Bruno Di Geronimo, Ph.D.

Curriculum Vitae

Postdoctoral Researcher | Georgia Institute of Technology |bdigeronimo3@gatech.edu

STATEMENT

I am Dr. Bruno Di Geronimo a pharmacist and computational biochemist currently working as senior postdoctoral researcher at Georgia Institute of Technology, in the Kamerlin lab. My career has been highly international, with research experience across Spain, Finland, the Czech Republic, Austria, and currently at the United States. Throughout these stages, my work has followed a clear and coherent trajectory: applying advanced computational methods to understand how protein structure and dynamics encode function, and translating this knowledge into enzyme engineering, biocatalysis, and therapeutic discovery. Trained originally as a pharmacist with honours at the Universidad Complutense de Madrid, I developed early expertise in biocatalysis and medicinal chemistry before completing a PhD focused on structure-based drug design and molecular dynamics of phosphatases and oncology targets. Subsequent postdoctoral work strengthened my mechanistic toolkit through QM/MM simulations, enhanced sampling, and virtual screening, applied to glycosidases, metalloenzymes, and ion channels. I am currently a senior postdoctoral researcher at Georgia where I focus on mechanistic enzymology and AI-enabled enzyme design. Across my career, I have progressively built independent collaborations, secured competitive funding and HPC resources, mentored students at multiple levels, and contributed to teaching and outreach. These experiences position me to lead an independent research program at the interface of computational enzyme engineering and computer-aided drug design.

EDUCATION

Ph.D. Computational Chemistry and Molecular Modeling on Drug Discovery 2015-2020
University San Pablo CEU, Madrid, Spain

Graduated in Pharmacy with honors 2009-2014
University Complutense of Madrid, Spain

RESEARCH POSITIONS

Postdoctoral Researcher, Georgia Institute of Technology, USA 2024-present
School of Chemistry and Biochemistry, Kamerlin lab

Postdoctoral Researcher, Medical University of Graz, Austria 2022-2024
Division of Medicinal Chemistry, Computer-Aided Molecular Design Lab

Research Assistant, Spanish National Cancer Research Center (CNIO), Spain 2019-2022
Experimental Therapeutics Program

Research Visit, Institute of Organic Chemistry and Biochemistry (IOCB), Czech Republic 2017
Theoretical Bioinorganic Chemistry

Pharmaceutical Industry Internship, GSK Aranda de Duero, Spain 2015

Erasmus SNS program, University of Helsinki, Finland 2013-2014
Division of Pharmaceutical Chemistry and Technology

PUBLICATIONS

JCR ARTICLES, H INDEX

https://orcid.org/0000-0003-1822-7142

Information obtained from **(Publons):** https://publons.com/researcher/1863029/bruno-bdg-di-geronimo/

Total Number of Publications: 16 | Total Times Cited: 187 | h-index: 9 | Verified peer reviews: 26

WoS Research ID: R-2454-2018 | SCOPUS ID: 57200032570 | ResearchGate: "Bruno Di Geronimo"

1. Elske van der Pol, Thomas Schlatzer, Gyula Hoffka, **Bruno Di Geronimo**, Johannes Eder, Anna K. Schweiger, Marianna Karava, Dominik Gross, Roland C. Fischer, Daniel Kracher, Romas Kazlauskas, Kenji Miyamoto, Shina Caroline Lynn Kamerlin, Rolf Breinbauer, and Robert Kourist. Mechanistic Elucidation and Stereochemical Consequences of Alternative Binding of Alkenyl Substrates by Engineered Arylmalonate Decarboxylase. *Journal of the American Chemical Society* **2025** *147* (43), 39271-39283. https://doi.org/10.1021/jacs.5c10721
2. Mandl, Š.; **Di Geronimo, B.**; Alonso-Gil, S.; Grininger, C.; George, G.; Ferstl, U.; Herzog, S. A.; Žagrović, B.; Nusshold, C.; Pavkov-Keller, T.; Sánchez-Murcia, P. A. A New View of Missense Mutations in α-mannosidosis Using Molecular Dynamics Conformational Ensembles. *Protein Science* **2025**, *34* (4). https://doi.org/10.1002/pro.70080.
3. **Di Geronimo, B.**; Mandl, Š.; Alonso-Gil, S.; Žagrović, B.; Reibnegger, G.; Nusshold, C.; Sánchez-Murcia, P. A. Digging out the Molecular Connections between the Catalytic Mechanism of Human Lysosomal α-Mannosidase and Its Pathophysiology. *J Chem Inf Model* **2025**. https://doi.org/10.1021/acs.jcim.4c02229
4. Llanos, S.; **Di Geronimo, B.**; Casajús, E.; Blanco-Romero, E.; Fernández-Leiro, R.; Méndez, J. Interference of Small Compounds and Mg2+ with DsRNA-Binding Fluorophores Compromises the Identification of SARS-CoV-2 RdRp Inhibitors. *Sci Rep* **2024**, *14* (1), 28250. https://doi.org/10.1038/s41598-024-78354-x.
5. Yehorova, D.; **Di Geronimo, B.**; Robinson, M.; Kasson, P. M.; Kamerlin, S. C. L. Using Residue Interaction Networks to Understand Protein Function and Evolution and to Engineer New Proteins. *Curr Opin Struct Biol* **2024**, *89*, 102922. https://doi.org/10.1016/j.sbi.2024.102922.
6. Rossmann, C., Ranz, C., Kager, G., Ledinski, G., Koestenberger, M., Wonisch, W., Wagner, T., Schwaminger, S. P., **Di Geronimo, B.**, Hrzenjak, A., Hallstöm, S., Reibnegger, G., Cvirn, G., & Paar, M. (2023). Metformin Impedes Oxidation of LDL In Vitro. *Pharmaceutics* **2023**, 15(8), 2111. https://doi.org/10.3390/pharmaceutics15082111
7. Nina Gubensäk, Theo Sagmeister, Christoph Buhlheller, **Bruno Di Geronimo**, Gabriel E Wagner, Lukas Petrowitsch, Melissa A Gräwert, Markus Rotzinger, Tamara M Ismael Berger Jan Schäfer, Isabel Usón, Joachim Reidl, Pedro A Sánchez-Murcia, Klaus Zangger, Tea Pavkov-Keller. Vibrio cholerae's ToxRS bile sensing system. *eLife.* **2023**; 12. 88721. https://doi.org/10.7554/eLife.88721
8. Paar M, Aziz F, Sourij C, Tripolt NJ, Kojzar H, Müller A, Pferschy P, Obermayer A, Banfic T, **Di Geronimo B**, Goswami N, Schlagenhauf A, Köstenberger M, Bärnthaler T, Wagner T, Hrzenjak A, Wonisch W, Reibnegger G, Raggam RB, Sourij H, Cvirn G. Only Subclinical Alterations in the Haemostatic System of People with Diabetes after COVID-19 Vaccination. *Viruses.* **2023**; 15(1):10. https://doi.org/10.3390/v15010010
9. Martínez-González, Sonia; Alvarez, Rosa María; Martín, José I.; García, Ana Belén; Riesco-Fagundo, Concepción; Varela, Carmen; Rodríguez-Hergueta, Antonio; González-Cantalapiedra, Esther; Albarrán, María Isabel; Gómez-Casero, Elena; Cebriá, Antonio; Aguirre, Enara; Ajenjo, Nuria; Cebrián, David; **Di Geronimo, Bruno**; Cunningham, Darren; O'Neill, Michael; Dave, Harish P.G.; Blanco-

Aparicio, Carmen; Pastor, Joaquín. Macrocyclization as a source of desired polypharmacology. Discovery of Triple PI3K/mTOR/PIM inhibitors. *ACS Medicinal Chemistry Letters.* **2021** *12* (11), 1794-1801. https://pubs.acs.org/doi/10.1021/acsmedchemlett.1c00412

10. Rosa M. Álvarez, Ana Belén García, Concepción Riesco-Fagundo, José I. Martín, Carmen Varela, Antonio Rodríguez Hergueta, Esther González Cantalapiedra, Julen Oyarzabal, **Bruno Di Geronimo**, Milagros Lorenzo, M Isabel Albarrán, Antonio Cebriá, David Cebrián, Sonia Martínez-González, Carmen Blanco-Aparicio, Joaquín Pastor. Omipalisib inspired macrocycles as dual PI3K/mTOR inhibitors. *European Journal Medicinal Chemistry.* **2021**, *211*, 113109. https://www.sciencedirect.com/science/article/pii/S0223523420310813?via=ihub
11. García-Marín J, Griera M, Sánchez-Alonso P, **Di Geronimo B**, Mendicuti F, Rodríguez-Puyol M, Alajarín R, de Pascual-Teresa B, Vaquero JJ, Rodríguez-Puyol D. Pyrrolo[1,2-a]quinoxalines: Insulin Mimetics that Exhibit Potent and Selective Inhibition against Protein Tyrosine Phosphatase 1B. *ChemMedChem*. **2020**. *15*, 1788-1801. https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/cmdc.202000446
12. Martínez, R.; **Di Geronimo, B.**; Pastor, M.; Zapico, J.M.; Coderch, C.; Panchuk, R.; Skorokhyd, N.; Maslyk, M.; Ramos, A.; de Pascual-Teresa, B. Multitarget Anticancer Agents Based on Histone Deacetylase and Protein Kinase CK2 Inhibitors. *Molecules*. **2020**, *25*, 1497. Open Access: https://www.mdpi.com/1420-3049/25/7/1497
13. Rangasamy, L.; **Di Geronimo, B.**; Ortín, I.; Coderch, C.; Zapico, J.M.; Ramos, A.; de Pascual-Teresa, B. Molecular Imaging Probes Based on Matrix Metalloproteinase Inhibitors (MMPIs). *Molecules*. **2019**, *24*, 2982. Open Access: https://www.mdpi.com/1420-3049/24/16/2982
14. Godoy, C.A.; Klett, J.; **Di Geronimo, B.**; Hermoso, J.A.; Guisán, J.M.; Carrasco-López, C. Disulfide Engineered Lipase to Enhance the Catalytic Activity: A Structure-Based Approach on BTL2. *International Journal of Molecular Science*. **2019**, *20*, 5245. Open Access: https://www.mdpi.com/1422-0067/20/21/5245
15. Rosalía Fernández-Calle, Marta Vicente-Rodríguez, Miryam Pastor, Esther Gramage, **Bruno Di Geronimo**, José María Zapico, Claire Coderch, Carmen Pérez-García, Amy W. Lasek, Beatriz de Pascual-Teresa, Ana Ramos, Gonzalo Herradón. Pharmacological inhibition of Receptor Protein Tyrosine Phosphatase beta/zeta (PTPRZ1) modulates behavioral responses to ethanol. *Neuropharmacology*. **2018**, *137*, 86-95. https://10.1016/j.neuropharm.2018.04.027
16. (**Author shared**) Pastor M, Fernández-Calle R, **Di Geronimo B**, Vicente-Rodríguez M, Zapico JM, Gramage E, Coderch C, Pérez-García C, Lasek AW, Puchades-Carrasco L, Pineda-Lucena A, de Pascual-Teresa B, Herradón G, Ramos A. Development of inhibitors of receptor protein tyrosine phosphatase β/ζ (PTPRZ1) as candidates for CNS disorders. *European Journal Medicinal Chemistry.* **2018**, *144*, 318-329. https://10.1016/j.ejmech.2017.11.080

- **Manuscript submitted**
  1) Zuson J, Helmer P.O, **Di Geronimo B**, Chánique A, Kavčiaková K, Teijeiro-Juiz R, Brickel S, Drienovská I, Kracher I, Kamerlin SCL, Loll B, Kourist B. Deciphering the evolutionary origin of the enantioselectivity of short-chain dehydrogenases from plants toward 1-borneol. DOI: 10.1101/2025.07.17.664155 (Submitted to *Nature Communications*)
  2) Myosin Post-translational Modifications Associated with Critical Illness Myopathy Ribeiro F, **Di Geronimo B**, Cacciani N, Widgren N, Hedström Y, S.Moriscot A, Kasson P, Kamerlin SCL, Bergquist J, Larsson L. DOI 10.1101/2025.08.18.25333907 (Submitted to *Journal of Acta Physiologica*)
  3) Alonso-Gil S, **Di Geronimo B**, Kashima T, Ishiwata A, Tanaka K, Fujita K, et al. GH172 difructose dianhydride I synthase: A two-stepped journey via glycosylation and cyclization using QM/MM metadynamics. DOI 10.26434/chemrxiv-2023-h76dn-v2 (Submitted to *ACS catalysis*)

- **Books**

  Biological Systems Workbook: Data modelling and simulations at molecular level. Javier Klett, Carlos Leon, **Bruno Di Geronimo.** Edition: 2021. Publisher: Universidad Carlos III de Madrid. Editor: Javier Klett. ISBN: 978-84-16829-65-1. Open Access: Biological Systems Workbook

- **Chapters**

  M. A. Albarrán, S. Llanos y **B. Di Geronimo.** La Contaminación del Aire como Factor de Riesgo en la Incidencia y el Desarrollo del Cáncer en el libro electrónico Contaminación, Salud y Políticas Públicas coordinado por J. J. Nogueira, Respira Madrid. Open Access: https://juannogueira0.wixsite.com/respiramadrid/post/contaminacion-cancer

- **Thesis**

  Computer-aided Drug Design based on Phosphatases (PTPRZ, PTPRGamma, PTP1B), Kinases (CK2) and Histone Deacetylases (HDAC1, HDAC6) as drug targets. 11/06/2020. Open Access: http://hdl.handle.net/10637/13014

PATENTS & LICENSE

1) **CNIO023-123:** This project focused on the identification and development of novel FOXO activators with potential applications in anti-aging therapeutics. Through a high-content screening campaign link at CNIO, a library of small molecules was evaluated, resulting in the identification of structurally diverse FOXO activators that function via mechanisms independent of classical pathways such as PI3K inhibition or nuclear transport interference. Key Contributions:
   - Curated and analyzed over 400 compounds across 23 chemical series.
   - Led structure-activity relationship (SAR) studies and mechanistic counter-screening.
   - Facilitated the licensing of top candidates to Refoxy Pharma for downstream development.

2) **Patent registration number: A55350/2025:** The present invention relates to pharmaceutical compositions for the treatment or prevention of infections or diseases involving microorganisms comprising a ToxRS or ToxRS-like system.
   Contributions:
   - Modelling of the system ToxRS
   - Virtual Screening
   - Hit-identification

ACHIEVEMENTS & AWARDS

Excellence of Doctoral Thesis awarded by the Paul Ehrlich MedChem Euro-PhD Network 2021

Ph.D. awarded with *cum laude* distinction 2020

Extraordinary Degree Award, Faculty of Pharmacy, Universidad Complutense de Madrid 2015

Academic recognition granted by the College of Pharmacists of Madrid for good academic record 2012

TEACHING EXPERIENCE

- **At Georgia Tech:**

Head of Teaching CHEM 3511 Survey on Biochemistry — Spring 2025

Teaching Assistance CHEM 8853 Introduction to Biomolecular Modeling — Fall 2025

Head of Teaching CHEM 6501 Biochemistry I — Spring 2024

Guest lecture at Chem6572-B, Structural Biology — Fall 2024
Prof. Hud, Nicholas (nick.hud@chemistry.gatech.edu)

Summer Theoretical and Computational Chemistry (STACC) Workshop — Fall 2024
Asst. Prof. Joshua Kretchmer (jkretchmer3@gatech.edu)

Guest lecture at CHEM-3511, Survey in Biochemistry. — Fall 2024

- **At Medical University of Graz:**

General Chemistry Laboratory with first year Medical Students, Practical Instructor — Spring 2022-2023

Mini-Workshop on Molecular Dynamics (MD) simulations — Fall 2023
Ass. Prof. Pedro Sánchez Murcia

Teaching assistance Workshop on Computer-Aided Drug Discovery — Fall 2022
Ass. Prof. Pedro Sánchez Murcia

- **At Universidad Carlos III:**

Guest lecture in Biological Systems — Spring 2021-2022
Ass. Prof. Javier Klett (javier.klett@uc3m.es)

Teaching assistance in Biological Systems — Spring 2020
Ass. Prof. Carlos León (cleon@ing.uc3m.es)

- **At University San Pablo CEU Faculty of Pharmacy:**

Teaching assistance at Master in Drug Discovery, practical lectures — Spring 2015-2021
Prof. Beatriz de Pascual Teresa (bpaster@ceu.es)

*During my Ph.D. (2015-2019) and part of my FPU grant I taught a total of 240 hours in different courses and practicum courses. Prof. Beatriz de Pascual Teresa (bpaster@ceu.es)

Teaching assistance at Organic Chemistry I Laboratory — 2015-2019
Teaching assistance at Pharmaceutical Chemistry I and II Laboratory — 2015-2019
Teaching assistance at Bioinformatics Laboratory — 2015-2019

GRANTS & CONTRACTS

Postdoctoral position, Georgia Institute of Technology, Kamerlin Lab — **2024-present**

Postdoctoral position LS-PHYCHE-2021-001331 — 2022-2024
Medical University of Graz, Division of Medicinal Chemistry

Fundación Martín Escudero Postdoctoral Grant — 2022-2024
Medical University of Graz, Division of Medicinal Chemistry

Sistema Nacional de Garantía Juvenil (SNGJ) 2019-2022
Spanish National Cancer Research Center (CNIO) in the Experimental Therapeutics Program

Full Scholarship from **Spanish government, Ministry of Education** to carry out PhD studies 2016-2019
FPU15/02857

PhD studies in the Department of Chemistry and Biochemistry. San Pablo CEU University 2015
FPI grant

CITIUS Scholarship at GSK Aranda de Duero (Spain) 2015

ERASMUS Student at University of Helsinki (Finland) 2014
MAREX project (EU FP7)

RESEARCH PROJECTS

- **Georgia Tech:**

Protein Tyrosine Phosphatases (PTPs). Investigation of loop dynamics and conformational mechanisms governing catalysis and functional evolution in protein tyrosine phosphatases, using molecular dynamics and enhanced sampling approaches. This project constitutes my main postdoctoral research activity in Prof. Shina C. L. Kamerlin's lab and is supported by the NSF Collaborative Grant *"Conformational Dynamics and Functional Evolution in Protein Tyrosine Phosphatases"* (NSF #2414074; 07/2024–06/2027; GT share $431K), which provides primary financial support for my postdoctoral position.

Polymerase. Elucidation of the catalytic reaction mechanism of DNA polymerase ε using advanced QM/MM and enhanced-sampling simulations, in collaboration with Prof. Erik Johansson at Umeå University (erik.tm.johansson@umu.se). This project forms the basis of my MSCA 2025 Postdoctoral Fellowship application (MSCA-2025-PF 101273744, POLS-4-DESIGN) in collaboration with Dr. Miguel de la Vega (CBM-CSIC), aimed at dissecting the role of water networks in polymerase catalysis and fidelity and translating these mechanistic insights into the rational redesign of the phi29 DNA polymerase toward high-fidelity RNA synthesis.

AMDase. Mechanistic dissection of AMDase regioselectivity across substrates and mutants using QM/MM metadynamics to resolve catalytic pathways and transition states. In collaboration with Prof. Robert Kourist (kourist@tugraz.at). My current work focuses on the *de novo* design of AMDase variants guided by conserved sequence motifs and targeted methionine substitutions using protein MPNN and MM(ML) guided metadynamics. Trought this collaboration, I have been invited as external advisory board at his European PhD programm BiotechPredict (DOC2686925).

SrBDH1. Mechanistic modeling of SrBDH1 catalysis with borneol and isoborneol, combining ML/MM simulations and funnel metadynamics to dissect enantioselective binding and turnover. Conducted with Prof. Robert Kourist (Graz University of Technology). These insights are now driving de novo design strategies to enhance enzyme thermostability without compromising selectivity.

Chemo-enzymatic antibiotic scaffolds. Collaborative project with Dr. Nicole Maria Hauser (nhauser@chem.au.dk) focused on the chemo-enzymatic optimization of nature-inspired antibacterial scaffolds. My contribution centers on QM/MM modeling and enzyme design of glycosyltransferases to elucidate and engineer glycosylation steps relevant for antibacterial activity. This work underpins the Sapere Aude DFF Starting Grant proposal *"Combating Antibiotic Resistance Chemo-Enzymatically with Nature-Inspired Scaffolds"* (requested budget €847K).

Myosine project. Modeling of how oxidative modifications in cardiac myosin affect structural flexibility and contractility, with a focus on specific residue interactions and their impact on motor function. In collaboration with Prof. Lars Larsson (lars.larsson@slu.se) from **Swedish University** and Prof. Kamerlin.

- **Medical University of Graz:**

Orai1-STIM1. Design of de novo binders to inhibit the interface between STIM1 and Orai1 using computational methods such as RFdiffusion, ProteinMPNN, AlphaFold2, and classical molecular dynamics. In collaboration with Prof. Schindl, Rainer (rainer.schindl@medunigraz.at) and Bernadett Bacsa (bernadett.bacsa@medunigraz.at) from the Medical University of Graz, Austria. This work is currently being developed in preparation for an FWF grant application focused on the de novo design of Orai1 mini-binders.

Alphaman2Brescued. Hit identification and discovery of novel positive allosteric modulators (PAMs) and Pharmacological Chaperones (PCs) for the treatment of mannosidosis. LS-PHYCHE-2021-001331. Project lead by, at the **Medical University of Graz**, Austria (pedro.murcia@medunigraz.at).

- **University of Graz:**

ToxR/S. Hit identification and discovery of potential antibiotics in the transcriptional transmembrane proteins ToxR/S from Vibrio Chloera. Collaboration with Dr. Nina Kerstin Gubensäk at University of Graz, Austria (nina.gubensaek@uni-graz.at). This work has led to a pending Austrian priority patent (*A55350/2025*) covering pharmaceutical compositions targeting ToxR/S or related systems, enabling strategic translational and industrial engagement. The project has supported the submission of a Proof-of-Concept grant (*P2514017: "Drug Repurposing – A Rapid Route for the Management of Pandemic Cholera"*, €80K funded of €107K total) and has attracted pharmaceutical industry interest, including engagement via the Inpart platform for potential collaborative and financially supported development.

- **At CNIO:**

Anti-aging discovering. Together with **Refoxy Pharma company**, we aimed to discovery potential anti-aging agents, particularly FOXO activators with novel mechanisms of action, not regulated by inhibition of PI3K or other known kinases or nuclear transport pathways (Patented). Head of Division Dr. Joaquín Pastor (jpastor@cnio.es)

Macrocycles modelling and design against PiK3CA and mTOR. Desing and model specific constrained macrocycles based on compounds under investigation with the aim to increase selectivity in kinases.

- **At CEU San Pablo University:**

PROTACs. Tumor-Targeted Inhibitors and Probes for Cancer Detection and treatment. Funding Body: MICINN (RTI2018-093539-B-I00). Project lead by Prof. Beatriz de Pascual Teresa, at the CEU San Pablo University, Spain. (bpaster@ceu.es)

Dual inhibitors. Multitarget modulators as a strategy for the design of new anticancer agents. MINECO (CTQ2014-52604-R). Project lead by Prof. Beatriz de Pascual Teresa, at the CEU San Pablo University, Spain.

PTPRZ1-inhibitors. Preclinical development of drug antagonists of PTPRZ1 receptor for the prevention of abuse consumption of alcohol. Ministerio de Sanidad (MSSSI). Plan Nacional Sobre Drogas (PNSD2015I001). Project lead by Prof. Gonzalo Herradón, at the CEU San Pablo University, Spain. (gherradon@ceu.es).

CONFERENCES & PRESENTATIONS

- **During my postdoctoral research at Georgia Tech:**

(Oral Presentation) Inversion & Innovation: Redefining C–C Bond Cleavage via Engineered AMDase with a de novo Edge. Bruno Di Geronimo, Gyula Hoffka, Elske van der Pol, Robert Kourist and Shina Caroline Lynn Kamerlin. European Society of Applied Biocatalysis, ESAB Congress 2025. Online, nvember 2025.

(Oral Presentation, Invited) Catalysis by Design: Computing Fundamental Chemical Reactivity. Bruno Di Geronimo and Shina Caroline Lynn Kamerlin. Beilstein Enzymology Symposium, Germany. September 2025.

(Oral Presentation, Invited) Harnessing Computational Methods and Protein Design in the Kamerlin Lab. Bruno Di Geronimo and Shina Caroline Lynn Kamerlin. The BioPhys Mex 2025 Conference Initiative. Ciudad de México, Mexico. May 2025.

(Oral Presentation-Invited) Pols and PRIMPOLs Reimagined: A Computational Roadmap to its mechanism of action, selectivity and fidelity**. Bruno Di Geronimo.** Next-Generation Computational Chemistry: Innovation, Collaboration, and Impact. Georgia Tech College of Sciences, School of Chemistry and Biochemistry. Atlanta, GA, USA. March 2025

(Oral presentation) Computational Insights into the Enforced Concerted Mechanism of AMDase Catalyzed Decarboxylation of Vinylic Substrates. **Bruno Di Geronimo**, Gyula Hoffka, Elske van der Pol, Thomas Schlatzer, Johannes Eder, Anna Schweiger, Marianna Karava, Roland C. Fischer, Daniel Kracher, Dominik Groß, Romas Kazlauskas, Kenji Miyamoto, Rolf Breinbauer, Robert Kourist, Shina Caroline Lynn Kamerlin. Postdoctoral Research Symposium. Georgia Tech College of Sciences, School of Chemistry and Biochemistry. Atlanta, GA, USA. November, 2024.

(Poster) Exploring STIM1-orai interaction. Juan Toledo-Marcos, Kata Horvát, **Bruno Di Geronimo**, Rainer Schindl, Benjamin Bourgeois, Tobias Madl, István Mándity, Pedro A Sánchez-Murcia and Bernadett Bacsa. 17th International Meeting of the European Calcium Society (ECS2024) Homerton College, Cambridge, UK. October 2024

(Oral presentation). Unraveling the Molecular Mechanisms of Alpha-Mannosidosis: Insights from QM/MM-Metadynamics Simulations. **Bruno Di Geronimo**, Shina Lynn Kamerlin, Pedro Sánchez Murcia. Spring Research Symposium. Georgia Tech College of Sciences, School of Chemistry and Biochemistry. Atlanta, GA, USA. June 2024. Awarded: SoCB Research Faculty High-Impact Communication Award (runner-up). chemistry.gatech.edu/postdoc-and-research-scientist-awards

- **During my postdoctoral research at the Medical University of Graz**

Unraveling the Mechanism of Covalent Lysine Attachment to Wortmannin: Insights from QM/MM studies. Jessica Meyr, Bernd Engels, **Bruno Di Geronimo.** 17th international congress of quantum chemistry (Awarded, best poster presentation). Bratislava, Slovakia. June 2023

(Flash presentation) On the pursuing of Chemical Rescuers for mannosidosis by Computer-Aided Molecular Design. **Bruno Di Geronimo** and Pedro A. Sánchez-Murcia. VI GEQB bienal meeting (ChemBioVI). Valencia, Spain. March 2023

(Poster) Allostery prediction of the human lysosomal α-mannosidase, disclosing new cryptic pockets by in silico tools. **Bruno Di Geronimo** and Pedro A. Sánchez-Murcia. "Robert Konrat's 60th: From Dynamics to Disorder and Beyond". Vienna, Austria. August 2022

(Oral presentation) The pathophysiology of alpha-mannosidosis, unveiling the mechanism of action and new cryptic pockets by in silico tools. **Bruno Di Geronimo.** "Frontiers in Integrative Strucural Biology and Biophysics". Medical University of Graz, Austria. Mayo 2022

Unveiling the role of enzyme dynamics on the pathophysiology of alpha-mannosidosis. **Bruno Di Geronimo**, Santiago Alonso-Gil and Pedro A. Sánchez-Murcia. Present and Future of Hybrid Quantum Chemical and Molecular Mechanical Simulations. Lecco, Italy. June 2022.

- **At CNIO**

(Oral presentation and Poster) Computational clustering methods in chemical libraries: development of a protein-protein interaction inhibitor focused library. **Bruno Di Geronimo**, Marina Moreno, Javier Klett. XXVI EFMC International Symposium on Medicinal Chemistry (EFMC-ISMC 2021), virtual event. August 2021. (Granted by the SEQT). Open Access presentation: https://www.youtube.com/watch?v=VJUlKAg-7Ns

- **During my Ph.D**

(Oral presentation) Computer-aided Drug Design based on Phosphatases (PTPRZ, PTPRGamma, PTP1B), Kinases (CK2) and Histone Deacetylases (HDAC1, HDAC6) as drug targets. **Di Geronimo, Bruno.** MedChem2021, Paul Ehrlich Virtual Meeting. June 2021. (**Excellence award**).

(Oral presentation) A proposed PROTAC binding mode in kinases. is an allosteric binding mode possible? **Di Geronimo, Bruno**; Viscovo, Marco; Coderch, Claire; Ramos, Ana & de Pascual-Teresa, Beatriz. National Congress from the Sociedad Española de Química Terapéutica (SEQT). Vitoria, Spain. 17/07/2019. (**Granted by the SEQT**).

(Poster) Behind allosteric pockets in PTPRZ1 & PTPRG. Breakthrough Molecular Dynamics (MD) simulations with mixed organic solvents. **Di Geronimo, Bruno**; Pastor, Miryam; Fernández-Calle, Rosalía; Coderch, Claire; Ramos, Ana; Herradón, Gonzalo & de Pascual-Teresa, Beatriz. MedChemSicily 2018 Italian-Spanish-Portuguese Joint Meeting in Medicinal Chemistry. Sicily, Italy. July 2018. (**Granted by the SEQT**).

(Poster) Behind allosteric pockets in PTPRZ1 & PTPRG. Breakthrough Molecular Dynamics (MD) simulations with mixed organic solvents. **Di Geronimo, Bruno**; Pastor, Miryam; Fernández-Calle, Rosalía; Coderch, Claire; Ramos, Ana; Herradón, Gonzalo & de Pascual-Teresa, Beatriz. MedChemSicily 2018 Italian-Spanish-Portuguese Joint Meeting in Medicinal Chemistry. Sicily, Italy. July 2018. (Granted by the SEQT).

(Oral presentation) Implicit or explicit approach? A DFT calculation of tbb alkylation reaction can be a good example. **B. Di Geronimo**, M. Pastor, C. Coderch, J.M. Zapico, A. Ramos and B. de Pascual-Teresa. V Young Symposium from SEQT. Madrid, Spain. June 2018. (Granted by the SEQT).

(Oral presentation) Pyrrolo[1,2-α]quinoxalines as new small molecules to modulate PTP1B activity by an allosteric mechanism. Javier García-Martín; Mercedes Griera; **Bruno Di Geronimo Quintero**; Patricia Sánchez-Alonso; Manuel, Rodriguez-Puyol; Ramón Alajarin; Beatriz Pascual-Teresa; Diego Rodriguez-Puyol; Julio Álvarez-Builla; Juan José Vaquero. Salamanca, Spain. January 2018.

(Oral presentation) Towards selective phosphatase inhibition: a new PTPRZ1 binding mode proposal promotes rational design of compounds that increase PTPRZ1/PTP1B selectivity. **Bruno Di Geronimo Quintero**; Miryam Pastor; Rosalia Fernández; Claire Coderch; Jose María Zapico; Gonzalo Herradón; Ana Ramos; Beatriz Pascual-Teresa. 18th Meeting of the Spanish Society of Medicinal Chemistry. Salamanca, Spain. January 2018 (Granted by the SEQT).

(Poster) DUAL INHIBITORS OF CK2 AND HDAC1: Multi-target drug discovery for infectious diseases. Regina Martínez; David Martin; Jose María Zapico; Claire Coderch; **Bruno Di Geronimo Quintero**; Beatriz Pascual-Teresa; Ana Ramos. 2nd Symposium on Medicinal Chemistry for Global Health. Madrid, Spain. June 2017.

(Poster) Novel drug discovery strategy against alcoholism, in silico approach to the Protein Tyrosine Phosphatase Receptor Z1 (PTPRZ1). **Bruno Di Geronimo**; Claire Coderch; Ana María Ramos; Beatriz Pascual-Teresa. 6th Meeting of the Paul Ehrlich Medchem Euro-phd network MUTALIG COST ACTION (CA15135) MEETING. Budapest, Hungary. November 2016.

(Poster) Exploring the Protein Tyrosin Phosphatase Receptor Z1 (PTPRZ1) in the search for new selective inhibitors for the prevention of alcohol abuse. **Bruno Di Geronimo**; Claire Coderch; Ana María Ramos; Beatriz Pascual-Teresa. 6th EuCheMS Chemistry Congress. Seville, Spain. September 2016.

(Poster and selected oral presentation) Novel approximation for alcoholism treatment through Protein Tyrosine Phosphatase Receptor Z1 modulation: Computer based design and discovery of small molecule drug candidates. **Bruno Di Geronimo**; Claire Coderch; Ana María Ramos; Beatriz de Pascual-Teresa. XXXVI ESMEC 2016 European School of Medicinal Chemistry. Urbino, Italy. June 2016. (Granted by the EFMC).

(Poster) Search for new selective inhibitors for alcoholism through virtual screening workflow, exploring the Protein Tyrosine Phosphatase Receptor Z1 (PTPRZ1). **Bruno Di Geronimo**; Claire Coderch; Beatriz de Pascual-Teresa. Medicinal Chemistry in Drug Discovery: The Pharma Perspective. Barcelona, Spain. June 2016. (Granted by the SEQT)

PEER-REVIEWED

https://www.webofscience.com/wos/author/record/R-2454-2018

https://orcid.org/0000-0003-1822-7142

- Nature communications (2)
- Protein Science (14)
- Journal of chemical theory and computation (1)
- Journal of chemical information and modeling (1)
- PLOS Computational Biology (5)
- Journal of biotechnology (2)
- Computational and Structural Biotechnology Journal (1)
- Chemistry & Biodiversity (3)
- ChemBioChem (5)
- ACS omega (3)

ACADEMIC SERVICES

Communication Captain at Kamerlin lab 2023-present

BiocatcodeExpander: Seminar about: Introduction of Molecular Dynamics. Berlin, Germany. 2024
https://biocatcodeexpander.com/ Ass. Prof. Ivana Drienovska (i.drienovska@vu.nl)

ENGAGES program at Georgia Institute of Technology: https://projectengages.gatech.edu/ 2024-2025

Atlanta Science festival, *"Imaging the Future"* 2024
Science ATL (alvaro@scienceatl.org)

Participation in the Doctoral Courses at Medical University of Graz (MolMed) 2022-2024

President of the committee Member 6th Young Researchers Symposium (Madrid, Spain) 2019
https://sites.google.com/view/yrs2019/home

Committee Member 7th Young Researchers Symposium. (Online event) 2020
https://sites.google.com/ucm.es/yrs-2021/home

Member of the SEQT (Spanish Society of Medicinal Chemistry) 2015-2022

Member of the RSEQ (Spanish Royal Society of Chemistry) 2016-present

Member of the CEINDO (CEU International School of Doctoral Studies) quality committee 2016-2020

- **Mentorship**

Ph.D. student: Gyula Hofka, Medical University University of Debrecen (hoffka.gyula@med.unideb.hu)

Ph.D. student: Juan Toledo Marcos, Medical University of Graz, Austria (juan.toledo-marcos@stud.medunigraz.at)

Ph.D. student: Gyula Hoffka, University of Debrecen, Hungary (hoffka.gyula@med.unideb.hu)

Master student (Biochemistry): Lukas Toth, Uppsala University, Sweeden (toth.lukacs.domokos@gmail.com)

Master student (Bioinformatics): Aaryesh Deshpande, Georgia Tech, USA (aaryeshad@gatech.edu)

Master student (Bioinformatics): Lucy Johns, Georgia Tech, USA (ljaisga9906@gmail.com)

Pregraduate student (Biochemistry): Sara M Dixon, Georgia Tech, USA (sdixon61@gatech.edu)

High School (ENGAGES program): Cordarius C. Williams, Mr. Richard Woods, State School, Georgia, Atlanta (cwilliams620@gatech.edu)

PROFESSIONAL DEVELOPMENT

1st EuChemS Chemical Biology School on Computational Chemical Biology 2025

Tech-to-Teaching Program 2025
(https://ctl.gatech.edu/tech-teaching)

ENGAGE Program 2024-2025

Mentoring Programme EFMC (European Federation of Medicinal Chemistry) 2022

EURORDIS Open Academy School on Medicines Research & Development 2021

Virtual Vienna Summer School on Drug Design 2021. Online event. 2021

Symposium Centennial of the Spanish Flu of 1918. 2018
Fundación Ramón Areces. Madrid, Spain

Symposium "Bioinformática estructural Ángel Ramírez Ortiz (in memoriam)" 2018
CBM Severo Ochoa. Madrid, Spain

Scientific Workshop Massive Computation for Ultrafast Molecular Breaking, MACUMB 2017
Red Española de Supercomputación (RES). Madrid, Spain

In silico tools in drug design and target discovery workshop. 2016
FIB Barcelona, Red Española de Supercomputación (RES). Barcelona, Spain

- **Courses:**

Large Language Models and their applications in Bioinformatics EMBO

PACE Trainings at Georgia Tech (https://pace.gatech.edu/pace-trainings/):
Python 101: Intro to Data Analysis with NumPy
Linux 101 & 102
Application of Machine Learning

ACS courses:
ACS Reviewer Lab

Medical University of Graz courses:
Induction course for New Supervisors of Doctoral Candidates

EdeX courses:
Introduction to Linux. LinuxFoundationX - LFS101x
Principles, Statistical and Computational Tools for Reproducible Data Science. HarvardX - PH527x

CEINDO courses during PhD (https://www.escueladoctorado.ceu.es/en/):
Training courses in experimental techniques: Technique: Statistics applied to research; X-ray technique
Ethical use of scientific documentation
Evaluation and assessment of scientific production
Advanced Search and Documentation Management Techniques applied to research