Chemistry, Journal of Physical Chemistry Letters, Nature Computational Sciences, Nature Communications, PLoSONE, Physical Chemistry Chemical Physics, Biochemistry (ACS), Scientific Reports, Protein Engineering, Design & Selection, Biophysical Journal, Journal of Molecular Recognition, ACS Omega, Spectrochimica Acta. Part A, Molecular and Biomolecular Spectroscopy, Journal of the Brazilian Chemical Society Brazil (*Invited Editor for special issue*) among other peer-reviewed journals

10.3. Reviewer Assistance for Funding Agencies and Panels (since 2010)

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), Institute Serrapilheira (Brazil), The National Science Centre Poland.

11. Invited Talks at International Events or Institutions (since 2010)

ACS on Campus Roadshow Chile (Santiago, Chile, 2024), II Cone Sul Symposium of Biomolecular Simulation (Buenos Ayres, Argentina, 2024), 47th Annual Meeting of the Brazilian Chemical Society (Águas de Lindoia, Brazil 2024), São Paulo Meeting on Soft and Biological Matter (São Paulo, Brazil, 2024), 47th Annual Meeting of the Brazilian Biophysical Society (Campinas, Brazil, 2023), XXII Brazilian Symposium on Theoretical Chemistry (Niterói, Brazil, 2023), 46th Annual Meeting of the Brazilian Chemical Society (Águas

de Lindoia, Brazil 2023), SBF-ATO (Brazil, 2022), Norwegian Chemical Society (Oslo, Norway 2021), RWTH Aachen University, (Juelich, Germany 2021), VII Encuentro Argentino de Materia Blanda (Virtual Meeting, 2021), 20th IUPAB-45th SBBf-50th SBBq (Virtual Meeting, 2021), University of Oslo (Oslo, Norway, 2021), 43th Annual Meeting of the Brazilian Chemical Society (Virtual Meeting, 2020), University of Oslo (Oslo, Norway, 2020), 48th Annual Meeting of the Brazilian Society of Biochemistry and Molecular Biology (Águas de Lindóia, Brazil, 2019), V Regional Meeting of the Brazilian Society of Biophysics (Recife, Brazil, 2019), Several presentations at the National Institute of Infectious Diseases (Japan Jan-Mar. 2019), VII STINT Workshop (Umeå, Sweden, 2018), VI STINT Workshop (Umeå, Sweden, 2017), XIX Brazilian Symposium of Theoretical Chemistry (Águas de Lindóia, Brazil, 2017), XLII Meeting of the Brazilian Biophysical Society. (Santos, Brazil, 2017), 6th Workshop on Microbial Adhesion and Surfaces (Sweden 2017), III Advanced School on Biomolecular Simulation (Recife, 2017), IV Brazilian School of Molecular Modeling (Santo André, Brazil, 2017), 4th International Workshop on Complex Physical Phenomena in Materials (Natal, Brazil, 2017), Several talks at the Department of Chemistry, Department of Molecular Biology and High Performance Computing Center at Umeå University (Sweden, Jun-Dec. 2016), Advanced Mini-Worskhop 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).

12. ACS Talks and Activities in Latin America

ACS on Campus - Road Show Chile 2024. Meet the ACS editor and Effective Scientific Writing.

Scientific Writing. 47th Annual Meeting of the Brazilian Biophysical Society. (2023). Águas de Lindóia, Brazil. Escrita Científica para a Publicação de Trabalhos com Revisão de Pares. Lecturer: Prof. Thereza A. Soares.

ACS on Campus - Open Access 2022. Meet the ACS Editors in Brazil. Professors Thereza A. Soares (JCIM), Osvaldo Oliveira Jr. (ACS Applied Materials & Interfaces), Monica Cotta (ACS CS Applied Nano Materials) and Frank Quina (ACS Omega).

Scientific Writing. 46th Annual Meeting of the Brazilian Biophysical Society. (2023). Campinas, Brazil. Escrita Científica para a Publicação de Trabalhos com Revisão de Pares. Lecturer: Prof. Thereza A. Soares.

ACS Publications Scientific Communication Course for the Institutes of Scientific Innovation from SENAI and CNI (4h course). Escrita Científica para a Publicação de Trabalhos com Revisão de Pares. Lecturer: Prof. Thereza A. Soares.

ACS on Campus at the 46th Annual Meeting of the Brazilian Chemical Society. Meet the Editor (2023). Escrita Científica para a Publicação de Trabalhos com Revisão de Pares. Lecturer: Prof. Thereza A. Soares.

ACS on Campus at Federal University of Ouro Preto (UFOP). 2022. Creating Your Title, Abstract, and TOC Graphic. Lecturer: Prof. Thereza A. Soares.

IX SeedMol. 2022. The Art of Scientific Writing and Publishing (4h course). Lecturer: Prof. Thereza A. Soares. November 8th and 9th. Access the event recordings for lecture 1 and lecture 2.

ACS on Campus at São Paulo State University (UNESP). 2021. 10 Tips for Scholarly Publishing. Lecturer: Prof. Thereza A. Soares.

ACS Publications Webinar Series. 2020. Moderator: Prof. Thereza A. Soares.

Webinar 1: *COVID-19: perspectivas sobre vacinas, terapêuticos e diagnósticos*.

Webinar 2: *COVID-19: possibilidades de interação universidade-indústria nas áreas de vacinas, terapêuticos e diagnósticos*.

Webinar 3: *COVID-19: O que falta para termos vacina?*.

13. Organization and Participation in Committees of Scientific Meetings

WATOC 2025 (Member of the Advisory Committee), Oslo, Norway, **2025**; 3rd ICTP-SAIFR Symposium on Current Topics in Molecular Biophysics (CTMB3) (Institute Principia), São Paulo, Brazil, **2024**. 11th Congress of International Association of Theoretical Chemical Physics (ISTCP-2024) (Member of the Advisory Committee), Qingdao, China, **2024**; Scientific Committee of the II Conesul Symposium on Biomolecular Simulations (Member of the Scientific Committee), Buenos Ayres, Argentina, **2024**; Advanced School of Molecular Simulation (Organizer), Campinas, Brazil, **2023**; XLVII Annual Meeting of the Brazilian Biophysical Society (Member of the Scientific Committee), Campinas, Brazil, **2023**; Advanced School of Molecular Simulation, Campinas, Brazil, **2023** (organizer); XLVI Annual Meeting of the Brazilian Society of Biophysics, Águas de Lindóia, Brazil, **2022** (Symposium Coordinator); V Regional Meeting of the Brazilian Society of Biophysics (organizer), Recife, Brazil, **2019**; 10th Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP-2019) (Member of the Advisory Committee), Trømso, Norway **2019**; III Advanced School on Biomolecular Simulation, Recife, Brazil, **2017** (organizer); UCMR Mini-Symposium on Structural Dynamics of Biological Membranes, Umeå, Sweden, **2016** (organizer); V STINT Workshop on Understanding Biocompatibility of Polymeric Biomaterial Surfaces, Recife, **2015** (organizer); I Advanced School on Biomolecular Simulation, Recife, Brazil, **2015** (organizer); III School of Chemistry Prof. Ricardo Ferreira, Recife, **2014** (organizer); XVII Brazilian Symposium of Theoretical Chemistry, Angra dos Reis, **2013** (Member of the Advisory Committee); II STINT Workshop on Understanding Biocompatibility of Polymeric Biomaterial Surfaces, Recife, **2012** (Organizer); I School of Chemistry Prof. Ricardo Ferreira, Recife, **2012** (Organizer).

14. Publications

Publications in peer-reviewed journals (July 10th 2026)

(**H-index 31, Citations 3,680 without self-citations 3,466 on ISI**)

(**H-index 36, Citations 5,232 i10-index 72 on Google Scholar**)

Publications in computational simulations of biomaterials and biocompatible materials.

1. D.E.S. Santos, R.L. Longo, T.A. Soares. A Numerical Implementation to Calculate Elastic Properties of Biological Membrane Simulations. *J. Chem. Inf. Mod.,* **2026**, 66, 8203–8214. **(Issue Cover)** DOI:10.1021/acs.jcim.6c00143
2. D. L. Z. Caetano, A.A. do Espírito Santo, D. Lima, D.E.S. Santos, T.A. Soares. SuAVE-Scatter: A Module for Integrating Simulations and SAXS/SANS Analyses. *J. Chem. Inf. Mod.,* **2026**, 66, 9, 5026–5034.
3. B. Tran, D.C.A. Lima, L. Sandblad, M. Ramstedt, T.A. Soares, S. Salentinig. LL-37 Driven Phase Transition and Stacking in Oligolamellar Gram-Negative Bacterial Membrane Models. *Adv. Funct. Mat.,* **2026**, *36, e32053*.
4. E.R. Almeida**,** V.F. dos Santos, M. Ramstedt, T.A. Soares. Exploring the Interactions Between Methyl Methacrylate Polymers and the Bacterial Outer Membrane via Coarse-Grained Molecular Dynamics Simulations. *J. Chem. Inf. Mod.,* **2026.** 66, 7138–7153. **(Issue Cover)**
5. T.M. Tsubone, P.N. Oliveira, G. Scanavachi, V.F. dos Santos, A.R. da Cunha, A.P. Ramos, T.A. Soares, R. Itri. Acidic pH Modulates Headgroup Orientation and Packing in Bis(monoacylglycero)phosphate Bilayers. *ACS Phys. Chem. Au*, **2026.** 6, 483–492. **(Issue Cover)**
6. D.C.A. Lima, V.F. Dos Santos, R. Ward, T.A. Soares. The Many Dimeric Faces of Lys49 PLA2-Like Proteins: Conformational Plasticity and Membrane Binding Drive Functional Dimer States. *Protein Science*, **2026**, 35, 1-19.
7. D.C.A. Lima, G.V. Bossa, P. Ciancaglini, A.P. Ramos, T.A. Soares. The Effect of Ceramide Ratio on the Membrane Curvature of Mimetic Models of Matrix Vesicles. *ACS Phys. Chem. Au,* **2025**, 5, 456–466. **(Issue Cover)**
8. V.F. dos Santos, E.R. Almeida, L.M.P. Souza, A.S. Pimentel, M. Ramstedt, T.A. Soares. Coarse-Grained Parameters for Simulations of Methyl-Methacrylate-Based Polymer Brushes That Reproduce Experimental Swelling Coefficients. *Macromol.*, **2025**, 58, 5431–5443.
9. M. Frigerio, R.V.M. Freire, T.A. Soares, M.E. Leser, S. Salentinig. Interfacial Structurization between Triolein and Water from pH and Buffer Ions. *J. Coll. Inter. Sci.*, **2024**, 665, 1091–1101.
10. R.C. Prati, B.S.M. Rodrigues, I. Aragão, T.A. Soares, M.G. Quiles, J.L.F. da Silva. The Impact of Interdisciplinary, Gender and Geographic Distributions on the Citation Patterns of the Journal of Chemical Information and Modeling. *J. Chem. Inf. Mod.,* **2024**, 62, 6297-6301.
11. M. Carrer, J. Eilsø-Nielsen, H.M. Cezar, R. Lund, M. Cascella, T.A. Soares. Accelerating Lipid Flip-Flop at Low Concentrations: A General Mechanism for Membrane Binding Peptides. *J. Phys. Chem. Lett.,* **2023,** 14, 7014-7019.
12. D.E.S. Santos, A. De Nicola, V.F dos Santos, G. Milano, T.A. Soares. Exploring the Molecular Dynamics of a Lipid-A Vesicle at the Atom Level: Morphology and Permeation Mechanism. *J. Phys. Chem. B.,* **2023,** 127, 30, 6694–6702.
13. L.G. Maciel, M.V. F. Ferraz, A.A. Oliveira, R.D. Lins, J.V. Dos Anjos, R.V.C. Guido, T.A. Soares. (2023) Inhibition of 3-Hydroxykynurenine Transaminase from *Aedes aegypti* and *Anopheles gambiae*: A Mosquito-Specific Target to Combat the Transmission of Arboviruses. *ACS Bio Med & Chem Au*, **2023**, 3, 211–222.

14. D.E.S. Santos, K. Coutinho, T.A. Soares. Surface Assessment via Grid Evaluation (SuAVE): For Every Surface Curvature and Cavity Shape. *J. Chem. Inf. Mod.,* **2022**, 62, 4690-4701. **(Issue Cover)**
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