

Ariela Patricia Vergara Jaque, PhD
Associate Professor, Faculty of Engineering, Universidad de Talca, Chile

CONTACT
INFORMATION

Email: arvergara@utalca.cl
Date of Birth: October 9, 1984
Nationality: Chilean

Address: Center for Bioinformatics
Simulation and Modeling. Av. Lircay s/n,
Talca, Chile
Phone: +56 9 4492 3917

EDUCATION

Course "Innovative Leadership: Transforming Higher Education in the Digital Age", organized by the IAP – International Academic Program with institutional support from Universidad Autónoma de Madrid (UAM) in collaboration with The David Rockefeller Center for Latin American Studies at Harvard University. Campus of Harvard University in Cambridge, MA, USA **(2023)**

Diploma in Competency-Based Education, Universidad de Talca, Talca–Chile **(2017)**

PhD. in Applied Sciences, Universidad de Talca, Talca–Chile **(2009 – 2013)**

Thesis: "Dendritic nanoparticles used as an optimal mechanism for transport and controlled delivery of drugs"

Thesis advisor: Dra. Claudia Sandoval and Dr. Leonardo Silva Santos

Date of graduation: September, 2013

Bioinformatics Engineer, Universidad de Talca, Talca–Chile **(2003 – 2009)**

Thesis: "Structural and electrostatic properties in the ion conduction pathway of *Shaker* potassium channel"

Thesis advisor: Dr. Danilo González-Nilo and Dr. David Naranjo

Date of graduation: January, 2009

RESEARCH AREA

Integrative modeling and simulation of biomolecular systems

I have extensive experience in applying computational approaches to study biomolecular systems, with a particular focus on membrane proteins, which play essential roles in numerous cellular processes and represent important targets for therapeutic intervention. My research group employs advanced methodologies in bioinformatics, molecular modeling, and molecular dynamics simulations to investigate biomolecular interactions, including protein–ligand and protein–protein interactions. These approaches enable us to characterize molecular mechanisms and support the rational design of drug-like molecules that target specific biological pathways.

HIGHER EDUCATION
ADMINISTRATION

Research, development, and innovation

I have served as a senior executive in the field of innovation, leading initiatives to strengthen research, development, innovation, and technology transfer at the University of Talca. My work has focused on fostering a culture of intellectual property, supporting the commercialization of research results, and promoting science- and technology-based entrepreneurship. In addition, I have actively contributed to national initiatives aimed at advancing the digital transformation of higher education institutions in Chile.

PROFESSIONAL
EXPERIENCE

Director of the Graduate School of the Faculty of Engineering (2026 – present)
Universidad de Talca, Chile.

Associate Professor (2024 – present)

Center for Bioinformatics, Simulation and Modeling (CBSM), Bioinformatics Department, Faculty of Engineering, Universidad de Talca, Chile.

Research area: Integrative modeling and simulation of biomolecular systems.

Director of Innovation and Technology Transfer (2024 – 2026)

Universidad de Talca, Chile.

Executive Secretary of Metared TIC-Chile (2023 – 2026)

Santander Universidades, Chile.

Vice Chancellor of Innovation (2022 – 2024)

Universidad de Talca, Chile.

Director of the Bioinformatics School (2020 – 2022)

Faculty of Engineering, Universidad de Talca, Chile.

Assistant Professor (2017 – 2024)

Center for Bioinformatics, Simulation and Modeling (CBSM), Bioinformatics Department, Faculty of Engineering, Universidad de Talca, Chile.

Research area: Computational structural biology applied to membrane proteins.

Postdoctoral Researcher (2015 – 2017)

Institute of Computational Comparative Medicine, Nanotechnology Innovation Center of Kansas State. Department of Anatomy and Physiology, Kansas State University, USA.

Supervisor: Dr. Jeffrey Comer

Research area: Molecular modeling and molecular dynamics simulation of membrane proteins.

Interactions between biomolecules and nanomaterials.

Postdoctoral Researcher (2014 – 2015)

Computational Structural Biology Section, National Institute of Neurological Disorders and Stroke, National Institutes of Health, USA.

Supervisor: Dr. Lucy Forrest

Research area: Exploring the structural basis of membrane transporters function through computational methods.

Research Assistant (2013 – 2014)

Center for Bioinformatics and Molecular Simulations, Universidad de Talca, Chile.

Supervisor: Dra. Wendy González

Research area: Design and evaluation of inhibitors for ion channels.

PEER-REVIEWED
JOURNAL ARTICLES

48. De-la-Torre P, Valencia M, Gálvez J, Flores del Pino V, Gómez del Campo A, Romero S, Mendoza E, Rinné S, Kiper A, Prent L, **Vergara-Jaque A**, Mazola Y, Olivera-Fuentes C, Zúñiga R, Márquez Montesinos J, Rojas B, Peña L, Quiroga J, Pertusa M, Decher N, Zúñiga L, González W and Madrid R. The TASK-1 and TASK-3 activator JG-C3-98 attenuates cold and mechanical responses in primary somatosensory neurons. *Front. Pharmacol.* Volume 17 - 2026. doi.org/10.3389/fphar.2026.1844406.
47. Rosales-Rojas R, Fernández C, González-Avendaño M, **Vergara-Jaque A**, Cáceres M. Targeting Protein-Protein Interactions (PPIs) to Drive Functional Annotation: An Integrative Methodology to Study Senescence-Associated PPIs Using TMPRSS11a as Model Interactor. *Biomolecules*. 2026 May 13;16(5):714. doi: 10.3390/biom16050714.
46. González-Avendaño M, Rosales-Rojas R, **Vergara-Jaque A**. Computational Mapping and Targeting of BK Channel Protein-Protein Interactions in Breast Cancer. *J Chem Inf Model*. 2026 Apr 13;66(7):3999-4011. doi: 10.1021/acs.jcim.6c00191. Epub 2026 Mar 17.
45. EPeña-Vilches N, González-Avendaño M, Soto-García N, Maureira D, Silva I, Avilés J, Manríquez-Benítez E, Medina E, Cerda O, Galaz-Davison P, **Vergara-Jaque A**. Identification of 14-3-3 Proteins as Binding Partners of TRP Channels. *J Chem Inf Model*. 2026 Apr 13;66(7):3987-3998. doi: 10.1021/acs.jcim.6c00092. Epub 2026 Mar 16.

44. Espinoza-Arcos LG, González-Avendaño M, Zuñiga-Bustos M, Zamora RA, **Vergara-Jaque A**, Poblete H. Exploring a peripheral PIP2-binding site and its role in the alternative regulation of the TRP channel superfamily. *J Gen Physiol.* 2025 Nov 3;157(6):e202413574. doi: 10.1085/jgp.202413574.
43. Sánchez-Hernández R, Benítez-Angeles M, Talyzina IA, Llorente I, González-Avendaño M, Sierra F, Méndez-Reséndiz A, Mercado F, **Vergara-Jaque A**, Sobolevsky AI, Islas LD, Rosenbaum T. Structural basis of the inhibition of TRPV1 by analgesic sesquiterpenes. *Proc Natl Acad Sci U S A.* 2025 Jul 22;122(29):e2506560122. doi: 10.1073/pnas.2506560122.
42. Lavanderos B, Orellana-Serradell O, Maureira D, Cruz P, Silva I, Toledo J, González-Avendaño M, López J, Santos R, Arancibia F, Varela D, Cáceres M, **Vergara-Jaque A**, Cerda O. Rhotekin-1 is a novel interacting protein and regulator of TRPC6 activity. *FASEB J.* 2025 Mar 2. doi: 10.1111/febs.70028.
41. González-Avendaño M, López J, **Vergara-Jaque A***, Cerda O. The power of computational proteomics platforms to decipher protein-protein interactions. *Curr Opin Struct Biol.* 2024 Jul 13;88:102882. doi: 10.1016/j.sbi.2024.102882.
40. Bravo-Moraga F, Bedoya M, **Vergara-Jaque A**, Alzate-Morales J. Understanding the Differences of Danusertib's Residence Time in Aurora Kinases A/B: Dissociation Paths and Key Residues Identified using Conventional and Enhanced Molecular Dynamics Simulations. *J Chem Inf Model.* 2024 Jun 24;64(12):4759-4772. doi: 10.1021/acs.jcim.4c00387.
39. Adriana V. Treuer, Mario Faúndez, Roberto Ebensperger, Erwin Hovelmeyer, **Ariela Vergara-Jaque**, Yunier Perera-Sardiña, Margarita Gutierrez , Roberto Fuentealba and Daniel R. Gonzalez. New NADPH Oxidase 2 Inhibitors Display Potent Activity against Oxidative Stress by Targeting p22phox-p47phox Interactions. *Antioxidants (Basel).* 2023 Jul 18;12(7):1441. doi: 10.3390/antiox12071441.
38. Benitez-Angeles M, Romero AEL, Llorente I, Hernandez-Araiza I, **Vergara-Jaque A**, Real FH, Gutierrez Castaneda OE, Arciniega M, Morales-Buenrostro LE, Torres-Quiroz F, Garcia-Villegas R, Tovar-Y-Romo LB, Liedtke WB, Islas LD, Rosenbaum T. Modes of action of lysophospholipids as endogenous activators of the TRPV4 ion channel. *J Physiol.* 2023 Jan 9. doi: 10.1113/JP284262.
37. Benitez-Angeles M, Juarez-Gonzalez E, **Vergara-Jaque A**, Llorente I, Rangel-Yescas G, Thebault SC, Hiriart M, Islas LD, Rosenbaum T. Unconventional interactions of the TRPV4 ion channel with beta-adrenergic receptor ligands. *Life Sci Alliance.* 2022 Dec 22;6(3):e202201704. doi: 10.26508/lsa.202201704.
36. Bustos D, Hernandez-Rodriguez EW, Poblete H, Alzate-Morales J, Challier C, Boetsch C, **Vergara-Jaque A***, Beassoni P. Structural Insights into the Inhibition Site in the Phosphorylcholine Phosphatase Enzyme of Pseudomonas aeruginosa. *J Chem Inf Model.* 2022 Jun 27;62(12):3067-3078. doi: 10.1021/acs.jcim.2c00059.
35. Peña-Varas C, Kanstrup C, **Vergara-Jaque A**, Gonzalez-Avendano M, Crocoll C, Mirza O, Dreyer I, Nour-Eldin H, Ramirez D. Structural Insights into the Substrate Transport Mechanisms in GTR Transporters through Ensemble Docking. *Int J Mol Sci.* 2022 Jan 29;23(3):1595. doi: 10.3390/ijms23031595.
34. Rossino G, Rui M, Linciano P, Rossi D, Boiocchi M, Peviani M, Poggio E, Curti D, Schepmann D, Wünsch B, González-Avendaño M, **Vergara-Jaque A**, Caballero J, Collina S. Bitopic Sigma 1 Receptor Modulators to Shed Light on Molecular Mechanisms Underpinning Ligand Binding and Receptor Oligomerization. *J Med Chem.* 2021 Oct 28;64(20):14997-15016. doi: 10.1021/acs.jmedchem.1c00886. Epub 2021 Oct 8.
33. González-Avendaño M, Zúñiga-Almonacid S, Silva I, Lavanderos B, Robinson F, Rosales-Rojas R, Durán-Verdugo F, González W, Cáceres M, Cerda O, **Vergara-Jaque A***. PPI-MASS:

- An Interactive Web Server to Identify Protein-Protein Interactions From Mass Spectrometry-Based Proteomics Data. *Front Mol Biosci*. 2021 Jul 1;8:701477. doi: 10.3389/fmolb.2021.701477. eCollection 2021.
32. Fernandez C, Burgos A, Morales D, Rosales-Rojas R, Canelo J, **Vergara-Jaque A**, Vieira GV, da Silva RAA, Sales KU, Conboy MJ, Bae EJ, Park KS, Torres VA, Garrido M, Cerda O, Conboy IM, Cáceres M. TMPRSS11a is a novel age-altered, tissue specific regulator of migration and wound healing. *FASEB J*. 2021 May;35(5):e21597. doi: 10.1096/fj.202002253RRR.
 31. Comer J, Bassette M, Burghart R, Loyd M, Ishiguro S, Azhagiya Singam ER, **Vergara-Jaque A**, Nakashima A, Suzuki K, Geisbrecht BV, Tamura M. Beta-1,3 Oligoglucans Specifically Bind to Immune Receptor CD28 and May Enhance T Cell Activation. *Int J Mol Sci*. 2021 Mar 18;22(6):3124. doi: 10.3390/ijms22063124.
 30. Rojas G, Orellana I, Rosales-Rojas R, García-Olivares J, Comer J, **Vergara-Jaque A***. Structural Determinants of the Dopamine Transporter Regulation Mediated by G Proteins *J Chem Inf Model*. 2020 Jul 27;60(7):3577-3586. doi: 10.1021/acs.jcim.0c00236.
 29. Rivas J, Díaz N, Silva I, Morales D, Lavanderos B, Álvarez A, Saldías MP, Pulgar E, Cruz P, Maureira D, Flores G, Colombo A, Blanco C, Contreras HR, Jaña F, Gallegos I, Concha ML, **Vergara-Jaque A**, Poblete H, González W, Varela D, Trimmer JS, Cáceres M, Cerda O. KCTD5, a novel TRPM4-regulatory protein required for cell migration as a new predictor for breast cancer prognosis. *FASEB J*. 2020 Jun;34(6):7847-7865. doi: 10.1096/fj.201901195RRR.
 28. Sarkar SK, Foo ACY, Matyas A, Asikhia I, Kosenko T, Goto NK, **Vergara-Jaque A**, Lagace TA. A transient amphipathic helix in the prodomain of PCSK9 facilitates binding to low-density lipoprotein particles. *J Biol Chem*. 2020 Feb 21;295(8):2285-2298.
 27. Rossino G, Orellana I, Caballero J, Schepmann D, Wünsch B, Rui M, Rossi D, González-Avendaño M, Collina S, **Vergara-Jaque A***. New Insights into the Opening of the Occluded Ligand-Binding Pocket of Sigma1 Receptor: Binding of a Novel Bivalent RC-33 Derivative. *J Chem Inf Model*. 2019 Dec. doi: 10.1021/acs.jcim.9b00649.
 26. Dreyer I, **Vergara-Jaque A**, Riedelsberger J, González W. Exploring the fundamental role of potassium channels in novel model plants. *J Exp Bot*. 2019 Nov; 70(21):5985-5989. doi: 10.1093/jxb/erz413.
 25. Riedelsberger J, **Vergara-Jaque A**, Piñeros M, Dreyer I, González W. An extracellular cation coordination site influences ion conduction of OsHKT2;2. *BMC Plant Biol*. 2019 Jul; 19(1):316. doi: 10.1186/s12870-019-1909-5.
 24. **Vergara-Jaque A**, Palma-Cerda F, Lowet AS, de la Cruz Landrau A, Poblete H, Sukharev A, Comer J, Holmgren M. A structural model of the inactivation gate of voltage activated potassium channels. *Biophys J*. 2019 Jul; 17(2):377-387. doi: 10.1016/j.bpj.2019.06.008.
 23. Blanco C, Morales D, Mogollones I, **Vergara-Jaque A**, Vargas C, Alvarez A, Riquelme D, Leiva-Salcedo E, Gonzalez W, Morales D, Maureira D, Aldunate I, Caceres M, Varela D and Cerda O. EB1- and EB2-dependent anterograde trafficking of TRPM4 regulates focal adhesion turnover and cell invasion. *FASEB J*. 2019 Aug; 33(8):9434-9452. doi: 10.1096/fj.201900136R.
 22. Carrasco-Sanchez V, Marican A, **Vergara-Jaque A**, Folch-Cano C, Comer J, Laurie VF. Polymeric substances for the removal of ochratoxin A from red wine followed by computational modeling of the complexes formed. *Food Chem*. 2018 Nov; 265:159-164. doi: 10.1016/j.foodchem.2018.05.089.
 21. Mena-Ulecia K, Gonzalez-Norambuena F, **Vergara-Jaque A**, Poblete H, Tiznado W, Caballero J. Study of the affinity between the protein kinase PKA and homoarginine-containing peptides derived from kemptide: Free energy perturbation (FEP) calculations. *J Comput Chem*. 2018 Feb; 39(16):986-992. doi: 10.1002/jcc.25176.
 20. **Vergara-Jaque A**, Fong P, Comer J. Iodide Binding in Sodium-Coupled Cotransporters. *J Chem Inf Model*. 2017 Nov; 57(12):3043-3055. doi: 10.1021/acs.jcim.7b00521.

19. Vergara-Jaque A, Comer J, Sepulveda-Boza S, Santos LS, Mascayano C, Sandoval-Yañez C. Study of specific interactions in inclusion complexes of amine-terminated PAMAM dendrimer/flavonoids by experimental and computational methods. *Int J Polym Mater*. 2017 Jan; 66(10):485-494. doi: 10.1080/00914037.2016.1252345.
18. Yaffe D, Vergara-Jaque A, Shuster Y, Listov D, Meena S, Singh SK, Forrest LR, Schuldiner S. Emulating proton-induced conformational changes in the vesicular monoamine transporter VMAT2 by mutagenesis. *Proc Natl Acad Sci U S A* 2016 Nov; 113(47):E7390-E7398. doi: 10.1073/pnas.1605162113.
17. Mulligan C, Fenollar-Ferrer C, Fitzgerald GA, Vergara-Jaque A, Kaufmann D, Li Y, Forrest LR, Mindell JA. The bacterial dicarboxylate transporter VcINDY uses a two-domain elevator-type mechanism. *Nat Struct Mol Biol*. 2016 Mar; 23(3):256-63. doi: 10.1038/nsmb.3166.
16. Comer J, Chen R, Poblete H, Vergara-Jaque A, Riviere JE. Predicting adsorption affinities of small molecules on carbon nanotubes using molecular dynamics simulation. *ACS Nano*. 2015 Dec; 9(12):11761-74. doi: 10.1021/acsnano.5b03592.
15. Vergara-Jaque A, Fenollar-Ferrer C, Mulligan C, Mindell JA, Forrest LR. Family resemblances: A common fold for some dimeric ion-coupled secondary transporters. *J Gen Physiol*. 2015 Nov; 146(5):423-34. doi: 10.1085/jgp.201511481.
14. Vergara-Jaque A, Fenollar-Ferrer C, Kaufmann D, Forrest LR. Repeat-swap homology modeling of secondary active transporters: updated protocol and prediction of elevator-type mechanisms. *Front Pharmacol*. 2015 Sep; 6:183. doi: 10.3389/fphar.2015.00183.
13. Mansour-Hendili L, Blanchard A, Pottier NL, Roncelin I, Lourdel S, Treard C, González W, Vergara-Jaque A, Morin G, Colin E, et al. Mutation update of the Clcn5 gene responsible for dent disease. *Hum Mutat*. 2015 Aug; 36(8):743-52. doi: 10.1002/humu.22804.
12. Guerra FP, Reyes L, Vergara-Jaque A, Campos C, Gutiérrez A, Pérez R, Blaudez D, Ruíz S. Populus deltoides Kunitz trypsin inhibitor 3 confers metal tolerance and binds copper, revealing a new defensive role against heavy metal stress. *Environmental and Experimental Botany*. 2015 Jul; 115:28-37. doi:10.1016/j.envexpbot.2015.02.005.
11. Yaffe D, Vergara-Jaque A, Shuster Y, Listov D, Meena S, Singh SK, Forrest LR, Schuldiner S. Functionally important carboxyls in a bacterial homologue of the Vesicular Monoamine Transporter (VMAT). *J Biol Chem*. 2014 Dec; 289(49):34229-40. doi: 10.1074/jbc.M114.607366.
10. Mena-Ulecia K, Vergara-Jaque A, Poblete H, Tiznado W, Caballero J. Study of the affinity between the protein Kinase PKA and peptide substrates derived from Kemptide using molecular dynamics simulations and MM/GBSA. *PLoS One*. 2014 Oct; 9(10):e109639. doi: 10.1371/journal.pone.0109639.
9. Carrasco-Sánchez V, Vergara-Jaque A, Zuñiga M, Comer J, John A, Nachtigall FM, Valdes O, Duran-Lara EF, Sandoval C, Santos LS. In situ and in silico evaluation of amine- and folate-terminated dendrimers as nanocarriers of anesthetics. *Eur J Med Chem*. 2014 Feb; 73:250-7. doi: 10.1016/j.ejmech.2013.11.040.
8. Vergara-Jaque A, Comer J, Monsalve L, González-Nilo FD, Sandoval C. Computationally efficient methodology for atomic-Level characterization of dendrimer-drug complexes: A comparison of amine- and acetyl-terminated PAMAM. *J Phys Chem B*. 2013 Jun; 117(22):6801-13. doi: 10.1021/jp4000363.
7. Moscoso C, Vergara-Jaque A, Márquez-Miranda V, Sepúlveda RV, Valencia I, Díaz-Franulic I, González-Nilo F, Naranjo D. K⁺ conduction and Mg²⁺ blockade in a *Shaker* Kv-channel single point mutant with an unusually high conductance. *Biophys J*. 2012 Sep; 103(6):1198-207. doi: 10.1016/j.bpj.2012.08.015.
6. Vergara-Jaque A, Poblete H, Lee EH, Schulten K, González-Nilo F, Chipot C. Molecular basis of drug resistance in A/H1N1 virus. *J Chem Inf Model*. 2012 Oct; 52(10):2650-6. doi: 10.1021/ci300343w. **Cover Art of the Journal.**

5. Muñoz C, Adasme F, Alzate-Morales JH, **Vergara-Jaque A**, Kniess T, Caballero J. Study of differences in the VEGFR2 inhibitory activities between semaxanib and SU5205 using 3D-QSAR, docking, and molecular dynamics simulations. *J Mol Graph Model*. 2012 Feb; 32:39-48. doi: 10.1016/j.jmgm.2011.10.005.
4. Caballero J, Alzate-Morales JH, **Vergara-Jaque A**. Investigation of the differences in activity between hydroxycycloalkyl N1 substituted pyrazole derivatives as inhibitors of B-Raf kinase by using docking, molecular dynamics, QM/MM, and fragment-based de novo design: study of binding mode of diastereomer compounds. *J Chem Inf Model*. 2011 Nov; 51(11):2920-31. doi: 10.1021/ci200306w.
3. Alzate-Morales JH, **Vergara-Jaque A**, Caballero J. Computational study on the interaction of N1 substituted pyrazole derivatives with B-raf kinase: an unusual water wire hydrogen-bond network and novel interactions at the entrance of the active site. *J Chem Inf Model*. 2010 Jun; 50(6):1101-12. doi: 10.1021/ci100049h.
2. Caballero J, **Vergara-Jaque A**, Fernández M, Coll D. Docking and quantitative structure-activity relationship studies for sulfonyl hydrazides as inhibitors of cytosolic human branched-chain amino acid aminotransferase. *Mol Divers*. 2009 Nov; 13(4):493-500. doi: 10.1007/s11030-009-9140-1.
1. Alzate-Morales JH, Caballero J, **Vergara Jaque A**, González Nilo FD. Insights into the structural basis of N2 and O6 substituted guanine derivatives as cyclin-dependent kinase 2 (CDK2) inhibitors: prediction of the binding modes and potency of the inhibitors by docking and ONIOM calculations. *J Chem Inf Model*. 2009 Apr; 49(4):886-99. doi: 10.1021/ci8004034.

BOOK CHAPTERS

1. **A Vergara-Jaque**, M Zúñiga, H Poblete. Computational Methodologies for Exploring Nano-engineered Materials. *Nanoengineering Materials for Biomedical Uses*, 2019, pages 57-79. Springer, Cham.

GRANTS

- FONDECYT Regular N° 1260205 (**2026-2030**). Structure-based engineering of toxin-derived peptides for therapeutic applications: a strategy inspired by protein-protein interactions modulating ion channels. **Principal Investigator**. Amount: CLP \$270,000,000.
- FONDECYT Regular N° 1260886 (**2026-2030**). Disrupting Antibiotic Resistance in *Pseudomonas aeruginosa*: Peptide Inhibitors Targeting the Assembly of the OprM protein with the MexAB, MexXY, MexCD and MexEF efflux pumps. **Co-Investigator**.
- EXPLORACION N° 13250060 (**2025-2029**). Targeting ABC transporters with peptide-based strategies to combat hospital-acquired infections caused by *Staphylococcus aureus* and *Klebsiella pneumoniae*. **Principal Investigator**. Amount: CLP \$384,000,000.
- OTL (**2023-2027**). OTL UTalca: Consolidación de la Oficina de Transferencia y Licenciamiento de la Universidad de Talca. **Director**.
- FONDECYT Postdoctorate N° 3240319 (**2024-2027**). Molecular basis behind channel regulation: structure and dynamics of the TRPM4 and 14-3-3gamma interaction. **Sponsoring Researcher**.
- InES CD54 (**2022-2024**). Transformando la innovación basada en ciencia hacia un enfoque transdisciplinario con perspectiva de género para resolver problemas complejos desde el territorio, con un horizonte 2030. **Director**.
- FONDECYT Regular N°1220110 (**2022-2026**). Structural and functional properties regulating the association of TRP channels and 14-3-3 proteins: new insights into protein-protein interactions for drug discovery. **Principal Investigator**. Amount: CLP \$266,246,000.
- FONDECYT Regular N°1221308 (**2022-2026**). TRPV3 and Cav3.2 channels interaction modulates cortical granule release and polyspermy blockade in mammalian eggs. **Co-Investigator**.

- FONDECYT Regular N°1211143 (**2021-2025**). Computational nanotechnology: rational design of peptide-based functional biomaterials to enhance molecular recognition. **Co-investigator**.
- CONICYT International Networking between Research Centers N°190025 (**2019-2021**). In-SecTr-International Network to Study Secondary Metabolite Transport in Plants. **Associated Researcher**.
- NVIDIA Academic GPU (**2018**). Exploring the structural basis of membrane transporter dysfunction through computational methods. **Principal Investigator**. *Donation*: NVIDIA Titan Xp graphics card for research purposes.
- FONDECYT Postdoctorate N° 3180484 (**2018-2021**). Heteroaryl-acrylonitrile derivatives as inhibitors of NADPH Oxidases in an isoform-specific manner. **Sponsoring Researcher**.
- FONDECYT research initiation N° 11170223 (**2017-2020**). Exploring the structural basis of membrane transporter dysfunction associated with neural and endocrine diseases. **Principal Investigator**. *Amount*: CLP \$104,400,000.
- Millennium Nucleus of Ion Channels-Associated Diseases (MiNICAD) (**2017-2023**). **Young Investigator**.
- Universidad de Talca research support (**2017-2020**). Desarrollo Núcleo Científico Multidisciplinario. **Principal Investigator**. *Amount*: CLP \$15,000,000.

AWARDS AND HONORS

- Recognized in the “Periodic Table of Chilean Women Scientists 2026,” an initiative promoted by the Library of the National Congress (BCN), highlighting 118 researchers for their contributions to scientific development. (**2026**)
- “Visionary Women 2025” Recognition, Direction of Innovation and Technology Transfer, University of Talca. (**2025**)
- Recognized as “Pioneer Woman Engineer in Chile” 2025 by the *Mujeres Ingenieras de Chile* program (**2025**)
- Winner of Santander W50 Chile 2025, the prestigious international women’s leadership program (**2025**)
- Project FONDECYT Regular N°1220110, reviewed by Evaluation Group BIOLOGY 3, ranked 1st place (**2022**)
- Nominated by Columbus Association for participation in the 68th Lindau Nobel Laureate Meeting, Lindau, Germany (**2018**)
- Project FONDECYT research initiation 11170223, reviewed by Evaluation Group BIOLOGY 3, ranked 1st place. (**2017**)
- L’Oréal-UNESCO award “International Rising Talent” (**2015**)
- L’Oréal Chile-UNESCO award “For Women in Science” (**2013**)
- CONICYT PhD thesis support (**2012 – 2013**)
- CONICYT doctoral fellowship (**2011 – 2013**)
- Universidad de Talca doctoral fellowship (**2009 – 2010**)

INVITED TALKS

- 3rd Student Research Congress of the Maule Region, University of Talca. (**2025**)
- Conesul Symposium on Biomolecular Simulations - CSBS, together with the XII Regional Symposium of the SBB (Sociedade Brasileira de Biofísica). “Understanding the impact of protein-protein interactions on TRP ion channel function: A computational approach”. Vergara-Jaque A. Porto Alegre, Brasil (**2023**)
- Talk for doctors specializing in Nuclear Medicine at the Chilean Nuclear Energy Commission. “Computational simulation of biological systems for therapeutic purposes”. (**2022**)

- IIBM extraordinary - Seminar. “Computational approaches to study protein-protein interactions regulating the expression of membrane proteins”. Pontificia Universidad Católica de Chile **(2022)**
- MM Col Seminars. “Computational approaches to study protein-protein interactions regulating the expression of membrane proteins”. Molecular Modeling Colombia **(2021)**
- First Scientific Outreach Conference KawScience, “Simulation of Biological Systems using Computational Tools”. Universidad Yachay Tech - Ecuador **(2021)**
- III International Symposium on Integrative Bioinformatics. “Protein-protein interactions regulating the function of ion channels and membrane transporters”. Pucon, Chile **(2019)**
- Protein Biophysics at the End of the World (PBATEOTW). “Protein-protein interactions regulating the function of ion channels and membrane transporters”. Montevideo, Uruguay **(2019)**
- First International Conference on Research, Innovation and Technology. “Strategies for the search of therapeutic targets to combat neurological disorders”. Lima, Perú **(2018)**
- Department of Biochemistry, Microbiology and Immunology, University of Ottawa Heart Institute. “Computational structural biology methods applied to membrane proteins”. Ottawa, Canada **(2018)**
- Institute of Biological Sciences, Universidad de Talca. “Molecular basis of the mechanism of *Shaker* potassium channel inactivation”. Talca, Chile **(2017)**
- Department of Anatomy and Physiology, Institute of Computational Comparative Medicine, Kansas State University. “A structural model of the inactivation gate of voltage activated potassium channels”. Manhattan, Kansas, USA **(2016)**
- First International Conference in Bioinformatics, Simulation and Modeling. “Predicting transport mechanisms in membrane proteins through the repeat-swap homology modeling technique”. Talca, Chile **(2015)**
- International Seminar Germany-Chile: From Plant Biology to Computational Chemistry and Molecular Bioinformatics. “Dendritic nanoparticles used as an optimal mechanism for transport and controlled drug delivery”. Talca, Chile **(2013)**
- Workshop of Computational Modeling and Simulations of Biological Systems, Universidad La República. “A molecular model for the BKCa channel and the location of $\beta 1$ in the $\beta 1$ - α subunit complex”. Montevideo, Uruguay **(2010)**

CONFERENCES ATTENDED

- 15th European Biophysics Congress. “Modulation of TRPC channel-protein complexes through peptide inhibition”. Ariela Vergara-Jaque. Rome, Italy **(2025)**
- II Conesul Symposium on Biomolecular Simulation. “Coevolution-based prediction of binding interfaces in TRP-14-3-3 complexes”. Nicolás Peña-Vilches, Pablo Galaz-Davison, Ariela Vergara-Jaque. Buenos Aires, Argentina **(2024)**
- 3ra Reunión Anual Sociedad Chilena de Bioinformática. “Elucidating TRP channel-protein interactions to characterize critical binding domains for targeted drug design”. Vergara-Jaque A. Concepción, Chile **(2024)**
- XLV Annual Meeting Sociedad de Bioquímica y Biología Molecular de Chile. “Computational approaches to study protein-protein interactions regulating the expression and function of membrane proteins”. Vergara-Jaque A, Cerda O. Cuncumen, Chile **(2022)**
- First Women in Bioinformatics and Data Science LA Conference. “Protein-protein interactions regulating the function of membrane proteins”. Virtual Meeting. **(2020)**
- XLII Annual Meeting Sociedad de Bioquímica y Biología Molecular de Chile. “Molecular determinants of the TRPC6 channel association with VAPA endoplasmic reticulum contact proteins”. Vergara-Jaque A, Álvarez A, Díaz J, Poblete H, González W, Silva I, Lavanderos B and Cerda O. Iquique, Chile, **(2019)**

- SGP 73rd Annual Symposium/SOBLA Annual Meeting. “Molecular determinants of the TRPC6 channel association with VAPA endoplasmic reticulum contact proteins”. Vergara-Jaque A, Álvarez A, Díaz J, Poblete H, González W, Silva I, Lavanderos B and Cerda O. Valparaíso, Chile, **(2019)**
- V Research Conference Ion Channels in the Valley. “A structural model of the inactivation gate of voltage activated potassium channels” Vergara-Jaque A, Poblete P, Comer J, Holmgren M. Montegrande, Chile **(2019)**
- XLI Annual Meeting Sociedad de Bioquímica y Biología Molecular de Chile. “Molecular insights into the dopamine transporter inhibition mediated by G proteins” Orellana I, Rojas G, Vergara-Jaque, A. Iquique, Chile **(2018)**
- XL Annual Meeting Sociedad de Bioquímica y Biología Molecular de Chile. “Structural similarities between SMCT1 and NIS: Clues to the origin of apical iodide transport in the thyroid” Vergara-Jaque, A., Comer, J., Fong, P. Puerto Varas, Chile **(2017)**
- Biophysical Society 61st Annual Meeting. “A Structural Model of the Inactivation Gate of Voltage Activated Potassium Channels” Ariela Vergara-Jaque, Francisco Palma-Cerda, Horacio Poblete, Adam Lowet, Alexander Sukharev, Jeffrey Comer, Miguel Holmgren. New Orleans, Louisiana, USA **(2017)**
- Biophysical Society 61st Annual Meeting. “Insights into the Gating Mechanism of Excitatory Amino Acid Transporters-Associated Anion Channel” Delany Torres-Salazar, Horacio Poblete, Aneysis Gonzalez-Suarez, Ariela Vergara-Jaque, Jennie Garcia-Olivares, Jeffrey Comer, Susan G Amara. New Orleans, Louisiana, USA **(2017)**
- Biophysical Society 60th Annual Meeting. “Is Sodium Monocarboxylate Transporter (SMCT1) A Protein Involved in the Apical Iodide Transport?” Ariela Vergara-Jaque, Peking Fong, Jeffrey Comer. Los Angeles, USA **(2016)**
- Biophysical Society 60th Annual Meeting. “Elucidating the Anion Channel Gating Mechanism in Excitatory Amino Acid Transporters” Delany Torres Salazar, Horacio Poblete, Aneysis Gonzalez, Ariela Vergara-Jaque, Jeffrey Comer, Susan G. Amara. Los Angeles, USA **(2016)**
- Biophysical Society 60th Annual Meeting. “Computational Studies of Elevator-Like Movements in Secondary Transport” Cristina Fenollar-Ferrer, Claudio Anselmi, Ariela Vergara Jaque, Hossein Ali Karimi-Verzaneh, Horacio Poblete-Vilches, Christopher Mulligan, Ian C. Forster, Joseph A. Mindell, and Lucy Forrest. Los Angeles, USA **(2016)**
- Biophysical Society 59th Annual Meeting. “Carboxyl Residues Required for Transport by a Vesicular Monoamine Transporter Homolog from *Brevibacillus Brevis* (BbMAT)” Ariela Vergara-Jaque, Dana Yaffe, Yonatan Shuster, Dina Listov, Sitaram Meena, Satinder K. Singh, Shimon Schuldiner, Lucy R. Forrest. Baltimore, USA **(2015)**
- Biophysical Society 59th Annual Meeting. “Proton Permeation in Ci-Hv1 Voltage-Gated Proton Channels occurs through a Proton Wire Involving Residues D160 and D222 and It is Modulated by N264” Amaury Pupo, David Baez-Nieto, Ester Otarola, Osvaldo Yañez, Ariela Vergara-Jaque, Wendy Gonzalez, Karen Castillo, Gustavo Contreras, H. Peter Larsson, Ramón Latorre, Carlos Gonzalez. Baltimore, USA **(2015)**
- XXXVII Annual Meeting Sociedad de Bioquímica y Biología Molecular de Chile. “Theoretical study of the affinity between the Protein Kinase PKA and peptide substrates derived from Kemptide using MM-GBSA” Caballero, J., Mena-Ulecia, K., Vergara-Jaque, A., Poblete, H., Tiznado, W. Puerto Varas, Chile **(2014)**
- XXXV Reunión Anual Sociedad de Bioquímica y Biología Molecular. “Molecular dynamics simulations of the binding of Phosphorylcholine to Phosphorylcholine Phosphatase” Bustos, D., Vergara-Jaque, A., Beassoni, P., Alzate-Morales, J. Puerto Varas, Chile **(2012)**
- XXXV Reunión Anual Sociedad de Bioquímica y Biología Molecular. “Evaluation of polyamidoamine (PAMAM) dendrimers as drug carriers using Tramadol and Morphine as model drugs”

Zúñiga, M., Vergara-Jaque, A., Carrasco, V., Comer, J., Santos L., Sandoval, C. Puerto Varas, Chile **(2012)**

- XXXV Reunión Anual Sociedad de Bioquímica y Biología Molecular. “Molecular Characterization of Shaker Potassium Channel Inactivation” Vergara-Jaque, A., Poblete, H., Holmgren, M. Puerto Varas, Chile **(2012)**
- XXXIV Reunión Anual Sociedad de Bioquímica y Biología Molecular. “Dendritic nanoparticles (PAMAM) used as an optimal mechanism for transport and controlled drug delivery” Vergara-Jaque A., Monsalve L., Sandoval C. and González-Nilo F.D. Valdivia, Chile **(2011)**
- Biophysical Society 55th Annual Meeting. “Ion Conduction in a Shaker Potassium Channel Mutant Having an Unusually High Single Channel Conductance” David Naranjo, Ignacio Valencia, Cristian Moscoso, Katherine Stack, Valeria Márquez, Ariela Vergara, Marcos Sotomayor, Fernando González-Nilo. Baltimore, USA **(2011)**
- 17th Workshop of Computational Chemistry and Molecular Spectroscopy. “Understanding the ligand-protein Interactions in B-Raf Kinase through Molecular Dynamics and Hybrid Calculation Methods” J. H. Alzate-Morales, A. Vergara-Jaque, J. Caballero. Punta de Tralca, Chile **(2010)**
- XXXIII Reunión Anual Sociedad de Bioquímica y Biología Molecular. “Structural analysis of A/H1N1 neuraminidase interacting with Peramivir, Oseltamivir and Relenza” Bernardita Poblete, Ariela Vergara-Jaque, Horacio Poblete, Danilo González-Nilo. Termas de Chillán, Chile **(2010)**
- First International Conference on Bioinformatics, SOIBIO. “Molecular dynamics and free energy perturbation analysis of Oseltamivir and Zanamivir interacting with neuraminidase mutants of human influenza virus (A/H1N1)” Ariela Vergara-Jaque, Horacio Poblete, Danilo González, Christophe Chipot. Termas de Chillán, Chile **(2010)**
- First International Conference on Bioinformatics, SOIBIO. “Structural properties that determine the affinity of classical agonists of the nicotinic acetylcholine receptor $\alpha 7$ ” Francisco Adasme Carreño, Ariela Vergara-Jaque, Jans Alzate-Morales y Patricio Iturriaga. Termas de Chillán, Chile **(2010)**
- First International Conference on Bioinformatics, SOIBIO. “In-silico analysis of the interaction between the VEGFR2 receptor and Semaxanib derivatives” Camila Muñoz G., Ariela Vergara-Jaque, Jans Alzate-Morales, Julio Caballero. Termas de Chillán, Chile **(2010)**
- First International Conference on Bioinformatics, SOIBIO. “In silico approach to understand structure/function relationship of exopolyphosphatase from *Escherichia coli*” Cristhian Boetsch, Ariela Vergara-Jaque, Angela T. Lisa and Paola R. Beassoni. Termas de Chillán, Chile **(2010)**
- First International Conference on Bioinformatics, SOIBIO. “Phosphorylcholine phosphatase from *Pseudomonas aeruginosa*. Some key residues involved in substrate interaction” Cristhian Boetsch, Ariela Vergara-Jaque, Lisandro H. Otero, Danilo González-Nilo, Paola R. Beassoni. Termas de Chillán, Chile **(2010)**
- 6th Annual McGill Biophysical Chemistry Symposium. “A molecular model for the BKCa channel and the location of $\beta 1$ in the $\beta 1$ - α subunit complex” Cristian A. Zaelzer, Clark Hyde, Ariela Vergara, Horacio Poblete, Daniel Aguayo, Walter Sandtner, Fernando D. González-Nilo, Francisco Bezanilla, Ramón Latorre. Montreal, Canada **(2010)**
- Biophysical Society 54th Annual Meeting. “A molecular model for the BKCa channel and the location of $\beta 1$ in the $\beta 1$ - α subunit complex” Cristian A. Zaelzer, Clark Hyde, Ariela Vergara, Horacio Poblete, Daniel Aguayo, Walter Sandtner, Fernando D. González-Nilo, Francisco Bezanilla, Ramón Latorre. San Francisco, USA **(2010)**
- III Reunión de Biología Vegetal. “A Conformational Dynamics Study of Potassium Channels Involved in Salinity Tolerance in *Arabidopsis Thaliana*” Morales-Navarro, S., González, W., Vergara, A., Aguayo, D., Dreyer, I., González, F. Paso Pehuenche, Chile **(2008)**

- XXXI Reunión Anual de la Sociedad de Bioquímica y Biología Molecular de Chile. “Structural and electrostatic properties in the permeation pathway of *Shaker* potassium channel and the mutant P475D” Vergara-Jaque, A., Naranjo, D., González-Nilo, F. Termas de Chillán, Chile (2008)
- XXX Reunión Anual de la Sociedad de Bioquímica y Biología Molecular de Chile. “*Shaker* K⁺ Channel Inactivation” Vergara, A., Urbina, H., González-Nilo, F, Gonzalez, C., Holmgren, M. Termas de Chillán, Chile (2007)
- XXIX Reunión Anual de la Sociedad de Bioquímica y Biología Molecular de Chile. XVIII Reunión Anual Sociedad de Botánica de Chile. ‘Molecular aspects of nucleotide phosphoenolpyruvate carboxykinase interaction” Vergara, A., Arenas, M., Gonzalez-Nilo, F., Cardemil, E. XLIX Reunión anual de la Sociedad de Biología de Chile. Pucón, Chile (2006)

TEACHING EXPERIENCE

- Course “Structural Bioinformatics”, Biochemistry, Universidad de Talca, Chile (2022-2026)
- Course “Introduction to Bioinformatics”, Bioinformatics Engineering, Universidad de Talca, Chile (2011, 2026)
- Course “Programming in Science and Technology”, PhD on Sciences mention Modeling of Biological and Chemical Systems, Universidad de Talca, Chile (2020-2022)
- Course “Biophysics and Modeling of biomolecular systems”, PhD on Sciences mention Modeling of Biological and Chemical Systems, Universidad de Talca, Chile (2022-2023)
- Course “Molecular Evolution”, Bioinformatics Engineering, Universidad de Talca, Chile (2018-2022)
- Course “Molecular Dynamics Simulation”, Bioinformatics Engineering, Universidad de Talca, Chile (2018-2023)
- Course “Parallel and Distributed Computing”, Bioinformatics Engineering, Universidad de Talca, Chile (2017-2018, 2021)
- Course “Molecular simulation and its application on biotechnology and health”, IPDIE–Universidad Tecnológica del Perú, Lima, Perú (2017)
- Course “Molecular simulation applied to biological systems”, Bioinformatics Engineering, Universidad de Talca, Chile (2017)
- Course “Bioinformatics II”, Bioinformatics Engineering, Universidad de Talca, Chile (2011,2017)
- Special cycle courses “Structural Bioinformatics”, Master in Bioinformatics (PEDECIBA), Universidad de la República de Uruguay, Uruguay (2010)
- Course “Bioinformatics and Society”, Bioinformatics Engineering, Universidad de Talca, Chile (2010)
- Course “Introduction to molecular simulation of biological systems”, PhD on Sciences mention Cellular and Molecular Biology, Universidad Austral, Valdivia, Chile (2010)
- Course “Molecular simulation of proteins”. Universidad Nacional de Río Cuarto, Argentina (2008)

MENTORING

Isidora Valdebenito. Master thesis student (2026-present)
 Benjamin Cerpa. Master thesis student (2026-present)
 Magdalena Lolos. Undergraduate thesis student (2026-present)
 Benjamin Cerpa. Undergraduate thesis student (2025-2026)
 Joaquin Arriagada. Undergraduate thesis student (2024-2025)
 Lucciano Ducci. Undergraduate thesis student (2024-2025)
 Pablo Galaz. Postdoctoral researcher (2024-2027)
 Nicolás Peña. PhD student (2022-present)
 Mariela González. PhD student (2021-2026)

Roberto Rosales. PhD student **(2019-2026)**
 Nicole Soto. Undergraduate thesis student **(2022-2023)**
 Valentina Garrido. Undergraduate thesis student **(2022-2023)**
 Martina Inostroza. Undergraduate thesis student **(2022-2023)**
 Tiaren Ruiz. Undergraduate thesis student **(2021-2022)**
 Isabel García. Undergraduate thesis student **(2021-2022)**
 Lady Belen Maldonado. Undergraduate thesis student. Yachay Tech University. Ecuador **(2020-2021)**
 Simón Zuñiga. Undergraduate thesis student **(2020-2021)**
 Nicolás Peña. Undergraduate thesis student **(2020-2021)**
 Julio Salgado. Undergraduate thesis student **(2020-2021)**
 Christa Kanstrup. Visiting PhD Student, University of Copenhagen, Denmark **(2019)**
 Mariela González. Undergraduate thesis student **(2019)**
 Adriana Treuer Moya. Postdoctoral researcher **(2018-2021)**
 Ivana Orellana. Undergraduate thesis student **(2018-2019)**
 Genoveva Rojas. Undergraduate thesis student **(2018-2019)**
 Héctor Montecino. Research assistant **(2018)**
 Supervision of undergraduate student thesis projects, Bioinformatics Engineering, Universidad de Talca, Chile **(2012 -present)**

OUTREACH AND TRAINING

- Discussion Forum: Women in Science. Liceo Marta Donoso Espejo **(2026)**
- Seminar: Women Who Transform. School of Biochemistry, University of Talca **(2026)**
- Engineering Connect Podcast, Faculty of Engineering, University of Talca **(2022)**
- Founding member of the Chilean Society of Bioinformatics (SCB), playing a crucial role as the coordinator of the Strategic Development Committee. **(2021-2022)**
- First Chilean Student Council Symposium. Discussion panel "Bioinformatics: Today's Challenges and the Future" **(2021)**
- Discussion panel "Cool Women in Bioinformatics" in commemoration of International Women's Day **(2021)**
- Talk for High School "How do I become a Bioinformatics Scientist?", Universidad de Talca, Talca. **(2019)**
- Symposium Present and Future of Science in Chile, Santiago, Chile. *Organizing Committee* **(2019)**
- Academic program "Al laboratorio con mi profesor", Millennium Nucleus of Ion Channels-Associated Diseases (MINICAD), Universidad de Talca, Talca. *Advisor* **(2018)**
- EXPLORA project's reviewer "Investigación Científica Escolar", Talca. **(2018-2019)**
- Talk for High School "How many opportunities I will have in life if I Study a Bachelor's Degree", Liceo Abate Molina, Talca. **(2014)**
- EXPLORA program "Mil Científicos, mil aulas", Colegio Alborada de Linares, Linares. **(2013)**

OTHER SKILLS

Languages: Spanish (native) and English (professional working proficiency).