

Curriculum Vitae

Name: **Amaury Pupo-Meriño**

Nationality: Cuban

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Education

- 1999-2004 B.S. in Biochemistry, Faculty of Biology, University of Havana, Cuba.
- 2003-2004 Master's course in Bioinformatics, Center for Genetic Engineering and Biotechnology (CIGB), Havana, Cuba.
- 2008 Master's Degree in Biochemistry (Mention Immunology), Faculty of Biology, University of Havana, Cuba.
- 2016 PhD in Science, mention Neuroscience. Universidad de Valparaíso. Chile.

Languages: Spanish (mother tongue), English.

Research Experience

- 2004-2006 Research on structure-function relationships of pore-forming proteins from marine origin. Center of Protein Studies, Faculty of Biology, University of Havana, Cuba.
- 2006-2008 Development of a new algorithm for prediction of class II T-cell epitopes. Study on the rotamericity of peptidic ligand side chains. Center of Molecular Immunology, Cuba.
- 2009-2013 Identification of MHC ligands presented in tumor cell lines and tissues by Mass Spectrometry. Center of Molecular Immunology, Cuba.
- 2011-2013 Design of chimeric proteins. B epitopes identification and reconstitution. Center of Molecular Immunology, Cuba.
- 2014- Structure-function relationship of Hv1 voltage-gated proton channel. Universidad de Valparaíso. Chile.

Teaching Experience

- 2004-2006 Seminars and laboratories in metabolism, enzymology, biochemical methods and bioinformatics. Faculty of Biology, University of Havana, Cuba.
- 2007-2013 Invited lectures about high throughput methodologies and Bioinformatics to Biochemistry students. Faculty of Biology, University of Havana, Cuba.

Expertise

- Bioinformatics. Data mining (R, RapidMiner).
- Structural biology. Protein design and modeling, protein-protein and protein-ligand docking, molecular dynamics (rosetta, modeller, namd, gromacs, autodock-vina).
- Computer system administration (Linux, Unix).
- High-Performance Computing Cluster set-up and administration.
- Programming (Python, bash, tcl, C, C++, Java).
- Liquid chromatography (HPLC): RP, IEC, affinity, 2D.
- Mass Spectrometry (MALDI, ESI, MSMS), proteomics, protein identification, quantization, sequencing and characterization, post-translational modifications.
- Biochemical methods. SDS and native PAGE, 2D electrophoresis.
- Electrophysiology, ion channel biophysics (patch-clamp, voltage-clamp, voltage-clamp fluorometry, cut-open, lipid-bilayers, kinetic models).

Publications

- Fernandez A, Pupo A, Mena-Ulecia K, Gonzalez C. Pharmacological modulation of proton channel Hv1 in cancer therapy: Future perspectives. *Mol Pharmacol*. 2016 Jun 3. pii: mol.116.103804.
- Pinto BI, García IE, Pupo A, Retamal MA, Martínez AD, Latorre R, González C. Charged residues at the first transmembrane region contribute to the voltage dependence of connexins slow gate. *J Biol Chem*. 2016 May 3. pii: jbc.M115.709402.
- García IE, Prado P, Pupo A, Jara O, Rojas-Gómez D, Mujica P, Flores-Muñoz C, González-Casanova J, Soto-Riveros C, Pinto BI, Retamal MA, González C, Martínez AD. Connexinopathies: a structural and functional glimpse. *BMC Cell Biol*. 2016 May 24;17 Suppl 1:17. doi: 10.1186/s12860-016-0092-x.
- García IE, Bosen F, Mujica P, Pupo A, Flores-Muñoz C, Jara O, Gonzalez C., Willecke K, Martinez AD. From hyperactive Connexin26 hemichannels to impairments in epidermal calcium gradient and permeability barrier in the Keratitis-Ichthyosis-Deafness syndrome. *Journal of Investigative Dermatology*. Jan 2016.
- Retamal MA, Garcia IE, Pinto B, Pupo A, Baez-Nieto D, Stebberg J, Del Rio R, Gonzalez C. Extracellular Cysteine in Connexins: Role as Redox Sensors. *Frontiers in Physiology* 12/2015.
- Morera FJ, Saravia J, Pontigo JP, Vargas-Chacoff L, Contreras GF, Pupo A, Lorenzo Y, Castillo K, Tilegenova C, Cuello LG, Gonzalez C. Voltage-dependent BK and Hv1 channels expressed in non-excitabile tissues: New therapeutics opportunities as targets in human diseases. *Pharmacol Res*. 2015 Nov; 01:56-64. doi: 10.1016/j.phrs.2015.08.011.
- Castillo K, Pupo A, Baez-Nieto D, Contreras GF, Morera FJ, Neely A, Latorre R, Gonzalez C. Voltage-gated proton (Hv1) channels, a singular voltage sensing domain. *FEBS Lett*. 2015 Nov 14;589(22):3471-8. doi: 10.1016/j.febslet.2015.08.003.
- Retamal MA, León-Paravic CG, Ezquer M, Ezquer F, Rio RD, Pupo A, Martínez AD, González C. Carbon monoxide: A new player in the redox regulation of connexin hemichannels. *IUBMB Life*. 2015 May 29. doi: 10.1002/iub.1388.

- Castillo K, Contreras GF, Pupo A, Torres YP, Neely A, González C, Latorre R. Molecular mechanism underlying $\beta 1$ regulation in voltage- and calcium-activated potassium (BK) channels. *Proc Natl Acad Sci U S A*. 2015 Apr 14;112(15):4809-14. doi: 10.1073/pnas.
- Pupo A, Gonzalez León C. In pursuit of an inhibitory drug for the proton channel. *Proc Natl Acad Sci U S A*. 2014 Jun 11. pii: 201408808.
- Tundidor Y, García-Hernández CP, Pupo A, Infante YC, Rojas G. Delineating the functional map of the interaction between nimotuzumab and the epidermal growth factor receptor. *MAbs*. 2014 Jul 1;6(4):1013-25. doi: 10.4161/mabs.28915. Epub 2014 Apr 23.
- Pupo A, Baez-Nieto D, Martínez A, Latorre R, González C. Proton channel models: Filling the gap between experimental data and the structural rationale. *Channels (Austin)*. 2014 Apr 22;8(3).
- Infante YC, Pupo A, Rojas G. A combinatorial mutagenesis approach for functional epitope mapping on phage-displayed target antigen: application to antibodies against epidermal growth factor. *MAbs*. 2014 May-Jun;6(3):637-48. doi: 10.4161/mabs.28395.
- Rojas G, Cabrera Infante Y, Pupo A, Carmenate T. Fine epitope specificity of antibodies against Interleukin-2 explains their paradoxical immunomodulatory effects. *MAbs*. 2014 Jan 1;6(1):273-85. doi: 10.4161/mabs.27224. Epub 2013 Nov 19.
- Alvarez-Ginarte YM, Montero-Cabrera LA, García-de la Vega JM, Bencomo-Martínez A, Pupo A, Agramonte-Delgado A, Marrero-Ponce Y, Ruiz-García JA, Mikosch H. Integration of ligand and structure-based virtual screening for identification of leading anabolic steroids. *J Steroid Biochem Mol Biol*. 2013 Nov;138:348-58. doi: 10.1016/j.jsbmb.2013.07.004. Epub 2013 Jul 18.
- Lamdan H, Gabilondo JV, Muñoz Y, Pupo A, Huerta V, Musacchio A, Pérez L, Ayala M, Rojas G, Balint RF, Larrick JW. Affinity maturation and fine functional mapping of an antibody fragment against a novel neutralizing epitope on human vascular endothelial growth factor. *Mol Biosyst*. 2013 Aug;9(8):2097-106. May 24.
- Rojas G, Pupo A, Gómez S, Kregel U, Moreno E. Engineering the binding site of an antibody against N-glycolyl GM3: from functional mapping to novel anti-ganglioside specificities. *ACS Chem Biol*. 2013 Feb 15;8(2):376-86. doi: 10.1021/cb3003754. Epub 2012 Nov 21.
- Rojas G, Pupo A, Leon K, Avellanet J, Carmenate T, Sidhu S. Deciphering the molecular bases of the biological effects of antibodies against Interleukin-2: a versatile platform for fine epitope mapping. *Immunobiology*. 2013 Jan;218(1):105-13. doi: 10.1016/j.imbio.2012.02.009. Epub 2012 Feb 16.
- Bencomo-Martínez, A., Sablón-Carrazana, M., Rivera-Marrero, S., Rodríguez-Tanty, C., Álvarez-Ginarte, Y. M., Pupo-Meriño, A., Rivera-, S., et al. Identificación y caracterización in silico de la zona de interacción entre el péptido beta-amiloide y compuestos derivados del naftaleno. *Revista CENIC Ciencias Químicas*, 2012, 43(1).
- Talavera A, Friemann R, Gómez-Puerta S, Martinez-Fleites C, Garrido G, Rabasa A, López-Requena A, Pupo A, Johansen RF, Sánchez O, Kregel U, Moreno E. Nimotuzumab, an antitumor antibody that targets the epidermal growth factor receptor, blocks ligand binding while permitting the active receptor conformation. *Cancer Res*.

2009 Jul 15;69(14):5851-9. Epub 2009 Jul 7. *Erratum in: Cancer Res.* 2009 Aug 15;69(16):6758.

- Pupo A, Moreno E. Do rotamer libraries reproduce the side-chain conformations of peptidic ligands from the PDB? *J Mol Graph Model.* 2009 Jan;27(5):611-9.
- Rojas G, Pupo A, Del Rosario Aleman M, Vispo NS. Preferential selection of Cys-constrained peptides from a random phage-displayed library by anti-glucitolysine antibodies. *J Pept Sci.* 2008 Nov;14(11):1216-21.
- Valiente PA, Batista PR, Pupo A, Pons T, Valencia A, Pascutti PG. Predicting functional residues in Plasmodium falciparum plasmepsins by combining sequence and structural analysis with molecular dynamics simulations. *Proteins.* 2008 Nov 1;73(2):440-57.
- Pazos F, Valle A, Martínez D, Ramírez A, Calderón L, Pupo A, Tejuca M, Morera V, Campos J, Fando R, Dyszy F, Schreier S, Horjales E, Alvarez C, Lanio ME, Lissi E. Structural and functional characterization of a recombinant sticholysin I (rSt I) from the sea anemone Stichodactyla helianthus. *Toxicon.* 2006 Dec 15;48(8):1083-94.

Patents

- Recombinant antibodies against endothelial growth factor (VEGF) obtained through mutagenesis of variable regions. Humberto Lamdan Ordaz, Jorge Victor Gavilondo Cowley, Marta Ayala Avila Muñoz, Yasmiana Well, Amaury Pupo Meriño, Gertrudis Rojas Dorantes, Lincidio Perez Sanchez. Granted on April 8, 2013. Certificate No.: 23895. Havana. Cuba.
- Polypeptides derived from TGF β and uses thereof. OSORIO Ángel de Jesús CORRIA, MONZÓN Kalet LEÓN, Portilla Tania Carmenate, MERIÑO Amaury PUPO, RODRÍGUEZ Saumel PÉREZ. Solicited on October 30th, 2013. WO 2014071894 A1.

Awards-Scholarships

- 1997 Member of the Cuban team to the III Iberoamerican Chemistry Olympiads, Rio de Janeiro, Brazil (winner of silver medal).
- 1998 Member of the Cuban teams to IV Iberoamerican Chemistry Olympiads, Bogota, Colombia (winner of gold medal).
- 2006 Mention to the best poster, in one of the sessions of the III International Symposium on Biochemistry and Molecular Biology, Havana, Cuba.
- 2014 Doctoral scholarship from CONICYT, Chile.
- 2015 National Prize from the Cuban Academy of Sciences, for the work "Study of the molecular basis of the Antibodies effects: development and application of a new platform for fine epitope mapping", Havana, Cuba.

Conferences, meetings

- Amaury Pupo, David Baez-Nieto, Ester Otarola, Osvaldo Yañez, Ariela Vergara-Jaque, Wendy Gonzalez, Karen Castillo, Gustavo Contreras, Ramón Latorre, Carlos Gonzalez. Permeation mechanism of the voltage-gated proton channel Hv1. Ion Channels in the Valley 2015. Valle del Elqui, Chile.

- Tundidor Y, García-Hernández CP, Pupo A, Cabrera Infante Y, Rojas G. Delineating the functional map of the interaction between nimotuzumab and the Epidermal Growth Factor Receptor. PepTalk 2015. January 19– 23. San Diego, California, USA.
- Amaury Pupo, Ester Otarola, David E. Baez-Nieto, Gustavo Contreras, Wendy González, Karen Castillo, Peter Larsson, Ramon Latorre and Carlos Gonzalez. Understanding the structural basis of permeation and selectivity in Hv1 proton channel. OMICS 2014. October 28-30th. Varadero, Cuba.
- Castillo Karen, Pupo Amaury, Torres Yolima, Lorenzo Yenislad, Alvarez Osvaldo, Neely Alan, Gonzalez Carlos, Latorre Ramón. The B Subunit N-Terminus is Involved in the Modulation of α -Subunit Voltage Sensor of BK Channels. X Annual Meeting. Sociedad Chilena de Neurociencia. Hotel Villa del Río, October 1-4, 2014. Valdivia, Chile.
- Pupo A, Otarola Este, Baez-Nieto David, Miño Germán, Contreras Gustavo, Yañez Osvaldo, Castillo Karen, Gonzalez Wendy, Latorre Ramón, Gonzalez Carlos. Mechanism Of The Permeation Pathway in Hv1 Channel. X Annual Meeting. Sociedad Chilena de Neurociencia. Hotel Villa del Río, October 1-4, 2014. Valdivia, Chile.
- Karen Castillo, Gustavo F., Contreras, Amaury Pupo, Yolima Torres, Sara Granados, Yenislady Lorenzo, Osvaldo Alvarez, Alan Neely, Carlos Gonzalez, and Ramon Latorre. The beta1 subunit N-terminus is involved in the modulation of alfa subunit voltage sensor of BK channels. Gordon Research Conference. Ion Channels. The Molecular Basis of Excitability and Disease. July 6-11, 2014. Mount Holyoke College. South Hadley, MA.
- Amaury Pupo, Ester Otarola, David E. Baez-Nieto, Gustavo Contreras, Osvaldo Yañez, Wendy Gonzalez, German Miño, Peter Larsson, Ramon Latorre and Carlos Gonzalez. Role of C-terminal of S4 in the permeation pathway of Ciona Intestinalis Hv1 Channel. Gordon Research Conference. Ion Channels. The Molecular Basis of Excitability and Disease. July 6-11, 2014. Mount Holyoke College. South Hadley, MA.
- José Alberto Gómez Pérez, Ana Victoria Casadeús, Marilyn Clavel, Amaury Pupo Meriño, Alejandro López Requena, Kalet León Monzón, MALDI MS characterization of the shift from N-glycolyl- to N-acetyl-sialic acid of the GM3 ganglioside in the mouse lymphocytic leukemia cells, 5^o Congresso Brasileiro de Espectrometria de Massas -BrMASS, BRASIL, 2013.
- Amaury Pupo Meriño, Alberto Bencomo Martínez, Yaima Cires Pérez, Kalet león Monzón, Computational design of chimeric proteins for B cell epitopes reconstruction, 9th Seminars of Advanced Studies of Molecular Design and Bioinformatics, CUBA, 2013.
- Amaury Pupo, José Alberto Gómez, MALDI-TOF-TOF application being developed at CIM, Humboldt Kolleg 2012: Challenges and Frontiers of Physics and Chemistry to Modern Biology, CUBA, 2012.
- Alberto Bencomo, Rodríguez Ch., Álvarez Y., Sablón M., Pupo A., In Silico study of naphthalene derivated compounds as possible inhibitors of beta-amyloid aggregation, QuimiCuba 2012, CUBA, 2012.
- Alberto Bencomo Martínez, M. Sablón Carrazana, S. Rivera Marrero, C. Rodriguez Tanty, Y. M. Álvarez Ginarte, A. Pupo Meriño, Identification and characterization in silica of the interaction zone between the beta-amyloidal peptide and naphthalene derived compounds, 4to Seminario Internacional de Nanociencias y Nanotecnologías, CUBA, 2012.
- A. Bencomo Martínez, C. Rodríguez Tanty, A. Pupo Meriño, Identification and characterization of the interaction sites between compounds derived from Naphtalene and beta-amyloid peptide, 20 Chemistry Conference, CUBA, Santiago de Cuba, 2011

- Alberto Bencomo Martínez, Amaury Pupo Meriño, Chryslaine Rodríguez Tanty, Identification and characterization of the interaction sites between compounds derived from naphthalene and beta-amyloid peptide, Seadim 8, CUBA, 2011.
- Amaury Pupo, José Alberto Gómez Pérez, Peptidomics: Analyzing complex mixtures of peptides with two-dimensional HPLC plus MALDI-TOF-TOF mass spectrometry, IT-2010, CUBA, 2010.
- A. Pupo, E. Moreno, A new hybrid, structure and artificial intelligence-based method for prediction of class II T-cell epitopes., 1st Ibero-american Congress on Chemistry, Biochemistry and Chemical Engineering., CUBA, 2009.
- Amaury Pupo, Un nuevo método híbrido basado en la estructura e inteligencia artificial para la predicción de epítodos T para MHC-II, XIII EXPOSICION FORJADORES DEL FUTURO, CUBA, La Habana, 2009.
- Amaury Pupo Meriño, Ernesto Moreno Frías, A new hybrid, structure and artificial intelligence-based method for prediction of class II T-cell epitopes, Seadimb 7, CUBA, 2009.
- Amaury Pupo, Desarrollo de un nuevo método de predicción de epitopos T de clase II, IV Conferencia Científica UCICIENCIA, CUBA, 2008.
- Amaury Pupo, Ernesto Moreno, A new hybrid, structure and artificial intelligence-based method for prediction of class II T-cell epitopes, IT-2008 Implementing Combinations, CUBA, 2008.
- A. Pupo, P. Valiente, M. E. Lanio, T. Pons, Similitud de estructura tridimensional y de secuencia aminoacídica entre actinoporinas, otras familias de toxinas formadoras de poros tipo-b, y proteínas que unen carbohidratos y lípidos., 6th International Congress on Chemistry and Chemical Engineering, CUBA, 2006.
- Pedro Valiente, Amaury Pupo, Maya Chávez, Maria Elena Lanio, Tirso Pons, Predicción de los residuos aminoacídicos funcionales en las plasmepsinas de Plasmodium falciparum: implicaciones para el Diseño de drogas antimaláricas, XXVII Congreso Latinoamericano de Química., CUBA, 2006.
- Aisel Valle, Pedro Valiente, Amaury Pupo, Maria Elena Lanio, Carlos Álvarez Valcarcel, Caracterización Estructural y funcional de Sticolisina I recombinante (RstI) de la anémona marina Stichodactyla helianthus., XXVII Congreso Latinoamericano de Química., CUBA, 2006.
- Pedro Valiente, Amaury Pupo, Maya Chávez, Tirso Pons, Prediction of functional residues from Plasmodium falciparum plasmepsins: implications in the antimalarial drugs design, ISBM, BRASIL, 2006.