Curriculum Vitae

Contact Information

Full Name: César Raúl García Jacas

Position: Professor and researcher of *Grupo de Investigación de Bioinformática, Centro de Estudio de Matemática Computacional*.

Job Address: Universidad de las Ciencias Informáticas. Carretera a San Antonio de los Baños, Km. 2 ½. Torrens, Municipio La Lisa. La Habana, Cuba.

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http://www.researchgate.net/profile/Cesar_Garcia-Jacas

Education and Training

2012 - 2015 Ph.D. Technical Sciences (Computer Science) from *Centro de Estudios Informáticos (CEI), Universidad Central "Marta Abreu" de Las Villas (UCLV), Santa Clara, Cuba*.

Definition of novel 3D molecular descriptors based on concepts of tensor algebra in order to codify chemical information between more than two atoms of a molecule, as well as its application in chemo-informatics tasks. Also, a parallel and distributed software was developed to compute the novel indices.

2011 - 2013 Master in Computer Science from *Centro de Estudios Informáticos (CEI), Universidad Central "Marta Abreu" de Las Villas (UCLV), Santa Clara, Cuba*.

Definition of novel 3D molecular descriptors based on bilinear, quadratic and linear algebraic maps and its application in chemo-informatics tasks.

2004 - 2009 Bachelor in Informatics Sciences from *Universidad de las Ciencias Informáticas (UCI), La Habana, Cuba*. Graduated *summa cum laude*.

Development of a multi-server computing system to carry out distributed calculations by using non-dedicated idle workstations allocated in the local network and its application in bio-chemo-informatics tasks.

Professional Experience

2015 - now Invited Professor, "*Pontificia Universidad Católica del Ecuador Sede Esmeraldas (PUCESE)*"

Teaching Data Structures, Programming Language and Software Engineering.

2013 - 2016 Researcher of "*Grupo de Investigación de Bioinformática, Centro de Estudio de Matemática Computacional (CEMC), Universidad de las Ciencias Informáticas (UCI)* "

Definition of novel 3D molecular descriptors and its application in the modeling of biological and toxicological activities. Development of software to carry out virtual screening of compound datasets using the QSAR models built with the novel 3D indices. High throughput computing applied to chemo-informatics applications.

2009 - 2016 Assistant Professor, Programming Techniques and Artificial Intelligence Department, "*Universidad de las Ciencias Informáticas (UCI)*"

Teaching Object Oriented Programming, Data Structures, Logic Programming, Artificial Intelligence and Machine Learning.

Awards

2016* National Mention of the Ministry of Science, Technology and Environment (CITMA) of the Republic of Cuba in the category of Researcher Young.

2015* National Award of the Cuban Academy of Sciences in Natural and Exact Sciences: "*Algorithms based on tensor algebra for the geometric characterization of organic molecules. Application to the prediction of biological activity*". **[main author]**

2015* Honorific National Mention to the Best Scientific Work, Technological and Innovation in Exact Sciences of the Republic of Venezuela: "*Novel global and local 3D atom-based linear descriptors of the Minkowski distance matrix: theory, diversity–variability analysis and QSPR applications*". **[co-author]**

2015 Rector Award of the "*Universidad de las Ciencias Informáticas (UCI)*" to the work of the highest originality and scientific impact: "*Algorithms based on tensor algebra to extract geometric features of organic molecules. Application to the prediction of biological activity*". **[main author]**

2009 Rector Award of the "*Universidad de las Ciencias Informáticas (UCI)*" for being the best student in the scientific research.

2008 Rector Award of the "*Universidad de las Ciencias Informáticas (UCI)*" to the work of the highest originality and scientific impact (student category): "*Distributed Computing Platform*". **[main author]**

2007 First Award in the Cuban National Computer Contest.

Publications (8)

2016* ***García-Jacas, C. R.***; Contreras-Torres, E.; Marrero-Ponce, Y.; Pupo-Meriño, M.; Barigye, S. J.; Cabrera-Leyva, L., Examining the predictive accuracy of the novel 3D N-linear algebraic molecular codifications on benchmark datasets. *Journal of Cheminformatics*. 2016, 8:10. **DOI:** 10.1186/s13321-016-0122-x

2015 Marrero-Ponce, Y.; ***García-Jacas, C. R.***; Barigye, S. J.; Valdés-Martiní, J. R.; Rivera-Borroto, O. M.; Pino-Urias, R. W.; Cubillán, N.; Alvarado, Y. J., Optimum Search Strategies or Novel 3D Molecular Descriptors: is there a Stalemate? *Current Bioinformatics*. 2015, 10 (5), 533-564. **DOI:** 10.2174/1574893610666151008011457

2015 Cubillán, N.; Marrero-Ponce, Y.; Ariza-Rico, R.; Barigye, S. J.; ***García-Jacas, C. R.***; Valdés-Martiní, J. R.; Alvarado, Y. J., Novel global and local 3D atom-based linear descriptors of the Minkowski distance matrix: theory, diversity–variability analysis and QSPR applications. *Journal of Mathematical Chemistry*. 2015, 53 (9), 2028-2064. **DOI:** 10.1007/s10910-015-0533-3

2015 Marrero-Ponce, Y.; Contreras-Torres, E.; ***García-Jacas, C. R.***; Barigye, S. J., Cubillán, N.; Alvarado, Y. J., Novel 3D bio-macromolecular bilinear descriptors for protein science: Predicting protein structural classes. *Journal of Theoretical Biology*. 2015, 374, 125-137. **DOI:** 10.1016/j.jtbi.2015.03.026

2015* Pino-Urias, R. W.; Barigye, S. J.; Marrero-Ponce, Y.; ***García-Jacas, C. R.***; Valdés-Martiní, J. R.; Pérez-Giménez, F., IMMAN: Free Software for Information Theory-based Chemometric Analysis. *Molecular Diversity*. 2015, 19 (2), 305-319. **DOI:** 10.1007/s11030-014-9565-z

2015* ***García-Jacas, C. R.***; Aguilera-Mendoza, L.; González-Pérez, R.; Marrero-Ponce, Y.; Acevedo-Martínez, L.; Barigye, S. J.; Avdeenko, T.; Multi-Server Approach for High-Throughput Molecular Descriptors Calculation based on Multi-Linear Algebraic Maps. *Molecular Informatics*. 2015, 34 (1), 60-69. **DOI:** 10.1002/minf.201400086

2014* ***García-Jacas, C. R.***; Marrero-Ponce, Y.; Acevedo-Martínez, L.; Barigye, S. J.; Valdés-Martiní, J. R.; Contreras-Torres, E., QuBiLS-MIDAS: A Parallel Free-Software for Molecular Descriptors Computation based on Multi-Linear Algebraic Maps. *Journal of Computational Chemistry*. 2014, 35 (18), 1395–1409. **DOI:** 10.1002/jcc.23640

2014 ***García-Jacas, C. R.***; Marrero-Ponce, Y.; Barigye, S. J.; Valdés-Martiní, J. R.; Rivera-Borroto, O. M.; Verbel, J. O., N-Linear Algebraic Maps to Codify Chemical Structures: is a suitable generalization to the atom-pairs approaches? *Current Drug Metabolism.* 2014, 15 (4), 441-469. **DOI:** 10.2174/1389200215666140605124506

International Congresses and Conferences

2016 XI International Congress of Informatics in the Health, *Multimodal Methodology in Quantitative Structure-Activity Relationships*. La Habana, Cuba, March 2016.

2015 III Colombian Congress of Computational Biology and Bioinformatics, *Novel 3D Multi-Linear Algebraic Molecular Descriptors*. Medellín, Colombia, September 2015.

2014 I International Scientific Conference of Computational Mathematic (UCIencia), *Software for parallel and distributed computing of the QuBiLS-MIDAS molecular descriptors*. La Habana, Cuba, March 2014.

2013 VIII Colombian Congress of Computation (8CCC). *Multi-Server Approach for Distributed Tasks*. Armenia, Quindío, Colombia, August 2013.

2010 III International Meeting of Computational Modeling, *Platform of Distributed Tasks*. Petrópolis, Rio de Janeiro, Brazil, January 2010.

2008 International Congress of Telematics and Telecommunications (CITTEL´08), *Distributed Computing System*. La Habana, Cuba, December 2008.

2007 XXXIII Congress of Theoretical Chemists of Latin Expression (QUITEL XXXIII), *Distributed Quantum-Chemistry Calculation*. La Habana, Cuba, September 2007.

Developed Software

2015 Software IMMAN for Information Theory-based Chemometric Analysis (http://mobiosd-hub.com/feature-selection-variable-screening/) **[collaborator]**

2015 Software QuBiLS-MAS for Topological Molecular Descriptors Computation Based on Bilinear, Quadratic and Linear Algebraic Maps (http://tomocomd.com/) **[collaborator]**

2014 Software QuBiLS-MIDAS for Geometric Molecular Descriptors Computation Based on Multi-linear Algebraic Maps (http://tomocomd.com/) **[main developer]**

2013 Multi-Server Distributed Computing System (http://tomocomd.com/) **[main developer]**

Undergraduate Teaching

- Object Oriented Programming
- Algorithms and Data Structures
- Logic Programming
- Artificial Intelligence
- Machine Learning
- Software Engineering

Postgraduate Teaching

- Distributed and Parallel Computing