



# Pablo Ricardo Arantes

PHD

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## Curriculum Vitae

October 1, 2022

MARCH 7TH, 1988

BRAZILIAN

## Current Position

### 2019-Currently Research Fellow

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

### 2018-2019 Research Fellow

PPGBio - UFCSPA - Porto Alegre, BR

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

PPGBCM - UFRGS - Porto Alegre, BR

"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

PPGBCM - UFRGS - Porto Alegre, BR

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

Supervisor: Dr. Hugo Verli

### 2007-2012 Bachelor of Pharmacy

UFRGS - Porto Alegre, BR

"Conformation-toxicity relationship on oversulfated chondroitin sulfate"

Supervisor: Dr. Hugo Verli

## Languages

- Portuguese Native speaker
- Fluent English
- Intermediate Spanish

## Skills and Abilities

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### A) EXTENSIVE EXPERIENCE

- Molecular Dynamics Simulations;
- Molecular Docking;
- Metadynamics Simulations;
- Force Field Parameterization;
- OpenMM engine;
- AMBER Simulation Suite;
- GROMACS Simulation Suite;
- Molecular Modelling;
- Conformational Characterization of Biomolecules

### B) EXPERIENCE

- Python and Shell Scripting Languages;
- Quantum Mechanics Calculations;
- Supervising Undergraduate and Graduate Students.

### C) EXTENSIVE KNOWLEDGE

- 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) Arantes, P. R.; Patel, A. C.; Palermo, G. *Journal of Molecular Biology* **2022**, 167518.
- (2) Belato, H. B.; Alexandra, M.; Nierzwicki, L.; Arantes, P. R.; Jogl, G.; Palermo, G.; Lisi, G. P. *Journal of Structural Biology* **2022**, 214, 107814.
- (3) Nierzwicki, Ł.; East, K. W.; Binz, J.; Hsu, R. V.; Ahsan, M.; Arantes, P. R.; Skeens, E.; Pacesa, M.; Jinek, M.; Lisi, G. P.; Palermo, G. *Nature Catalysis* **2022**, *accepted*.
- (4) 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**, *accepted*.
- (5) 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.
- (6) 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.
- (7) Sagini, J. P.; Arantes, P. R.; Pedebos, C.; Ligabue-Braun, R. *Macromol* **2022**, 2, 100–112.
- (8) Saha, A.; Arantes, P. R.; Palermo, G. *Current Opinion in Structural Biology* **2022**, 75, 102400.
- (9) 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.
- (10) Arantes, P. R.; Polêto, M. D.; Pedebos, C.; Ligabue-Braun, R. *Journal of Chemical Information and Modeling* **2021**, 61, 4852–4856.
- (11) 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.
- (12) Nierzwicki, Ł.; Arantes, P. R.; Saha, A.; Palermo, G. *Wiley Interdisciplinary Reviews: Computational Molecular Science* **2021**, 11, e1503.

- (13) Nierzwicki, L.; East, K. W.; Morzan, U. N.; Arantes, P. R.; Batista, V. S.; Lisi, G. P.; Palermo, G. *Elife* **2021**, *10*, e73601.
- (14) 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.
- (15) 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.
- (16) Arantes, P. R.; Saha, A.; Palermo, G. *ACS Central Science* **2020**, *6*, 1654–1656.
- (17) 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.
- (18) 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.
- (19) Arantes, P. R.; Pedebos, C.; Polêto, M. D.; Pol-Fachin, L.; Verli, H. *Journal of chemical information and modeling* **2019**, *60*, 631–643.
- (20) 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.
- (21) Arantes, P. R.; Pérez-Sánchez, H.; Verli, H. *Journal of Biomolecular Structure and Dynamics* **2018**, *36*, 4045–4056.
- (22) Pedebos, C.; Arantes, P. R.; Giesel, G. M.; Verli, H. *Glycobiology* **2015**, *25*, 1183–1195.
- (23) 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.
- (24) Arantes, P. R.; Sachett, L. G.; Graebin, C. S.; Verli, H. *Molecules* **2014**, *19*, 5421–5433.
- (25) 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) Saha, A.; Ahsan, M.; Arantes, P. R.; Schmitz, M.; Chanez, C.; Jinek, M.; Palermo, G. *bioRxiv* **2022**.
- (2) Arantes, P. R.; Polêto, M. D.; Pedebos, C.; Ligabue-Braun, R. *ChemRxiv* **2021**.
- (3) 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.; Hałasa, 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.

**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

## 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 Ipomotaosides. 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.

## Awards and Titles

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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".