

## CURRICULUM VITAE

### PERSONAL DATA

**Name** : **Fernando Danilo González Nilo**  
**Birth date** : December 9, 1968.  
**Address** : Full professor and Director of Center for Bioinformatics and Integrative Biology (CBIB),  
Facultad de Ciencias Biológicas, Universidad Andres Bello, Av. República 217, Santiago,  
Chile.  
**Phone** : +56 9 88085872  
**E-mail** : [fernando.gonzalez@unab.cl](mailto:fernando.gonzalez@unab.cl), [danilo.gonzaleznilo@gmail.com](mailto:danilo.gonzaleznilo@gmail.com)

Degree: Chemistry PhD. (2000) Facultad de Química y Biología. Universidad de Santiago de Chile (USACH).  
Santiago, Chile. Postdoc (2001) National Cancer Institute-USA.

Research Group: I directly supervise 3 Postdocs, 2 PhD Students, 1 Master Student and 7 Bioinformatics  
Engineers. Additionally, I direct a research Center where there are other 5 principal investigators.

Present position: Professor (Senior Lecturer), Director of the Center for Bioinformatics and Integrative  
Biology, and Director of the School of Bioinformatics Engineering. PI of Centro Interdisciplinario de  
Neurociencias de Valparaíso (CINV), PI of PMI UNAB for Bionanotechnology, and PI of Fraunhofer Chile  
Research Fundation.

### Summary:

Fernando Danilo González Nilo, Ph.D. in Chemistry (45) is currently full professor and director of the Center  
for Bioinformatics and Integrative Biology (CBIB), at Universidad Andrés Bello, Santiago. To date, he has  
founded two Centers for Bioinformatics in Chile. His current research team includes 3 postdocs, 2 PhD  
students, 1 Master student, and 8 bioinformatics engineers. Additionally, the CBIB hosts another 4 principal  
investigators for whom prof. González-Nilo serves as faculty mentor. The Center for Bioinformatics and  
Integrative Biology (CBIB) of Universidad Andrés Bello houses a trans-disciplinary team whose main goal is  
to develop research strategies that bring together the benefits of computational and experimental validation  
methods. The CBIB highly integrated approach favors an iterative research cycle based on observation,  
modeling, simulation, and experimental validation. This approach is supported by a high performance  
computing system (SGI ICE 8400 with 1.536 cores and 3TB of RAM), enabling the development and use of  
high-performance molecular simulation and bioinformatics tools in areas as diverse as Bio-Nanotechnology,  
Molecular Design, Protein Engineering, and Omics-Technologies. The computer system is tightly integrated  
to the enzyme-informatics and genomic enzymology, molecular simulations of bio-nanosystems, molecular  
biophysics, bionanotechnology and microbiology, and biomacromolecule characterization laboratories.

Among his most important awards is his selection as a member of the Science of Frontier project of the  
Chilean Academy of Sciences (2007). He also participated in the commission of agricultural innovation and  
biotechnology, from the Ministry of Agriculture of the Government of Chile (2007-2009) and in the  
Commission for International Collaboration NCI (USA) - Ministry of Health: Pilot Project for Breast Cancer  
(2008-2009).

In the scientific field, Dr. González-Nilo has been honored by the President of the Republic of Chile, Ricardo  
Lagos, for having one of the highest scores in a scientific grant submitted to FONDECYT (2004). In regards  
to his international activities, he was awarded a young scientist travel fellowship (2000) from the IUBMB /  
FEBS / Biochemical Society and a fellowship from the Organization of American States (OAS) for the  
Regular Training Program at the National Cancer Institute-US (1999). Currently, the group of Dr. Gonzalez-  
Nilo is in close collaboration with leading research groups in Molecular Simulation and Bionanotechnology in  
USA, Europe and Latin America (CNRS (France), Beckmann Institute, NIH, NCI (USA), HMG (Spain), LNCC  
(Brazil), etc.).



Another of Dr. Gonzalez-Nilo's important scientific activity is developing the first database of Nanobiotechnology structure, Collaboratory for Structural Nanobiology (CSN, <http://nanobiology.utalca.cl>). CSN was developed in collaboration with the NCI-USA. In the field of education he serves as Professor of Molecular Simulation of Proteins in several PhD programs in Chile and South America. At the University Andrés Bello he provides specialized lectures in undergraduate, Master and Ph.D. programs. Among his scientific papers are two articles published in the journal Proc. Nat Acad. Sci USA, 5 Cover Figure (FEBS Letters, JBC, JGP, JCTC and JCIM), and over 80 articles published in ISI journals.

#### **RELEVANT HONORS:**

- 2013 : Par Evaluador CAN de Facultad de Ingeniería de la Pontificia Universidad Católica de Chile.
- 2011 : Invited for an interview at Fundación Imagen de Chile. International Press Conference.
- 2008-2009 : Commission for international collaboration NCI (USA)-Ministry of Health: Pilot Project for Breast Cancer. Ministry of Health, Government of Chile.
- 2007-2009 : Award by the Science Academy of Chile under Project "Science of Frontier".
- 2007-2008 : Commission for Innovation for Biotechnology. Ministry of Agriculture, Government of Chile.
- 2004 : Award by the President of Chile as the best FONDECYT project in the Biology 2 scientific group
- 2000 : Travel Fellowship for Young Scientist from the IUBMB/FEBS/Biochemical Society.
- 1999 : Scholarship from the Organization of American States (OAS) for the Regular Training Program at the National Cancer Institute-USA

#### **PATENTS**

1. "Synthetic proteins based on dendrimers", submitted as a provisional patent application to the United States Patent and Trademark Office. The application number is 61/692,464 and it was filed on August 23, 2012. Fraunhofer Chile Research/Universidad Andres Bello.
2. "Powdered gas", submitted as a provisional patent application to the United States Patent and Trademark Office. Universidad Andres Bello. 2014.
3. "Use of compounds that selectively modulate astrocytic release of substances through hemichannels of connexins and pannexins, without influencing gap junctions, for the treatment of psychiatric disorders", submitted as a provisional patent application to the United States Patent and Trademark Office. The application number is PCT/IB2013/054486 and it was filed on May 31, 2013. Universidad Andres Bello

#### **INDUSTRIAL CONSULTANT**

- 2010-2014 : Medimmune AstraZeneca, Washington DC, USA.
- 2008-2013 : Implementation of Bioinformatics Platform for TTechnologies, Chile

#### **GRANTS**



- 2014-2017 : Alternate Director: **Proyecto Corfo**, Línea 2, Proyecto de I+D Aplicada. “Desarrollo de potenciales fármacos usando los Astrocitos como blanco farmacológico para el tratamiento de enfermedades psiquiáticas”. Universidad Andrés Bello.
- 2014-2015 : Principal Investigator: **US Army of USA**, “Rational Design of Pain Inhibitors: target TRPV1 channel”.
- 2015 : Principal Investigator: **Air-Force of USA**, “Cross-Discipline Bio-Nanostructured Enhanced Multimode-Sensor Science”.
- 2015 : Principal Investigator: **USA-Army/Air-Force of USA**, “Green Energetic Materials”.
- 2014-2015 : Principal Investigator: **Proyecto Fondecip** EQM140174, Programa de Equipamiento Científico y Tecnológico, Fondecip. Universidad Andrés Bello.
- 2013-2016 : Principal Investigator: **PMI Project**, Convenio De Desempeño Apoyo A La Innovación En Educación Superior, Ministerio De Educación De Chile. Fortalecimiento De Las Capacidades De Innovación Basadas En Ciencia, Bio-Nanotecnología. Universidad Andrés Bello.
- 2013-2016 : Director of Line Research: Nano-Biomedicine, **Corfo** Attracting Program Centers International Excellence CEI For Competitiveness. Fraunhofer Chile Research Center For Systems Biotechnology.
- 2013-2015 : Co-Investigator: **Fondecip** Idea Program, Applied Science, Conicyt. “Powder gas: A New Tool Nano-microtechnology For Managing Maturation, Senescence and Decay In Fruits Of Export in Post-Harvest”. Universidad Andrés Bello.
- 2013-2015 : Principal Investigator. **FONDECYT Regular** # 1131003, Study of structural and dynamic properties that govern selectivity and conductance of K channels under non-equilibrium conditions. Universidad Andrés Bello.
- 2012-2015 : Director Proyecto Anillo Científico de Ciencia y Tecnología, **Conicyt**. Integración de la Biología estructural al desarrollo de la Biotecnología. Universidad Andrés Bello.
- 2011-2016 : Principal Investigator: Iniciativa Equipamiento Mayor **Conicyt**. National Laboratory for HighPerformance Computing.
- 2011-2020 : Principal Investigator: Iniciativa Científica Milenio, **Ministerio de Planificación**. Centro Interdisciplinario de Neurociencia de Valparaíso (CINV).
- 2011-2020 : Director of Line Research: Nano-Biotechnology in Food, **CORFO** Attracting Program Centers International Excellence CEI For Competitiveness. Fraunhofer Chile Research Center for Systems Biotechnology.
- 2010-2012 : Principal Investigator. **FONDECYT** Concurso Inserción de Investigadores/as en la Academia, N° 79090038. Fortalecimiento del área de Nano-Biotecnología y su potencial aplicación en la agroindustria y biomedicina.



- 2011-2014 : Co-investigador. Proyecto **FONDECYT** Regular, BASES MOLECULARES DE LA SENSIBILIDAD TERMICA EN CANALES TRP. Titular: R. Latorre (U. Valparaíso)
- 2009-2011 : Co-investigador. Proyecto **FONDECYT** Regular, # 1090493, IONIC CONDUCTION IN K CHANNELS. Titular: D. Naranjo (U. Valparaíso)
- 2008-2010 : Principal Investigator. FONDECYT Programa de Cooperacion Cientifica Internacional – PCCI **CONICYT / DAAD** (Alemania) N° 2008 – 141. NIAPOC- New Interdisciplinary Approaches to Gain Molecular Insights into the Regulation of Potassium Channels in Plants. Contraparte Alemania: Ingo Dreyer, Potsdam University.
- 2009 : Co-investigador. **Innova-Corfo**-"Gestión de la innovación en empresas chilenas": "Instalación de capacidades de innovación en eslabones empresariales del cluster porcícola nacional".
- 2009-2011 : Alternate Director. **FONDEF TIC-EDU**. " Collaboratory learning system based on GRID facilities (SACGRID): Applications for Biological Science and Biotechnology (Sistema de Aprendizaje Colaborativo Basado en Infraestructura GRID (SACGRID): Aplicaciones en Ciencias Biológicas y Biotecnología)"
- 2008-2009 : PI, **National Cancer Institute-USA, SAIC**. Development of nanoparticle database: Collaboratory for Structural Nanobiology 2008-2009 : PI, **FP7-ICT-2007-2** International Cooperative Action on Grid Computing and Biomedical Informatics between the European Union@\*Latin America, the Western Balkans and North Africa ACTION-Grid
- 2007-2009 : PI, **Research Rings in Science and Technology** (ACT/24), Bicentenary Program for Science and Technology (PBCT). Computer Simulation Laboratory of Nanomaterials and Biological Systems of Experimental Interest.
- 2006-2010 : : Co-investigador. FONDECYT-Chile (National Fund for Scientific and Technological Development) Research Grant # 1060198, Regulación alosterica diferencial de transportadores de glucosa de clase I y clase III por inhibidores exofaciales y endofaciales
- 2005-2006 : PI, **FONDECYT-Chile**. International Cooperation.
- 2004-2007 : PI. **FONDECYT-Chile**. Research Grant # 1040254. "Molecular aspects that govern the conductance of the potassium channels".
- 2003-2007 : Co-investigador. **FONDECYT-Chile**. Research Grant #1030760. "Structure and catalytic mechanism of phosphoenolpyruvate carboxykinase".
- 2003-2005 : Co-investigador. **FONDEF-Chile** (National Fund for the Promotion of Scientific and Technological Development), # GO2P1002. "Plataforma Científico-Tecnológica para el Desarrollo de la Genómica vegetal en Chile. Etapa I: Genómica Funcional en Vid", director of bioinformatics area.
- 2004-2005 : PI. **Hewlett Packard** Mobile Technology for Teaching Grant. MOBI-LAB: Bioinformatics Tools Applied to Biochemical and Chemical Labs.



- 2003-2005 : PI. **Fundación ANDES** C-18360. "Structural and dynamics study of water around the proteins and its role in protein-protein interactions."
- 1997-1999 : PI. **FONDECYT-Chile** PhD Research Grant # 2970090, "Experimental and molecular modeling study of polyelectrolyte".

### **Organization International Meeting**

Co-Organizer: International Dendrimer Symposium (IDS7), June 26 - July 1, 2011 at NIST Campus in Gaithersburg, MD. USA.

Organizer: The 1st International Conference on Bioinformatics SOIBIO 2010, September 26-28, 2010 at Termas de Chillan, Chillan, Chile

### **PUBLICATIONS** (relevant paper from 2004. Total number of articles to date: 95, h-index: 15)

25. Anaerobiospirillum succiniciproducens phosphoenolpyruvate carboxykinase. Mutagenesis at metal site 1. Jabalquinto AM, Gonzalez-Nilo FD, Laivenieks M, Cabezas M, Zeikus JG, Cardemil E. *Biochimie. Jan*;86(1):47-51. (2004)
26. Surface characterization of poly(4-vinylpyridine) quaternized with tetradecyl bromide: effect of the degree of quaternization. Gargallo L, Miranda B, Leiva A, Rios H, Gonzalez-Nilo F, Radic D. *J Colloid Interface Sci. Mar 1*;271(1):181-6. (2004)
27. Substrate binding to fluorescent labeled wild type, Lys213Arg, and HIS233Gln Saccharomyces cerevisiae phosphoenolpyruvate carboxykinases. Bueno C, Gonzalez-Nilo FD, Victoria Encinas M, Cardemil E. *Int J Biochem Cell Biol. May*;36(5):861-9 (2004)
28. Role of the HIT-Like Motif in Nucleotide Hydrolysis by the Rotavirus RNAPackaging Protein NSP2. Rodrigo Vasquez-Del Carpio, Fernando D. González-Nilo, Hariharan Jayaram, Eugenio Spencer, B. V. Venkataram Prasad, John T. Patton and Zenobia F. Taraporewala. *J. Biol. Chem., Vol. 279(11), 10624-10633, 2004. Cover Figure*
29. Relative solvation and strength of polycyano- and polynitromethanes in water: a study with molecular dynamics. Nelson Carrasco, Fernando Gonzalez-Nilo, Marcos Caroli. *J. Physc Org. Chem. 17, 1-6, (2004)*
30. Structure-Antioxidant Activity Relationships of Flavonoids Isolated from the Resinous Exudate of Heliotropium sinuatum. Brenda Modak, Leonor Contreras, Fernando Gonzalez-Nilo and Rene Torres. *Bioorg Med Chem Lett. 2005 Jan 17*;15(2):309-12.
31. Chilean effort for improving fruit quality in grapevine: a genomic approach to understand seed formation, fruit ripening and response to pathogen. Peña-Cortés, H., Valdés, J., Prieto, H., Rosales, M., Hinrichsen, P., Jashes, M., Fichet, T., Pinto, M., Riquelme, A., González, D., González, E. and Ruíz, S. *Acta Horticulturae 689: 505-512. (2005)*

32. Nucleotide specificity of *Saccharomyces cerevisiae* phosphoenolpyruvate carboxykinase: Kinetics, fluorescence spectroscopy, and molecular simulation studies. José M. Villarreal, Claudia Bueno, Felipe Arenas, Ana M. Jabalquinto, Fernando D. González-Nilo, María V. Encinas and Emilio Cardemil.  
*The International Journal of Biochemistry & Cell Biology*, 2006, 38(4), 576-588.
33. Site-directed mutagenesis study of the microenvironment characteristics of Lys213 of *Saccharomyces cerevisiae* phosphoenolpyruvate carboxykinase. Alejandro Yévenes, Rodrigo Espinoza, Jaime A. RivasPardo, José M. Villarreal, Fernando D. González-Nilo and Emilio Cardemil.  
*Biochimie*, 2006, 88(6), 663–672
34. Molecular dynamics simulation of the aqueous solvation shell of cellulose and xanthate ester derivatives. Eduardo Humeres, Carolina Mascayano, Gonzalo Riadi and Fernando Gonzalez-Nilo.  
*J. Phys. Org. Chem.* 2006, 19:1–6.
35. Gating of two-pore domain K<sup>+</sup> channels by extracellular pH. María Isabel Niemeyer, Fernando D. González-Nilo, Leandro Zúñiga, Wendy González, L. Pablo Cid and Francisco V. Sepúlveda.  
*Biochemical Society Transactions*, 2006, 34(5):899-902
36. Histidine Triad-Like Motif of the Rotavirus NSP2 Octamer Mediates Both RTPase and NTPase Activities. Rodrigo Vasquez-Del Carpio, Fernando D. Gonzalez-Nilo, Gonzalo Riadi, Zenobia F. Taraporewala, and John T. Patton.  
*Journal of Molecular Biology*, 2006, 362(3):663-672.
37. Blends Containing Amphiphilic Polymers. V. Compatibilization of N-Alkylitaconamic Acid-co-Styrene Copolymers with Interacting Polymers. Marcela Urzua, Claudia Sandoval, Fernando Gonzalez-Nilo, Angel Leiva, Ligia Gargallo, Deodato Radic´.  
*Journal of Applied Polymer Science*, 2006, 102 (3): 2512 – 2519.
38. Relevance of phenylalanine 216 in the affinity of *Saccharomyces cerevisiae* phosphoenolpyruvate carboxykinase for Mn(II). Yevenes A, Gonzalez-Nilo FD, Cardemil E.  
*Protein J.*, 2007, 26(2): 135-41.
39. Neutralization of a single arginine residue gates open a two-pore domain, alkali-activated K<sup>+</sup> channel. María Isabel Niemeyer, Fernando D. González-Nilo, Leandro Zúñiga, Wendy González, L. Pablo Cid & Francisco V. Sepúlveda.  
*Proceeding of the National Academy of Sciences*, 2007, 104 (2): 666-671.
40. Dissection of the Components for PIP<sub>2</sub> activation and Thermosensation in TRP Channels. Brauchi S., Orta G., Mascayano C., Salazar M., Raddatz N., Urbina H., Rossenmann E., Gonzalez-Nilo F., Latorre R.  
*Proceeding of the National Academy of Sciences*, 2007, 104(24):10246-10251.
41. In-silico nano-biodesign. A new frontier in computational biology. Cachau, R.E, Gonzalez-Nilo, FD, Ventura, O.N. and Fritts, M.J.  
*Curr Top Med Chem.* 2007;7(15):1537-40. **Review.**
42. Quantitative structure–activity relationship of rubiscoin analogues as  $\delta$  opioid peptides using Comparative Molecular Field Analysis (CoMFA) and Comparative Molecular Similarity Indices



- Analysis (CoMSIA). J. Caballero, M. Saavedra, M. Fernández and F.D. González-Nilo. *J. Agric. Food Chem.* 2007, 55, 8101-8104. (ISI-IF2006: 2.322).
43. 2D autocorrelation, CoMFA and CoMSIA modeling of protein tyrosine kinases' inhibition by substituted pyrido[2,3-d]pyrimidine derivatives. J. Caballero, M. Fernández, M. Saavedra and F.D. González-Nilo. *Bioorg Med Chem.* 2008 Jan 15;16(2):810-21. Epub 2007 Oct 13.
44. Loss of TP53-DNA interaction induced by p.C135R in lung cancer. Aranda M, Gonzalez-Nilo F, Riadi G, Díaz V, Perez J, Martel G, Hainaut P, Mimbacas A. *Oncol Rep.* 2007 Nov;18(5):1213-7.
45. Intrinsic electrostatic potential in the BK channel pore: role in determining single channel conductance and block. Carvacho I, Gonzalez W, Torres YP, Brauchi S, Alvarez O, Gonzalez-Nilo FD, Latorre R. *J. Gen. Physiol.* 2008 Feb;131(2):147-61. **Figure Cover**
46. *Proceedings of the Third Conference of the EELA Project.* R. Gavela, B. Marechal, R. Barbera et al. (Eds.) CIEMAT 2007. Gustavo Rivera<sup>1</sup>, Fernando González-Nilo, Tomás Perez-Acle, Raúl Isea and David S. Holmes.
47. Relevance of Arg457 for the nucleotide affinity of *Saccharomyces cerevisiae* phosphoenolpyruvate carboxykinase. Iván Tobar, Fernando D. González-Nilo, Ana M. Jabalquinto and Emilio Cardemil. *Int J Biochem Cell Biol.* 2008;40(9):1883-9. Epub 2008 Feb 12.
48. A CoMSIA study on the adenosine kinase inhibition of pyrrolo[2,3-d]pyrimidine nucleoside analogues. Caballero J, Fernández M, González-Nilo FD *Bioorg Med Chem.* 2008 May 1;16(9):5103-8.
49. Study of the Interaction between Progesterone and beta-Cyclodextrin by Electrochemical Techniques and Steered Molecular Dynamics. Caballero J, Zamora C, Aguayo D, Yañez C, González-Nilo FD. *J Phys Chem B.* 2008 Aug 21;112(33):10194-201.
50. Structural requirements of pyrido[2,3-d]pyrimidin-7-one as CDK4/D inhibitors: 2D autocorrelation, CoMFA and CoMSIA analyses. Caballero J, Fernández M, González-Nilo FD. *Bioorg Med Chem.* 2008 Jun 1;16(11):6103-15.
51. Role of electrostatics on membrane binding, aggregation and destabilization induced by NAD(P)H dehydrogenases. Implicance on membrane fusion. César L. Avila; Beatriz F. de Arcuri; Fernando Gonzalez-Nilo, Javier De Las Rivas, Rosana Chehín, Roberto Morero. *Biophys Chem.* 2008 Oct;137(2-3):126-32. Epub 2008 Aug 23.
52. 2D Autocorrelation, CoMFA, and CoMSIA modeling of protein tyrosine kinases' inhibition by substituted pyrido[2,3-d]pyrimidine derivatives. Caballero J, Fernández M, Saavedra M, González-Nilo FD. (ISI:2,662). *Bioorg Med Chem.* 2008 Jan 15;16(2):810-21. Epub 2007 Oct 13.
53. Docking and quantitative structure-activity relationship studies for the bisphenylbenzimidazole family of non-nucleoside inhibitors of HIV-1 reverse transcriptase. Lagos CF, Caballero J, Gonzalez-Nilo FD, David Pessoa-Mahana C, Perez-Acle T. (ISI:2,043). *Chem Biol Drug Des.* 2008 Nov;72(5):360-9.

54. Dielectric and dynamic-mechanical study of the mobility of poly(t-butylacrylate) chains in diblock copolymers: Polystyrene-b-poly(t-butylacrylate). Encinar M, Guzmán E, Prolongo M, Rubio R, Sandoval C, González-Nilo F, Gargallo L, Radic´ D. (ISI:3.065). *Polymer* 49 (2008) 5650–5658.
55. Antioxidant reactivity toward nitroxide probes anchored into human serum albumin. A new model for studying antioxidant repairing capacity of protein radicals. Aspée A, Orrego A, Alarcón E, LópezAlarcón C, Poblete H, González-Nilo D. *Bioorg Med Chem Lett.* 2009 Nov 15;19(22):6382-5.
56. Shared and group-specific features of the rotavirus RNA polymerase reveal potential determinants of gene reassortment restriction. McDonald SM, Aguayo D, Gonzalez-Nilo FD, Patton JT. *J Virol.* 2009 Jun;83(12):6135-48.
57. 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. Alzate-Morales JH, Caballero J, Vergara Jague A, González Nilo FD. *J Chem Inf Model.* 2009 Apr;49(4):886-99.
58. Distinct roles of the last transmembrane domain in controlling Arabidopsis K<sup>+</sup> channel activity. Gajdanowicz P, Garcia-Mata C, Gonzalez W, Morales-Navarro SE, Sharma T, González-Nilo FD, Gutowicz J, Mueller-Roeber B, Blatt MR, Dreyer I. *New Phytol.* 2009;182(2):380-91.
59. Photophysics and photochemistry of dyes bound to human serum albumin are determined by the dye localization. Alarcón E, Edwards AM, Aspee A, Moran FE, Borsarelli CD, Lissi EA, Gonzalez-Nilo D, Poblete H, Scaiano JC. *Photochem Photobiol Sci.* 2010 Jan;9(1):93-102.
60. Distributed Structures Underlie Gating Differences between the Kin Channel KAT1 and the Kout Channel SKOR. Riedelsberger J, Sharma T, Gonzalez W, Gajdanowicz P, Morales-Navarro SE, GarciaMata C, Mueller-Roeber B, González-Nilo FD, Blatt MR, Dreyer I. *Mol Plant.* 2010 Jan;3(1):236-45.
61. The pH-sensor of the plant K<sup>+</sup> uptake channel kat1 is built of a sensory cloud rather than of single key amino acids. Gonzalez W, Riedelsberger J, Morales-Navarro SE, Caballero J, Alzate-Morales JH, González-Nilo FD, Dreyer I. *Biochem J.* 2011 Nov 10.
62. Nanoinformatics: an emerging area of information technology at the intersection of bioinformatics, computational chemistry and nanobiotechnology. González-Nilo F, Pérez-Acle T, Guínez-Molinos S, Geraldo DA, Sandoval C, Yévenes A, Santos LS, Laurie VF, Mendoza H, Cachau RE. *Biol Res.* 2011;44(1):43-51.
63. Biosynthesis of methoxypyrazines: elucidating the structural/functional relationship of two Vitis vinifera O-methyltransferases capable of catalyzing the putative final step of the biosynthesis of 3-alkyl-2-methoxypyrazine. Vallarino JG, Lopez-Cortes XA, Dunlevy JD, Boss PK, Gonzalez-Nilo FD, Moreno YM. *J Agric Food Chem.* 2011 Jul 13;59(13):7310-6.



64. Site-directed mutations and kinetic studies show key residues involved in alkylammonium interactions and reveal two sites for phosphorylcholine in *Pseudomonas aeruginosa* phosphorylcholine phosphatase. Beassoni PR, Otero LH, Boetsch C, Domenech CE, González-Nilo FD, Lisa AT.  
*Biochim Biophys Acta*. 2011 Jul;1814(7):858-63.
65. Supramolecular complexes of quantum dots and a polyamidoamine (PAMAM)-folate derivative for molecular imaging of cancer cells. Geraldo DA, Duran-Lara EF, Aguayo D, Cachau RE, Tapia J, Esparza R, Yacaman MJ, Gonzalez-Nilo FD, Santos LS.  
*Anal Bioanal Chem*. 2011 Apr;400(2):483-92.
66. Gating of a pH-sensitive K(2P) potassium channel by an electrostatic effect of basic sensor residues on the selectivity filter. Zúñiga L, Márquez V, González-Nilo FD, Chipot C, Cid LP, Sepúlveda FV, Niemeyer MI.  
*PLoS One*. 2011 Jan 25;6(1).
67. Study of Interaction Energies between the PAMAM Dendrimer and Nonsteroidal Anti-Inflammatory Drug Using a Distributed Computational Strategy and Experimental Analysis by ESI-MS/MS. Avila-Salas F, Sandoval C, Caballero J, Guiñez-Molinos S, Santos LS, Cachau RE, González-Nilo FD.  
*J Phys Chem B*. 2012 Feb 23;116(7):2031-9.
68. The pH sensor of the plant K<sup>+</sup>-uptake channel KAT1 is built from a sensory cloud rather than from single key amino acids. González W, Riedelsberger J, Morales-Navarro SE, Caballero J, Alzate-Morales JH, González-Nilo FD, Dreyer I.  
*Biochem J*. 2012 Feb 15;442(1):57-63.
69. Nanoinformatics: developing new computing applications for nanomedicine. Maojo V, Fritts M, MartinSanchez F, De la Iglesia D, Cachau RE, Garcia-Remesal M, Crespo J, Mitchell JA, Anguita A, Baker N, Barreiro JM, Benitez SE, De la Calle G, Facelli JC, Ghazal P, Geissbuhler A, Gonzalez-Nilo F, Graf N, Grangeat P, Hermosilla I, Hussein R, Kern J, Koch S, Legre Y, Lopez-Alonso V, Lopez-Campos G, Milanesi L, Moustakis V, Munteanu C, Otero P, Pazos A, Perez-Rey D, Potamias G, Sanz F, Kulikowski C.  
*Comput Sci Eng*. 2012 Jun 1;94(6):521-539.
70. Molecular Basis of Drug Resistance in A/H1N1 Virus. Vergara-Jaque A, Poblete H, Lee EH, Schulten K, González-Nilo F, Chipot C. *J Chem Inf Model*. 2012 Oct 22;52(10):2650-6. **Figure Cover**
71. K(+) conduction and mg(2+) blockade in a shaker kv-channel single point mutant with an unusually high conductance. Moscoso C, Vergara-Jaque A, Márquez-Miranda V, Sepúlveda RV, Valencia I, Díaz-Franulic I, González-Nilo F, Naranjo D.  
*Biophys J*. 2012 Sep 19;103(6):1198-207.
72. Insight into the Properties of Cardiolipin Containing Bilayers from Molecular Dynamics Simulations, Using a Hybrid All-Atom/United-Atom Force Field. Aguayo, Daniel; Gonzalez-Nilo, Fernando D.; Chipot, Christophe  
*J of Chem. Theory and Computation*, 2012 May; 8 (5): 1765-1773. **Figure Cover**
73. Calculating position-dependent diffusivity in biased molecular dynamics simulations. Jeffrey Comer, Christophe Chipot and Fernando D. González-Nilo.  
*J. Chem. Theor. Comput*. 2013, [dx.doi.org/10.1021/ct300867e](https://doi.org/10.1021/ct300867e).

74. K<sup>+</sup> conduction and Mg<sup>2+</sup> blockade in a shaker Kv-channel single point mutant with an unusually high conductance. Moscoso C, Vergara-Jaque A, Márquez-Miranda V, Sepúlveda RV, Valencia I, DíazFranulic I, González-Nilo F, Naranjo D.  
*Biophys J.* 2012 Sep 19;103(6):1198-207
75. In silico analysis of putative paralytic shellfish poisoning toxins export proteins in cyanobacteria. SotoLiebe K, López-Cortés XA, Fuentes-Valdes JJ, Stucken K, Gonzalez-Nilo F, Vásquez M.  
*PLoS One.* 2013;8(2):e55664.
76. Paclitaxel-PHBV nanoparticles and their toxicity to endometrial and primary ovarian cancer cells. Vilos C, Morales FA, Solar PA, Herrera NS, Gonzalez-Nilo FD, Aguayo DA, Mendoza HL, Comer J, Bravo ML, Gonzalez PA, Kato S, Cuello MA, Alonso C, Bravo EJ, Bustamante EI, Owen GI, Velasquez LA.  
*Biomaterials.* 2013 May; 34(16):4098-108.
77. Computationally Efficient Methodology for Atomic-Level Characterization of Dendrimer-Drug Complexes: A Comparison of Amine- and Acetyl-Terminated PAMAM. Vergara-Jaque A, Comer J, Monsalve L, González-Nilo FD, Sandoval C.  
*J Phys Chem B.* 2013 Jun 6; 117(22):6801-13
78. *Penicillium purpurogenum* produces two GH family 43 enzymes with  $\beta$ -xylosidase activity, one monofunctional and the other bifunctional: biochemical and structural analyses explain the difference. María Cristina Ravanal, Melissa Alegría-Arcos, Fernando Danilo Gonzalez-Nilo and Jaime Eyzaguirre.  
*Archives of Biochemistry and Biophysics*, 2013.
79. The C-Terminal Regions Have an Important Role in the Activity of the Ferroxidase Center and the Stability of *Chlorobium tepidum* Ferritin. Brito C, Matias C, González-Nilo FD, Watt RK, Yévenes A.  
*Protein J.* 2014 Jun;33(3):211-20
80. pH-Dependent Nano-Capturing of Tartaric Acid using Dendrimers. Oana G. Schramm, a Xaviera LópezCortés, Leonardo S. Santos, V. Felipe Laurie, Fernando González Nilo, Michal Krolík, Rainer Fischer and Stefano Di Fiorea.  
*Soft Matter.* 2014 Jan 28;10(4):600-8.
81. Identification and functional expression of a glutamate- and avermectin-gated chloride channel from *Caligus rogercresseyi*, a southern Hemisphere sea louse affecting farmed fish. Cornejo I, Andrini O, Niemeyer MI, Marabolí V, González-Nilo FD, Teulon J, Sepúlveda FV, Cid LP.  
*PLoS Pathog.* 2014 Sep 25;10(9):e1004402.
82. The crystal structure of ferritin from *Chlorobium tepidum* reveals a new conformation of the 4-fold channel for this protein family. Arenas-Salinas M, Townsend PD, Brito C, Marquez V, Maraboli V, Gonzalez-Nilo F, Matias C, Watt RK, López-Castro JD, Domínguez-Vera J, Pohl E, Yévenes A.  
*Biochimie.* 2014 Nov;106:39-47.
83. Block Copolymers in the Synthesis of Gold Nanoparticles. Two New Approaches: Copolymer Aggregates as Reductants and Stabilizers and Simultaneous Formation of Copolymer Aggregates and Gold Nanoparticles. Angel Leiva, Irma Fuentes, Esteban Bossel, Marcela Urzua, Maximiliano Mendez, Maximiliano Pino, Deodato Radić, Valeria Márquez, Fernando. D. Gonzalez-Nilo.

- J. of Polymer Science, 2014.
84. AFAL: a web service for profiling amino acids surrounding ligands in proteins. Mauricio Arenas-Salinas • Samuel Ortega-Salazar • Fernando Gonzales-Nilo • Ehmke Pohl • David S. Holmes • Raquel Quatrini.  
J. Comput Aided Mol Des, 2014.
  85. Hydrogen peroxide and hypochlorous acid influx through the major S. Typhimurium porin OmpD is affected by substitution of key residues of the channel. Aguayo D, Pacheco N, Morales EH, Collao B, Luraschi R, Cabezas C, Calderón P, González-Nilo F, Gil F, Calderón IL, Saavedra CP.  
Arch Biochem Biophys. 2015 Feb 15;568:38-45.
  86. Nano-Detoxification Dendrimer Based Technology to Trap, Clear, Sense and Neutralize Organophosphate Agents. Esteban Durán-Lara, Fabian Ávila-Salas, Sebastian Galaz, Amalraj John, Adolfo Marican, Margarita Gutiérrez, Fabiane M. Nachtigall, Fernando D. Gonzalez-Nilo and Leonardo S. Santos.  
Journal of the Brazilian Chemical Society, Accepted 2014
  87. Synthesis, Biological Evaluation, and Molecular Simulation of Chalcones and Aurones as Selective MAO-B Inhibitors. Morales-Camilo N, Salas CO, Sanhueza C, Espinosa-Bustos C, Sepúlveda-Boza S, Reyes-Parada M, Gonzalez-Nilo F, Caroli-Rezende M, Fierro A.  
Chem Biol Drug Des. 2015 Jun;85(6):685-95.
  88. The BK Channel S6 Transmembrane Domain is a Stimuli Integration Node. Willy Carrasquel-Ursulaez, Gustavo F. Contreras, Romina V. Sepúlveda, Daniel Aguayo, Fernando González-Nilo, Carlos González and Ramón Latorre. Journal General Physiology. 2014. IF: 4.73
  89. Molecular determinants of phosphatidylinositol 4,5-bisphosphate (PI(4,5)P<sub>2</sub>) binding to transient receptor potential V1 (TRPV1) channels. Poblete H, Oyarzún I, Olivero P, Comer J, Zuñiga M, Sepulveda RV, Báez-Nieto D, González Leon C, González-Nilo F, Latorre R.  
J Biol Chem. 2015 Jan 23;290(4):2086-98. IF: 4.65
  90. On The Voltage-Dependent Gating of Trpv1 Channels. David Baez-Nieto, Osvaldo Alvarez, Carlos Gonzalez, Deny Cabezas, Pamela Sotelo-Hitschfeld, Camila Navas, Fernando Gonzalez-Nilo, Harley Kurata, Ramon Latorre, and Sebastian Brauchi.  
The Journal of Biological Chemistry, submitted 2015. IF: 4.65
  91. Experimental and theoretical binding affinity between polyvinylpolypyrrolidone and selected phenolic compounds from food matrices. Durán-Lara EF, López-Cortés XA, Castro RI, Avila-Salas F, González-Nilo FD, Laurie VF, Santos LS.  
Food Chem. 2015 Feb 1;168:464-70.
  92. Synthesis and characterization of an insoluble polymer based on polyamidoamine: applications for the decontamination of metals in aqueous systems. Valdés O, Vergara CE, Camarada MB, CarrascoSánchez V, Nachtigall FM, Tapia J, Fischer R, González-Nilo FD, Santos LS.  
J Environ Manage. 2015 Jan 1;147:321-9.
  93. PAMAM G4 dendrimers as inhibitors of the iron storage properties of human L-chain ferritin. Camarada MB, Márquez-Miranda V, Araya-Durán I, Yévenes A, González-Nilo F.  
Phys Chem Chem Phys. 2015 Jul 1.

94. Development of a nanoparticle-based oral vaccine for Atlantic salmon against ISAV using an alphavirus replicon as adjuvant. Rivas-Aravena A, Fuentes Y, Cartagena J, Brito T, Poggio V, La Torre J, Mendoza H, Gonzalez-Nilo F, Sandino AM, Spencer E. *Fish Shellfish Immunol.* 2015 Jul;45(1):157-66.
95. Hydrophobic interaction between contiguous residues in the S6 transmembrane segment acts as a stimuli integration node in the BK channel. Carrasquel-Ursulaez W, Contreras GF, Sepúlveda RV, Aguayo D, González-Nilo F, González C, Latorre R. *J Gen Physiol.* 2015 Jan;145(1):61-74.

#### **INVITED TALK, 2008-2014**

10th Congress of the World Association of Theoretical and Computational Chemists (WATOC) Santiago (Chile). 5-10 October, 2014. Structural analysis of the molecular self-assembly of amphiphilic dendrimer. Fernando González-Nilo, María Belen Camarada, Valeria Márquez-Miranda, Ingrid Araya, Lars Ratjen.

XXXVII Annual Meeting Sociedad de Bioquímica y Biología Molecular de Chile, Puerto Varas (Chile). September 30 – October 04, 2014. New computational strategies to understand the conductance mechanism in K<sup>+</sup> channels. Gonzalez, F, Sepúlveda, Romina, Bravo, Felipe, Latapiat, Veronica, Diaz-Franulic, I, Naranjo, David.

GIGA Institute, Belgium. June 16, 2014.

4ta. Conferencia Internacional de la Sociedad Iberoamericana de Bioinformática (SolBio) – Rosario, (Argentina). October 29-31, 2013. Assessing the Molecular Impact of Mutations in Protein Superfamilies Revealed by Whole-Exome Sequencing of Tumors. Fernando D. Gonzalez-Nilo, José I. Soto, Daniel A. Pizarro, Thomas A. Peterson, Maricel G. Kann, Daniel E. Almonacid

SUPFAB, International Dendrimer Symposium, Septiembre 30 – Octubre 4, 2012. Sao Paulo, Brasil. Plenary Talk

VII Simposio Brasileiro de Bioinformatica, Agosto 13-17, 2012. Campo Grande, Brasil. Plenary Talk

ISCB Latin America 2012, Conference on Bioinformatics, Marzo 17-21, Santiago Chile. Plenary Talk

Primer Congreso Colombiano de Biología Computacional (CCBCOL), Marzo 23 – 25, 2011, Bogotá D.C. Biblioteca Virgilio Barco, Colombia.

NEMO-Scientific Network (NSN). Advanced Microscopy and Image Processing in Neurobiology. NEMO-DFG Bilateral Meeting. January 17-21, 2011. Plenary Talk: New Challenges to Reach the Synergy between Electron Tomography and Molecular Simulations. Danilo Gonzalez.

Congreso de Sociedad Chilena de Biología, Noviembre 22, 2010. Symposium Ciencia de Frontera. Plenary Talk: Nanoinformatics: an emerging area of information technology at the intersection of bioinformatics, computational chemistry and nanobiotechnology. Danilo Gonzalez

Congreso de Sociedad Chilena de Bioquímica, Noviembre 2010. Symposium of Bioinformatics. Plenary Talk: Synergy between Electron Microscopy and Molecular Simulations. Danilo Gonzalez

Simposium de Biotecnología. Instituto de Biotecnología de Tarapaca. Universidad Arturo Prat, Iquique, November 2-5, 2010. Plenary talk: "Nanoinformatics: an emerging area of information technology at the intersection of bioinformatics, computational chemistry and nanobiotechnology". Danilo Gonzalez.

XXVII Congreso Nacional de Estudiantes de Bioquímica ANEB Chile, Universidad de Antofagasta, 4 al 7 de Agosto 2010. Plenary Talk, Simposium: Biomedicina y su importante rol en la sociedad

Workshop: Role of Bioinformatics in Medicine. January 26, 2009, School of Medicine, Faculty of Health Sciences, Universidad de Talca. Talca, Chile. Center for Bioinformatics and Molecular Simulations: Skills and Connections to Biomedicine. Plenary Lecture. Danilo Gonzalez.

Workshop: Computational Modelling and Simulations of Biological Systems. 21 Febrero- 25 marzo, 2010, Instituto Pasteur de Montevideo, Montevideo, Uruguay.

Workshop: Role of Bioinformatics in Medicine. January 26, 2009, School of Medicine, Faculty of Health Sciences, Universidad de Talca. Talca, Chile. Center for Bioinformatics and Molecular Simulations: Skills and Connections to Biomedicine. Plenary Lecture.

Startup Conference Medical Informatics, Facultad de Medicina, Universidad de Chile, Dic 10, 2009. Nano-BioMedical Informatics: the next frontier. Plenary Lecture.

Desafíos y Oportunidades para la Cooperación en TICs entre Chile y la Union Europea

Universidad Técnica Federico Santa Maria, March 25, 2010. Nano-Bio-Medical Informatics: ACTION-GRID. Plenary Lecture.

Bioinformsalud, March 2009, First European Commission-Funded Initiative to Analyse Biomedical Informatics, Grid Technologies and Nanoinformatics. Plenary Lecture.

6th Workshop of Computational Chemistry and Molecular Spectroscopy, Octubre 21-24, 2008. Punta de Talca, Chile. Plenary Lecture.

First Workshop for Proteomics in the New World. LNCC, Petropolis, Rio de Janeiro, Brasil. May 12-16, 2008. Plenary Lecture.