Mayk Caldas Ramos

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Education

Academic Qualifications

- **Federal University of Rio de Janeiro** — **Rio de Janeiro - Brazil**
  Bachelor of Chemical Engineering — *2012–2017*
  Thesis: A molecular dynamics study of water diffusion in LTA-type zeolites.
- **Federal University of Rio de Janeiro** — **Rio de Janeiro - Brazil**
  Masters in Chemical Sciences — *2017–2019*
  Thesis: Molecular dynamics simulations of PAMAM and PPI dendrimers using the GROMOS-compatible 2016H66 forcefield: structural properties for different generations and pH environments.
- **Federal University of Rio de Janeiro** — **Rio de Janeiro - Brazil**
  PhD in Chemical Sciences — *2019–Current*
  Thesis: Evaluation of the viability of PAMAM and PPI dendrimers in their use as drug carriers by molecular dynamics.

Professional Experience

- **Applied Thermodynamics and Molecular Simulation (ATOMS)** — **Rio de Janeiro - Brazil**
  Undergrad Student — *2015–2017*
  I studied transport properties by molecular dynamics simularion in a big group. It improved my team work and people management.
- **WIKKI Brasil** — **Rio de Janeiro - Brazil**
  CFD Engineer — *2016–2017*
  I worked as an intern in a CFD company. In there, I got experience with multi phase, multi compound and turbulent flow systems simulations using OpenFOAM.

Technical and Personal skills

- **Programming Languages:**
  - Proficient in: Python, Bash scripting, LaTeX
  - Familiar with: Fortran90 , C, C++
- **Known Softwares and libraries:** GROMACS, Lammps, Numpy, Matplotlib, Scipy, Pandas, Gaussian, ORCA, VMD, PyMol, Molden
- **Languages:** Portuguese (Native), English (Advanced).
- **General Business Skills:** Good presentation skills, Works well in a team, Linux administration.

Interests and Objectives

- **Molecular Modelling and Simulation**
  Apply published softwares and known techniques aiming to simulate and understand molecular systems
- **Simulation Techniques**
  Develop and implement new simulation techniques and create scripts for automating simulation processes
- **Data-driven Science and Software Development**
  I am interested in developing tool in the context of the inverse molecular design applying machine learning and computer vision in chemistry.

Events Participation

- **APS/ICTP-SAIFR Forum on Biological Physics: from Molecular to Macroscopic Scale (2020)**
  Poster presentation

  Title: Using multiple-restrained molecular dynamics to evaluate the loading capacity of quercetin molecules in PAMAM dendrimer.
- **XX Brazilian Symposium on Theoretical Chemistry (2019)**
  Poster and Oral presentations

  Title: Using steered molecular dynamics simulations for building models of dendrimer-drug complexes
- **XLIV Congress of the Brazilian Biophysical Society (2019)**
  Poster presentation

  Title: Creating models of dendrimer-drug complexes using steered molecular dynamics simulations
- **XLIII Annual Meeting of the Brazilian Biophysical Society (2018)**
  Poster presentation

  Title: Molecular Dynamics simulations of PAMAM and PPI dendrimers with the GROMOS-compatible 2016H66 force field

Publications

M. C. Ramos, P. K. Quoika, V. A. C. Horta, D. M. Dias, E. G. Costa, J. L. M. do Amaral, L. M. Ribeiro, K. R. Liedl, and B. A. C. Horta, "pyPolyBuilder: Automated Preparation of Molecular Topologies and Initial Configurations for Molecular Dynamics Simulations of Arbitrary Supramolecules," *Journal of Chemical Information and Modeling*, vol. 61, p. acs.jcim.0c01438, apr 2021.

M. C. Ramos and B. A. C. Horta, "Drug-Loading Capacity of PAMAM Dendrimers Encapsulating Quercetin Molecules: A Molecular Dynamics Study with the 2016H66 Force Field," *Journal of Chemical Information and Modeling*, p. acs.jcim.0c00960, jan 2021.

M. C. Ramos, V. A. C. Horta, and B. A. C. Horta, "Molecular Dynamics Simulations of PAMAM

and PPI Dendrimers Using the GROMOS-Compatible 2016H66 Force Field," *Journal of Chemical Information and Modeling*, vol. 59, pp. 1444–1457, apr 2019.