

## Ariane Nunes Alves starts as a junior group leader in UniSysCat

Start Time: Thursday, July 22, 2021

End Time:



In July 2021, Alexander von Humboldt fellow [Ariane Nunes Alves](#) has started as a junior group leader at Technische Universität Berlin. We're happy to welcome her in the UniSysCat team! Ariane's research goal is to understand how drugs and small molecules bind to their molecular partners. She is fascinated by ligand-protein binding kinetics and the consequences it can have for drug design and enzyme catalysis.

Ariane has a strong background in computational biochemistry and biophysics. In 2017, she obtained her Ph.D. in biochemistry from the University of São Paulo in Brazil under the supervision of Prof. Dr. Guilherme Menegon Arantes, where she worked on the application and development of computational methods to enhance sampling of ligand unbinding and protein unfolding. In 2018, she joined the [Molecular and Cellular Modeling group](#) of Prof. Dr. Rebecca Wade at the Heidelberg Institute for Theoretical Studies as a postdoctoral researcher, where she worked in simulations to characterize pathways for ligand dissociation and associated kinetic rates.

Within UniSysCat, Ariane will take the chance to establish her own research group. From now on, as a junior research group leader in the field of structural biology, she will work on the development and application of computational methods to study ligand binding kinetics and how kinetic rates can be used for optimizing enzyme catalysis and for tunnel engineering.

Ariane is also involved in initiatives to promote inclusion and visibility of women and minorities in science. In 2020, she co-organized “[LatinXChem](#)”, a poster conference on twitter for Latin American chemists and “[The impact of the COVID-19 crisis on women in science: challenges and solutions](#)”, a virtual conference to discuss the impact of the COVID-19 pandemic on female scientists.