

Pablo Ricardo Arantes

PHD

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Resume

July 25, 2023

MARCH 7TH, 1988

BRAZILIAN

Current Position

2019-Currently Research Fellow

University of California, Riverside, United States

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, 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

PPGBCM - 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

PPGBCM - 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

UFRGS - Porto Alegre, Brazil

"Conformation-toxicity relationship on oversulfated chondroitin sulfate"

Supervisor: Dr. Hugo Verli

Skills and Abilities

A) EXTENSIVE EXPERIENCE

- Molecular Modelling (AlphaFold2, RoseTTAFold);
- Molecular Dynamics Simulations;
- TorchANI (PyTorch implementation of ANI);
- GaMD Simulations;
- Metadynamics Simulations;
- Molecular Docking;
- Force Field Parameterization;
- Enhanced Sampling Methods;

- AMBER Simulation Suite;
- OpenMM engine;
- GROMACS Simulation Suite.

B) EXPERIENCE

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

C) EXTENSIVE KNOWLEDGE

- Protein Design
- Drug Design
- Structural Bioinformatics
- Structural Biology.
- Medicinal Chemistry;

- Protein Structure and Dynamics;

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

- (1) Kumar, A.; Arantes, P. R.; Saha, A.; Palermo, G.; Wong, B. M. *Molecules* **2023**, 28, 1277.
- (2) Sinha, S.; Pindi, C.; Ahsan, M.; Arantes, P. R.; Palermo, G. *Journal of Chemical Theory and Computation* **2023**.
- (3) 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.
- (4) Arantes, P. R.; Patel, A. C.; Palermo, G. *Journal of Molecular Biology* **2022**, 167518.
- (5) Belato, H. B.; Alexandra, M.; Nierzwicki, L.; Arantes, P. R.; Jogl, G.; Palermo, G.; Lisi, G. P. *Journal of Structural Biology* **2022**, 214, 107814.
- (6) 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.
- (7) 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.
- (8) 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.; Dalanhhol, C. S., et al. *International Journal of Pharmaceutics* **2022**, 617, 121584.
- (9) 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.
- (10) Sagini, J. P.; Arantes, P. R.; Pedebos, C.; Ligabue-Braun, R. *Macromol* **2022**, 2, 100–112.
- (11) Saha, A.; Arantes, P. R.; Palermo, G. *Current Opinion in Structural Biology* **2022**, 75, 102400.
- (12) 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.
- (13) Arantes, P. R.; Polêto, M. D.; Pedebos, C.; Ligabue-Braun, R. *Journal of Chemical Information and Modeling* **2021**, 61, 4852–4856.
- (14) 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.
- (15) Nierzwicki, Ł.; Arantes, P. R.; Saha, A.; Palermo, G. *Wiley Interdisciplinary Reviews: Computational Molecular Science* **2021**, 11, e1503.
- (16) Nierzwicki, L.; East, K. W.; Morzan, U. N.; Arantes, P. R.; Batista, V. S.; Lisi, G. P.; Palermo, G. *Elife* **2021**, 10, e73601.
- (17) 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.
- (18) 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.
- (19) Arantes, P. R.; Saha, A.; Palermo, G. *ACS Central Science* **2020**, 6, 1654–1656.
- (20) 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.
- (21) 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.
- (22) Arantes, P. R.; Pedebos, C.; Polêto, M. D.; Pol-Fachin, L.; Verli, H. *Journal of chemical information and modeling* **2019**, 60, 631–643.
- (23) 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.
- (24) Arantes, P. R.; Pérez-Sánchez, H.; Verli, H. *Journal of Biomolecular Structure and Dynamics* **2018**, 36, 4045–4056.
- (25) Pedebos, C.; Arantes, P. R.; Giesel, G. M.; Verli, H. *Glycobiology* **2015**, 25, 1183–1195.
- (26) 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.
- (27) Arantes, P. R.; Sachett, L. G.; Graebin, C. S.; Verli, H. *Molecules* **2014**, 19, 5421–5433.

- (28) 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.