

# Pablo Ricardo Arantes

PHD

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## Curriculum Vitae

February 23, 2024

MARCH 7TH, 1988

BRAZILIAN

## About Me

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PhD graduate in Cellular & Molecular Biology with a strong foundation in protein design and molecular dynamics simulations. Proficient in a wide range of techniques and simulation suites, including molecular docking, metadynamics simulations, and force field parameterization. Strong programming skills in Python and familiarity with several computational modeling packages and machine learning models to obtain potential energy surfaces and other physical properties of molecular systems. Demonstrated technical problem-solving skills and ability to develop and implement new ideas through a strong record of publications and conference presentations. Excellent verbal and written communication skills and ability to work both independently and as part of a diverse, multidisciplinary team.

## Current Position

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### 2019-Currently Postdoctoral Research

University of California, Riverside (UCR) - Riverside, USA

Research Project: "Structural and conformational characterization of proteins and nucleic acids involved in genome editing and regulation, which are promising against cancer and genetic diseases."

Supervisor: Dr. Giulia Palermo

## Education

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### 2018-2019 Postdoctoral Research

Federal University of Health Sciences of Porto Alegre (UFCSA) - Porto Alegre, Brazil

Research Project: "Structural and conformational characterization of Nek1 protein and new pyrimidine inhibitors with therapeutic potential in the treatment of glioblastoma".

Supervisor: Dr. Dinara Jaqueline Moura

### 2014-2018 PhD in Cellular & Molecular Biology

Federal University of Rio Grande do Sul (UFRGS) - Porto Alegre, Brazil

"Structural and Dynamic Bases of Biomolecules on the N-glycosylation pathway in Bacteria"

Supervisor: Dr. Hugo Verli

### 2013-2014 M.Sc. in Cellular & Molecular Biology

Federal University of Rio Grande do Sul (UFRGS) - Porto Alegre, Brazil

"Force Fields Reliability on the Description of protein complexed and uncomplexed siRNA"

Supervisor: Dr. Hugo Verli

### 2007-2012 Bachelor of Pharmacy

Federal University of Rio Grande do Sul (UFRGS) - Porto Alegre, Brazil

"Conformation-toxicity relationship on oversulfated chondroitin sulfate"

Supervisor: Dr. Hugo Verli

## Languages

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- Portuguese Native speaker
- Fluent English
- Intermediate Spanish

## Skills and Abilities

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### A) EXTENSIVE EXPERIENCE

- Computational Chemistry;
- Molecular Dynamics Simulations;
- Cheminformatics;
- Molecular Docking;
- Metadynamics Simulations;
- Force Field Parameterization;
- OpenMM engine;
- AMBER Simulation Suite;
- GROMACS Simulation Suite;
- Molecular Modelling;
- Conformational Characterization of Biomolecules
- Python and Shell Scripting Languages;

### B) EXPERIENCE

- Quantum Mechanics Calculations;
- Supervising Undergraduate and Graduate Students.

### C) EXTENSIVE KNOWLEDGE

- Drug Discovery;
- Medicinal Chemistry;
- Protein Structure and Dynamics;
- Structural Biology.

### D) SOFT SKILLS

- Self-Motivated and Positive Attitude.
- Verbal and Written Communication Skills;
- Working Both Collaboratively and Independently
- Working as Part of a Multidisciplinary and Diverse Team.

## Research Articles

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- (1) Saha, A.; Ahsan, M.; Arantes, P. R.; Schmitz, M.; Chanez, C.; Jinek, M.; Palermo, G. *Nature Communications* **2024**, *15*:1, 1–12.
- (2) Kumar, A.; Arantes, P. R.; Saha, A.; Palermo, G.; Wong, B. M. *Molecules* **2023**, *28*, 1277.
- (3) Sinha, S.; Pindi, C.; Ahsan, M.; Arantes, P. R.; Palermo, G. *Journal of Chemical Theory and Computation* **2023**.
- (4) Sinha, S.; Vargas, A. M. M.; Arantes, P. R.; Patel, A.; O'Connell, M. R.; Palermo, G. *Nucleic acids research. Accepted* **2023**.
- (5) Vargas, A. M. M.; Osborn, R.; Sinha, S.; Arantes, P. R.; Patel, A.; Dewhurst, S.; Palermo, G.; O'Connell, M. R. *Nucleic acids research. Accepted* **2023**.
- (6) Wang, J.; Arantes, P. R.; Ahsan, M.; Sinha, S.; Kyro, G. W.; Maschietto, F.; Allen, B.; Skeens, E.; Lisi, G. P.; Batista, V. S.; Palermo, G. *Frontiers in Molecular Biosciences* **2023**, *9*, 1393.

- (7) Wang, J.; Maschietto, F.; Qiu, T.; Arantes, P. R.; Skeens, E.; Palermo, G.; Lisi, G. P.; Batista, V. S. *Biophysical Journal* **2023**, *0*.
- (8) Arantes, P. R.; Patel, A. C.; Palermo, G. *Journal of Molecular Biology* **2022**, 167518.
- (9) Belato, H. B.; Alexandra, M.; Nierzwicki, L.; Arantes, P. R.; Jogl, G.; Palermo, G.; Lisi, G. P. *Journal of Structural Biology* **2022**, *214*, 107814.
- (10) Nierzwicki, Ł.; East, K. W.; Binz, J. M.; Hsu, R. V.; Ahsan, M.; Arantes, P. R.; Skeens, E.; Pacesa, M.; Jinek, M.; Lisi, G. P.; Palermo, G. *Nature Catalysis* **2022**, *5*, 912–922.
- (11) Pacesa, M.; Lin, C. H.; Cléry, A.; Saha, A.; Arantes, P. R.; Bargsten, K.; Irby, M. J.; Allain, F. H.; Palermo, G.; Cameron, P.; Donohoue, P. D.; Jinek, M. *Cell* **2022**, *185*, 4067–4081.e21.
- (12) Reinhardt, L. S.; Morás, A. M.; Henn, J. G.; Arantes, P. R.; Ferro, M. B.; Braganhol, E.; de Souza, P. O.; de Oliveira Merib, J.; Borges, G. R.; Dalanhol, C. S., et al. *International Journal of Pharmaceutics* **2022**, *617*, 121584.
- (13) Rossetti, M.; Merlo, R.; Bagheri, N.; Moscone, D.; Valenti, A.; Saha, A.; Arantes, P. R.; Ippodrino, R.; Ricci, F.; Treglia, I., et al. *Nucleic acids research* **2022**, *50*, 8377–8391.
- (14) Sagini, J. P.; Arantes, P. R.; Pedebos, C.; Ligabue-Braun, R. *Macromol* **2022**, *2*, 100–112.
- (15) Saha, A.; Arantes, P. R.; Palermo, G. *Current Opinion in Structural Biology* **2022**, *75*, 102400.
- (16) Wang, J.; Skeens, E.; Arantes, P. R.; Maschietto, F.; Allen, B.; Kyro, G. W.; Lisi, G. P.; Palermo, G.; Batista, V. S. *Biochemistry* **2022**, *61*, 785–794.
- (17) Arantes, P. R.; Polêto, M. D.; Pedebos, C.; Ligabue-Braun, R. *Journal of Chemical Information and Modeling* **2021**, *61*, 4852–4856.
- (18) Narkhede, Y. B.; Gautam, A. K.; Hsu, R. V.; Rodriguez, W.; Zewde, N. T.; Harrison, R. E.; Arantes, P. R.; Gaieb, Z.; Gorham Jr, R. D.; Kieslich, C., et al. *Frontiers in molecular biosciences* **2021**, *8*, 618068.
- (19) Nierzwicki, Ł.; Arantes, P. R.; Saha, A.; Palermo, G. *Wiley Interdisciplinary Reviews: Computational Molecular Science* **2021**, *11*, e1503.
- (20) Nierzwicki, L.; East, K. W.; Morzan, U. N.; Arantes, P. R.; Batista, V. S.; Lisi, G. P.; Palermo, G. *Elife* **2021**, *10*, e73601.
- (21) Seba, V.; de Lima, G. G.; Pereira, B. L.; Silva, G.; Reinhardt, L. S.; Arantes, P. R.; Chee, B. S.; Dos Santos, M. B.; França, S. C.; Regasini, L. O., et al. *Polymers* **2021**, *13*, 2611.
- (22) Wang, J.; Arantes, P. R.; Bhattarai, A.; Hsu, R. V.; Pawnikar, S.; Huang, Y.-m. M.; Palermo, G.; Miao, Y. *Wiley Interdisciplinary Reviews: Computational Molecular Science* **2021**, *11*, e1521.
- (23) Arantes, P. R.; Saha, A.; Palermo, G. *ACS Central Science* **2020**, *6*, 1654–1656.
- (24) Saha, A.; Arantes, P. R.; Hsu, R. V.; Narkhede, Y. B.; Jinek, M.; Palermo, G. *Journal of chemical information and modeling* **2020**, *60*, 6427–6437.
- (25) Steffens, L.; Morás, A. M.; Arantes, P. R.; Masterson, K.; Cao, Z.; Nugent, M.; Moura, D. J. *European Journal of Pharmaceutical Sciences* **2020**, *143*, 105183.
- (26) Arantes, P. R.; Pedebos, C.; Polêto, M. D.; Pol-Fachin, L.; Verli, H. *Journal of chemical information and modeling* **2019**, *60*, 631–643.
- (27) Arantes, P. R.; Polêto, M. D.; John, E. B.; Pedebos, C.; Grisci, B. I.; Dorn, M.; Verli, H. *The Journal of Physical Chemistry B* **2019**, *123*, 994–1008.
- (28) Arantes, P. R.; Pérez-Sánchez, H.; Verli, H. *Journal of Biomolecular Structure and Dynamics* **2018**, *36*, 4045–4056.
- (29) Pedebos, C.; Arantes, P. R.; Giesel, G. M.; Verli, H. *Glycobiology* **2015**, *25*, 1183–1195.
- (30) Valadão, A. L. C.; Abreu, C. M.; Dias, J. Z.; Arantes, P.; Verli, H.; Tanuri, A.; De Aguiar, R. S. *Molecules* **2015**, *20*, 11474–11489.
- (31) Arantes, P. R.; Sachett, L. G.; Graebin, C. S.; Verli, H. *Molecules* **2014**, *19*, 5421–5433.
- (32) Trindade, V. M. T.; Zanatta, G.; Arantes, P. R.; Blanco, I. D. S.; Demore, F. P.; Salbego, C. G. *Procedia-Social and Behavioral Sciences* **2013**, *106*, 3329–3334.

## Preprints

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- (1) Sinha, S.; Vargas, A. M. M.; Arantes, P. R.; Patel, A.; O’Connell, M. R.; Palermo, G. *bioRxiv* **2023**.
- (2) Vargas, A. M. M.; Osborn, R.; Sinha, S.; Arantes, P. R.; Patel, A.; Dewhurst, S.; Palermo, G.; O’Connell, M. R. *bioRxiv* **2023**.
- (3) Saha, A.; Ahsan, M.; Arantes, P. R.; Schmitz, M.; Chanez, C.; Jinek, M.; Palermo, G. *bioRxiv* **2022**.
- (4) Arantes, P. R.; Polêto, M. D.; Pedebos, C.; Ligabue-Braun, R. *ChemRxiv* **2021**.
- (5) Arantes, P. R.; Pedebos, C.; Poleto, M. D.; Pol-Fachin, L.; Verli, H. *ChemRxiv* **2019**.

## Book Chapters

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- (1) Reinhardt, L. S.; Barros Dias, M. C. H. d.; Gnoatto, J.; Wawruszak, A.; Hařasa, M.; Arantes, P. R.; Rowan, N. J.; Moura, D. J. In *Polymeric and Natural Composites*; Springer, Cham: 2022, pp 241–270.
- (2) Reinhardt, L. S.; Arantes, P. R.; Henn, J. G.; Moura, D. J. In *Biomedical Composites*; Springer, Singapore: 2021, pp 145–165.
- (3) Steffens, L.; de Barros Dias, M. C. H.; Arantes, P. R.; Henn, J. G.; Nugent, M.; Moura, D. J. In *Advances and Challenges in Pharmaceutical Technology*; Academic Press: 2021, pp 355–394.
- (4) Steffens, L.; de Barros Dias, M. C. H.; Arantes, P. R.; Gnoatto, J.; Raabe, M.; Moura, D. J. In *Tailor-Made Polysaccharides in Biomedical Applications*; Academic Press: 2020, pp 225–258.

## Oral Presentation in conferences

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**Pablo R. Arantes**, Giulia Palermo: Atomistic Understanding of the RNA-mediated Allosteric Crosstalk in Cas13a. ACS Spring 2022, COMP division – BIPOC MAKE COMP, March 20-24, 2022. San Diego, CA.

**Pablo R. Arantes**, Giulia Palermo: Assessing Structure and Dynamics of AlphaFold2 prediction of GeoCas9. ACS Spring 2022, COMP division – Molecular Mechanics, March 20-24, 2022. San Diego, CA.

**Pablo R. Arantes**, Giulia Palermo: Deciphering off-target effects in CRISPR-Cas9 through molecular dynamics. ACS Fall 2021, August 22 - 26, 2021. Atlanta, GA and Online.

**P. Arantes\***, C.G. Ricci, J.S. Chen, Y. Miao, M. Jinek, J.D. Doudna, J.A. Mccammon, G. Palermo: Oral Talk: Deciphering Off-Target Effects in CRISPR-Cas9 through Accelerated Molecular Dynamics. CRISPR 2021, June 1-10, 2021. Institute Pasteur, Paris, France.

**Arantes, P.R.**; Pedebos, C.; Polêto, M.D.; Verli, H.: SBBq-Conesul: Young Research Platform Session III: Biotechnology, Structural glycobiology of flippase Pglk in N-glycosylation pathway. XLVII Annual Meeting of the Brazilian Society for Biochemistry and Molecular Biology (SBBq), 2018, in the Convention Center of Expoville, in Joinville, SC, Brazil.

## Abstract published in proceedings of conferences

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Souvik Sinha, **Pablo R. Arantes**, Aakash Saha, Giulia Palermo. Atomistic understanding of the RNA-mediated allosteric crosstalk in Cas13a. *Biophysical Journal*, 121 (3), 286a. 2022.

Aakash Saha, **Pablo R. Arantes**, Mohd Ahsan, Martin Jinek, and Giulia Palermo. Multi-microsecond molecular dynamics unveils the mechanism of DNA traversal within CRISPR-Cas12a. *Biophysical Journal*, 121 (3), 322a. 2022.

Amun C. Patel, **Pablo R. Arantes\*** and Giulia Palermo. Domain dynamics and plasticity of the transposon-encoded cascade-TniQ system. *Biophysical Journal* 121 (3), 451a. 2022.

**Pablo R. Arantes**, Lukasz Nierzwicki, Helen Belato, MD Alexandra, Gerwald Jogl, George Lisi, Giulia Palermo. Assessing structure and dynamics of AlphaFold2 prediction of GeoCas9. *Biophysical Journal* 121 (3), 45a. 2022.

**P. Arantes**, L. Nierzwicki, A. Saha, A.C. Patel, P. Lawton, G. Palermo: Defining the allosteric mechanism in CRISPR-Cas9. CRISPR 2021, June 1-10, 2021. Institute Pasteur, Paris, France.

**Pablo R. Arantes**, Aakash Saha, Martin Jinek, Giulia Palermo. DNA-Induced Allosteric Control Regulates Activation of Cas12A. *Biophysical Journal*, 120, 17a-. 2021.

Aakash Saha\*, **Pablo R. Arantes\***, Rohaine V. Hsu, Yogesh B. Narkhede, Martin Jinek, and Giulia Palermo. Cooperative Dynamics of REC-Nuc Lobes Prime Cas12a for DNA Processing. *Biophysical Journal*, 120, 16a-17a. 2021.

**Arantes, P.R.**; Pedebos, C.; Polêto, M.D.; Verli, H.: Structural glycobiology of flippase Pglk in N-glycosylation pathway. XLVII Annual Meeting of the Brazilian Society for Biochemistry and Molecular Biology, 2018, Joinville/SC-BR.

**Arantes, P.R.**; Pedebos, C.; Polêto, M.D.; Verli, H.: Structural glycobiology of flippase Pglk in N-glycosylation pathway. XLVI Annual Meeting of the Brazilian Society for Biochemistry and Molecular Biology, 2017, Águas de Lindóia/SP-BR.

Pedebos, C.; **Arantes, P.R.**; Verli, H.: Atomic-level Evaluation of Key Components from the N-glycosylation Pathway in Prokaryota. XLVI Annual Meeting of the Brazilian Society for Biochemistry and Molecular Biology, 2017, Águas de Lindóia/SP-BR.

John E.O.; **Arantes, P.R.**; Polêto, M.D.; Verli, H.: Gromos53a6 Force Field Parameters For Chalcones And Flavonoids. XLVI Annual Meeting of the Brazilian Society for Biochemistry and Molecular Biology, 2017, Águas de Lindóia/SP-BR.

**Arantes, P.R.**; Pedebos, C.; Verli, H.: Dynamics Of Lipid-Linked, Membrane Soaked, Oligosaccharides: Biological Precursors For N-Glycosylation In Eukarya And Prokarya. XLV Annual Meeting of the Brazilian Society for Biochemistry and Molecular Biology, 2016, Natal/RN-BR.

John E.O.; **Arantes, P.R.**; Verli, H.: Gromos53a6 Force Field Parameters For Chalcones And Flavonoids. XLV Annual Meeting of the Brazilian Society for Biochemistry and Molecular Biology, 2016, Natal/RN-BR.

Pedebos, C.; Ligabue-Braun, R.; **Arantes, P.R.**; Verli, H.: Evolution and dynamics of the N-glycosylation pathway through oligosaccharyltransferases. XLV Annual Meeting of the Brazilian Society for Biochemistry and Molecular Biology, 2016, Natal/RN-BR.

Trindade, V.M.T.; **Arantes, P.R.**; Zanatta, G.; Salbego, C.G. XLV Annual Meeting of the Brazilian Society for Biochemistry and Molecular Biology, 2016, Natal/RN-BR.

**Arantes, P.R.**; Pérez-Sánchez, H.; Verli, H.: Effects of D-myo-inositol 3,4,5,6-Tetrakisphosphate (TMI) Binding on Antithrombin XLIV Annual Meeting of the Brazilian Society for Biochemistry and Molecular Biology, 2015, Foz do Iguaçu/PR-BR.

**Arantes, P.R.**; Verli, H.: Force Fields Reliability on the Description of Protein complexed and uncomplexed siRNA. XLIII Annual Meeting of the Brazilian Society for Biochemistry and Molecular Biology, 2014, Foz do Iguaçu/PR-BR.

Dallagnol, J. C. C.; **Arantes, P.R.**; Pedebos, C.; Braun, R. L.; Duarte, M. E.; Nosedá, M. D.; Ducatti, D. R. B.; Verli, H.; Gonçalves, A. G.: Influence of ring conformation on interactions of a carbohydrate based compound in a M1 muscarinic acetylcholine receptor model. 7th Brazilian Symposium on Medicinal Chemistry, 2014, Campos do Jordão/SP-BR.

Pedebos, C.; **Arantes, P.R.**; Verli, H.: Structural Glycobiology of the Oligosaccharyltransferase PglB from *Campylobacter lari*. XLIII Annual Meeting of the Brazilian Society for Biochemistry and Molecular Biology, 2014, Foz do Iguaçu/PR-BR.

Trindade, V.M.T.; **Arantes, P.R.**; Zanatta, G.; Salbego, C.G.: Virtual Determination of Liver and Muscle Glycogen Obtained from Fed Rats and from 24-Hour Fasted Rats. XLIII Annual Meeting of the Brazilian Society for Biochemistry and Molecular Biology, 2014, Foz do Iguaçu/PR-BR.

**Arantes, P.R.**; Verli, H.: Dynamics of siRNAs: Comparison of Force Fields Reliability. XLII Annual Meeting of the Brazilian Society for Biochemistry and Molecular Biology, 2013, Foz do Iguaçu/PR-BR.

Trindade, V.M.T.; **Arantes, P.R.**; Zanatta, G.; Zimmer, E.R.; Ewald, L.; Pettenuzzo, L.F.; Matté, C.; Salbego, C.G.: Evaluation of Serum Lactate Dehydrogenase Activity in a Virtual Environment. XLII Annual Meeting of the Brazilian Society for Biochemistry and Molecular Biology, 2013, Foz do Iguaçu/PR-BR.

**Arantes, P.R.**; Verli, H.: Conformational Characterization of Ipomatoosides. XLI Annual Meeting of the Brazilian Society for Biochemistry and Molecular Biology, 2012, Foz do Iguaçu/PR-BR.

**Arantes, P.R.**; Fernandes, C.L.; Andrade de Lima, M.; Cunha de Farias, E.H.; Verli, H.: Conformation-toxicity relationship on over-sulfated chondroitin sulfate. XL Annual Meeting of the Brazilian Society for Biochemistry and Molecular Biology, 2011, Foz do Iguaçu/PR-BR.

## Honors & Awards

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1. XXII Scientific Initiation Meeting, 2012: **Best presentation in the area of Exact and Earth Sciences - Session: Simulation and Molecular Modeling, UFRGS.** Conformational characterization of Ipomatosides. Advisor: Hugo Verli.
2. 7th Brazilian Symposium on Medicinal Chemistry, 2014: **Best Graduate Student Poster Of The Drug Discovery & Development Session**, with the poster entitled "Influence of ring conformation on interactions of a carbohydrate based compound in a M1 muscarinic acetylcholine receptor model".

3. **Awarded for best cover image at the Inaugural Symposium Center for RNA in Biology and Medicine** - University of California, Riverside - USA, 2022.

4. **Travel award for the Biophysical Society Meeting 2024** in Philadelphia, USA, 2024.

## **Grants for Computational Resources & Funding**

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PI: Giulia Palermo; Contributed significantly in writing and produce preliminary results for the following grants:

- Anton-2 by the COVID-19 HPC Consortium: 320,000 Service Units (SUs) & Comet CPU nodes: 580,000 SUs (MCB200150; Nov 2023).

- NERSC-DOE: 5,340 CPU Node Hours (2,100,000 NERSC Hours) (Jan 2022).

- National Science Foundation (NSF) grant on “Mechanistic Investigations of Conformational Activation and Catalysis in Emerging CRISPR-Cas Systems” (NSF CHE-2144823) (2022 – 2027).

- National Institutes of Health (NIH) grant on “Investigating the metal-dependent function, allostery and inhibition of CRISPR-Cas9” (NIH R01GM141329) (2021 – 2026).

- NSF at Extreme Science and Engineering Discovery Environment (XSEDE): 1.5 M core hours (\$600,000; Sep 2020).

- Microsoft Azure iCloud computing resources (\$350,000; Jul 2022).

- Anton-2 by the COVID-19 HPC Consortium: 320,000 Service Units (SUs) & Comet CPU nodes: 580,000 SUs (MCB200150; May 2020).