Marcelo D. Polêto

Research Associate · Biochemistry Department · Lemkul Lab

340 West Campus Dr. Blacksburg, VA 24061, United States

mdpoleto@vt.edu | www.mdpoleto.github.io | mdpoleto | @mdpoleto

Education

Ph.D. in Cell and Molecular Biology — *Brazil*

Universidade Federal do Rio Grande do Sul — *Mar. 2019*

- **Dissertation Title:** Molecular flexibility of ligands as a design strategy of ligand-receptor interactions.

M.Sc. in Cell and Molecular Biology — *Brazil*

Universidade Federal do Rio Grande do Sul — *Jul. 2016*

- **Thesis Title:** Parametrization strategies of aromatic rings commonly used in medicinal chemistry.

B.Sc. in Biochemistry — *Brazil*

Universidade Federal de Viçosa — *Dez. 2014*

- **Thesis Title:** Structural analysis of *Porcine circovírus 2* capsid protein: genetic diversity role on celular adsorption and viral stability.
- Science Without Border Fellowship - Uppsala Universitet (2013-2014)

Employment and Experience

Research Associate - Virginia Tech — *Blacksburg - VA, USA*

Supervisor: Justin A. Lemkul — *Nov. 2023 - Present*

Postdoctoral Associate - Virginia Tech — *Blacksburg - VA, USA*

Supervisor: Justin A. Lemkul — *Dez. 2020 - Nov. 2023*

Postdoctoral Associate - Universidade Federal de Viçosa — *Viçosa - MG, Brazil*

Supervisor: Juliana L.R. Fietto — *Apr. 2019 - Dez. 2020*

Graduate Researcher - Universidade Federal do Rio Grande do Sul — *Porto Alegre - RS, Brazil*

Advisor: Hugo Verli — *Mar. 2015 - Mar. 2019*

Skills

Programming Python, LaTeX, CHARMM, Matplotlib

Techniques Molecular Dynamics, Enhanced Sampling, Force field development, QM calculations

Softwares CHARMM, OpenMM, GROMACS, Plumed, Gaussian09, PyMol, VMD

Peer-Reviewed Publications

1. **Polêto, M.D.**; Allen, K.D.; Lemkul, J.A. *Structural dynamics of the methyl-coenzyme M reductase active site are influenced by coenzyme F_{430} modifications*. Biochemistry, 63 (14), 1783–1794, 2024.
2. **Polêto, M.D.**; Lemkul, J.A. *Differences in Conformational Sampling and Intrinsic Electric Fields Drive Ion Binding in Telomeric and TERRA G-Quadruplexes*. Journal of Chemical Information and Modeling, 63 (21), 6851-6862, 2023.
3. Giacon, N.,Lo Cascio, E., Davidson, D.S., **Polêto, M.D.**, Lemkul, J.A., Pennacchietti, V., Pagano,L., Zamparelli,C., Toto,A., Arcovito,A. *Structural and functional insights on the interaction between SARS-CoV-2 E protein and ZO1-PDZ2*. Computational and Structural Biotechnology Journal, 21: 3259-3271, 2023.
4. **Polêto, M.D.**; Lemkul, J.A. *TUPÃ: Electric field analyses for molecular simulations*. Journal of Computational Chemistry, 43(16), 2022.

5. **Polêto, M.D.**; Lemkul, J.A. *Integration of experimental data and use of automated fitting methods in developing protein force fields*. Communications Chemistry, 5(1), 2022.
6. Arantes, P.R.; **Polêto, M.D.**; Pedebos, C.; Ligabue-Braun, R. *Making it rain: cloud-based molecular simulations for everyone*. Journal of Chemical Information and Modeling, 61(10), 2021.
7. De Oliveira, T.V.; **Polêto, M.D.**; Barbosa, S.V.; Coimbra, J.S.R.; De Oliveira, E.B. *Impacts of Ca^{2+} cation and temperature on bovine α-lactalbumin secondary structures and foamability – Insights from computational molecular dynamics*. Food Chemistry, 367(15), 2021.
8. De Oliveira, T.V.; Guimarães, A.P.; Bressan, G.C.; Maia, E.R.; Coimbra, J.S.R.; **Polêto, M.D.**; De Oliveira, E.B. *Structural and molecular bases of angiotensin-converting enzyme inhibition by bovine casein-derived peptides: an in silico molecular dynamics approach*. Journal of Biomolecular Structure and Dynamics, 39(4), p. 1386-1403, 2020.
9. Rusu, V.H; Santos, D.E.S.; **Polêto, M.D.**; Galheigo, M.M.; Gomes, A.T.A.; Verli, H.; Soares, T.A.; Lins, R.D. *Rotational Profiler: A Fast, Automated, and Interactive Server to Derive Torsional Dihedral Potentials for Classical Molecular Simulations*. Journal of Chemical Information and Modeling, 60(12), p. 5923-5927, 2020
10. **Polêto, M.D.**; Grisci, B.I.; Dorn, M.; Verli, H. *ConfID: an analytical method for conformational characterization of small molecules using molecular dynamics trajectories*. Bioinformatics, 36(11), p. 3576–3577, 2020.
11. Arantes, P; Pedebos, C.; **Polêto, M.D.**; Pol-Fachin, L.; Verli, H. *The Lazy Life of Lipid-Linked Oligosaccharides in All Life Domains*. Journal of Chemical Information and Modeling, 2019 (online).
12. De Oliveira, A.S.; Gazolla, P.A.R.; Oliveira, A.F.C.S.; Pereira, W.L.; Viol, L.C.; Maia, A.F.S.; Santos, E.G.; Da Silva, I.E.P. ; Mendes, T.A.O.; Da Silva, A.M.; Dias, R.S.; Da Silva, C.C. ; **Polêto, M.D.**; Teixeira, R.R.; De Paula, S.O. *Discovery Of Novel West Nile Virus Protease Inhibitor Based On Isobenzonafuranone And Triazolic Derivatives Of Eugenol And Indan-1,3-Dione Scaffolds*. Plos One, v. 14, p. e0223017, 2019
13. **Polêto, M.D.**; Alves, M.P.; Ligabue-Braun, R.; Eller, M.R.; De Carvalho, A.F. *Role Of Structural Ions on the Dynamics of the Pseudomonas Fluorescens 07a Metalloprotease*. Food Chemistry, 286(15), p. 309-315, 2019.
14. Arantes, P; **Polêto, M.D.**; John, E.B.; Pedebos, C.; Grisci, B.I.; Dorn, M.; Verli, H. *Development of Gromos-Compatible Parameter Set for Simulations of Chalcones and Flavonoids*. Journal Of Physical-Chemistry B, 123(5), p. 994-1008, 2019.
15. Tesch, R.; Becker, C.; Müller, M.P.; Beck, M.E.; Quambusch, L.; Getlik, M.; Lategahn, J.; Uhlenbrock, N.; Costa, F.N.; **Polêto, M.D.**; De Sena, P.M.; Rodrigues, D.A.; Sant'Anna, C.M.; Ferreira, F.F.; Verli, H.; Fraga, C.A.M.; Rauh, Dl. *An Unusual Intramolecular Halogen Bond Guides Conformational Selection*. Angewandte Chemie-Internacional Edition, v. 57(31), p. 9970-9975, 2018.
16. **Polêto, M.D.**; Rusu, V.H. ; Grisci, B.I. ; Dorn, M.; Lins, R.D.; Verli, H. *Aromatic Rings Commonly Used In Medicinal Chemistry: Force Fields Comparison And Interactions With Water Toward The Design Of New Chemical Entities*. Frontiers In Pharmacology , v. 9, p. 395, 2018.
17. Fischer, N.M; **Polêto, M.D.**; Steuer, J.; Van Der Spoel, D. *Influence of Na^{+} And Mg^{2+} Ions on RNA Structures Studied With Molecular Dynamics Simulations*. Nucleic Acids Research (Online) , v. 46(10), p. 4872-4882, 2018
18. Lima, R.N.; Faheem, M.; Barbosa, J.A. R. G.; **Polêto, M.D.**; Verli, H.; Melo, F.L.; Resende, R.O. *Homology Modeling And Molecular Dynamics Provide Structural Insights Into Tospovirus Nucleoprotein*. BMC Bioinformatics , v. 17, p. 11-17, 2016.
19. Guimarães-Peixoto, R.P. M.; Pinto, P.S. A.; Santos, M. R.; **Polêto, Ma.D.**; Silva, L.F.; Silva-Júnior, A. *Evaluation Of a Synthetic Peptide From The Taenia Saginata 18kDA Surface/Secreted Oncospheral Adhesion Protein For Serological Diagnosis Of Bovine Cysticercosis*. Acta Tropica , v. 164, p. 463-468, 2016.
20. Figueira, F.; Farinha, A.S. F. ; Muteto, P.V. ; **Polêto, M.D.** ; Verli, H.; Gomes, M.T.S. R. ; Tomé, A.C. ; Cavaleiro, J.A. S. ; Tomé, J.P.C. *[28]Hexaphyrin Derivatives For Anion Recognition In Organic And Aqueous Media*. Chemical Communications (London. 1996. Print), v. 52, p. 2181-2184, 2016.
21. Ramos, C. ; Figueira, F.; **Polêto, M.D.** ; Amado, F.M.L ; Verli, H; Tomé, J.P.C ; Neves, M.G.P.M.S . *Esi-Ms/Ms Of Expanded Porphyrins: a Look Into Their Structure And Aromaticity*. Journal Of Mass Spectrometry (Print), v. 51, p. 342-349, 2016.
22. Siqueira, R.P.; Barbosa, E.A.A.; **Polêto, M.D.**; Righetto, G.L.; Seraphim, T.V.; Salgado, R.L.; Ferreira, J.G.; Barros, M.V.A.; De Oliveira, L.L.; Laranjeira, A.B.A; Almeida, M.R.; Júnior, A.S.; Fietto, J.L.R; Kobarg, J.; De Oliveira, E.B.;

Teixeira, R.R.; Borges, J.C.; Yunes, J.A.; Bressan, G.C. *Potential Antileukemia Effect And Structural Analyses Of SRPK Inhibition By N-(2-(Piperidin-1-Yl)-5-(Trifluoromethyl)Phenyl)Isonicotinamide (SRPIN340)*. Plos One, v. 10, p. e0134882, 2015.

23. Salgado, R.L.; Vidigal, P.M.P.; Gonzaga, N.F.; De Souza, L.F.L.; **Polêto, M.D.** ; Onofre, T.S.; Eller, M.R. ; Pereira, C.E.R.; Fietto, J.L.R.; Bressan, G.C. ; Guedes, R.M.C.; Almeida, M.R.; Silva Júnior, A. *A Porcine Circovirus-2 Mutant Isolated In Brazil Contains Low-Frequency Substitutions In Regions Of Immunoprotective Epitopes In The Capsid Protein*. Archives Of Virology, v. 160 (11), p. 2741-2748, 2015.

Journal Reviewer

- Journal of Chemical Information and Modeling
- The Journal of Physical Chemistry
- Journal of Biomolecular Structure and Dynamics
- Nature Communications Chemistry

Fellowships

Research Support Foundation of Minas Gerais State (FAPEMIG) — *Viçosa - MG, Brazil*
Undergrad Researcher - 2010-2011 — *2010-2011*

Research Support Foundation of Minas Gerais State (FAPEMIG) — *Viçosa - MG, Brazil*
Undergrad Researcher - 2011-2012 — *2011-2012*

Research Support Foundation of Minas Gerais State (FAPEMIG) — *Viçosa - MG, Brazil*
Undergrad Researcher - 2012-2013 — *2012-2013*

Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) — *Uppsala, Sweden*
Science without Borders - 2013-2014 — *2013-2014*

Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) — *Viçosa - MG, Brazil*
Postdoctoral Researcher - 2019-2020 — *2019-2020*

Invited Seminars and Presentations

American Chemical Society Meeting — *Indianapolis, USA*
Presenter of **Modulation of polyethylene terephthalate (PET) electronic properties by PET-degrading enzymes** — *March 2023*

Biophysical Society 67th Annual Meeting — *San Diego, USA*
Presenter of **Active-site electronic properties and conformational dynamics of PET-degrading enzymes.** — *February 2023*

Brazilian Congress of Industrial Biochemistry — *Online, Brazil*
Presenter of **Computational Biophysics: past, present and future** — *Jan 29 2021*

Proteomics and Protein Biochemistry Symposium — *Viçosa - MG, Brazil*
Presenter of **Computational Biophysics: past, present and future** — *Ago 14 2020*

Nacional Pharmaceutical Sciences Congress — *Online, Brazil*
Presenter of **Drug design: where we are and where we go from here** — *May 08 2020*

Courses Taught

Biophysical characterization of protein-ligand complexes — *Viçosa - MG, Brazil*
Credits: 1 — *Spring 2019*

BIO791 - Methods in Structural Bioinformatics — *Viçosa - MG, Brazil*
Credits: 3 — *Spring 2019*

Theory and Practice of Molecular Dynamics Simulations — *Viçosa - MG, Brazil*
Credits: 1 — *Spring 2017 and Fall 2018*

Bioinformatics for Biomedicine scholars — *Porto Alegre - RS, Brazil*
Credits (only practices): 2 — *Spring 2017*

Basic Bioinformatics — *Porto Alegre - RS, Brazil*
Credits (only practices): 1 — *Spring 2017*

Mentorship

Haley M. Michel — *PhD in Biochemistry*
Mentor — *2020 - Present*

Laura I. Gil-Pineda — *PhD in Biochemistry*
Mentor — *2020 - Present*

Thomás V. de Oliveira — *PhD in Food Technology*
Co-advisor — *2017 - 2020*

Marcel A. Diogo — *M.Sc. Student in Applied Biochemistry*
Co-advisor — *2019 - 2021*

João Victor B. de Moraes — *M.Sc. Student in Applied Biochemistry*
Co-advisor — *2021 - Present*

Júlia M. Ferreira — *B.Sc. Student in Biochemistry*
Co-advisor — *2019 - 2023*

Isabela S. Gomes — *B.Sc. in Chemical Engineering*
Co-advisor — *2019*

Gabriel Alves — *M.Sc. in Plant Pathology*
Co-advisor — *2023*

Other Professional Services

“Recent Advances in Molecular Force Fields” symposium — *ACS National Meeting*
Presider — *Spring 2021*

Softwares

TUPÃ - Electric field analyses
Website - https://github.com/mdpoleto/tupa/ — *2022*

ConfID - Conformational Identifier
Website - https://github.com/sbcblab/confid — *2019*

Technical Production

Making it Rain: cloud-based molecular simulations for everyone
Molecular dynamics tutorials using Google Colab — *2021*