

# Ernesto Estrada

## Curriculum Vitae

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### *Professor and Chair in Complexity Sciences*

Department of Mathematics and Statistics

Department of Physics

Institute of Complex Sciences at Strathclyde (ICSS)

University of Strathclyde, Glasgow G1 1XQ

<http://www.estradalab.org>

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## PERSONAL

Date of Birth: May 2, 1966

Place of Birth: Sancti Spíritus, Cuba

Citizenship: Spanish, Cuban

Marital status: Married (1 daughter)

## EDUCATION

Ph. D. (Chemistry). Central University of Las Villas, Cuba, 1997.

Dissertation Title: *Novel Graph-Theoretical Approaches to Molecular Design in Organic Chemistry*. Supervisor: Prof. L. A. Montero-Cabrera

M.A. (Chemistry), Central University of Las Villas, Cuba, 1990.

Dissertation Title: *Chemico-biological studies of antimicrobial 2-furylethylenes*

## HONORS AND AWARDS

- 1 Visiting Research Fellow of the Statistical and Applied Mathematical Sciences (SAMSI), North Carolina, USA, March-April 2011.
- 2 Visiting Research Fellow of the Institute of Industrial Science, The University of Tokyo, Japan, April-June 2008.
- 3 Fellowship of the Royal Society of Edinburgh International Exchange Programme and Edinburgh Mathematical Society for visiting the Department of Mathematics, University of Strathclyde, Scotland, U.K., 2008
- 4 “Outstanding Scientist” Award of the International Academy of Mathematical Chemistry, International Academy of Mathematical Chemistry, Dubrovnik, Croatia, 2007.
- 5 Elected as Full Member of the “*International Academy of Mathematical Chemistry*”, Dubrovnik, Croatia, 2005.
- 6 “Ramón y Cajal” Research Contract. Ministry of Education and Culture, Spain, 2003-2008.
- 7 “Foreign Scientists and Technologist in Spain” Postdoctoral Fellowship, Ministry of Education and Culture, Spain, 2001-2002.
- 8 “Lisa Mietner-Minerva Institute for Computational Quantum Chemistry” Postdoctoral Fellowship, Hebrew University of Jerusalem, 1999-2000.

- 9 National Prize of the Cuban Academy of Science, Section of Natural Science, La Habana, Cuba, 1998.
- 10 “Una Nau de Solidaritat” Postdoctoral Fellowship, Regional Government of Valencia, Spain, 1997.

## **APPOINTMENTS**

- 2008- Full Professor and Chair in Complexity Sciences, Department of Mathematics, Department of Physics and Institute of Complex Systems at Strathclyde, University of Strathclyde, Glasgow, U.K.
- 2003-2008 “Ramón y Cajal” Researcher in Complex Systems, University of Santiago de Compostela, Spain.
- 2002-2003 Research Scientist of Computational Chemistry, Safety & Environmental Assurance Centre (SEAC), Unilever, Colworth, U.K.
- 2001-2002 Postdoctoral Research Associate. Department of Organic Chemistry, University of Santiago de Compostela, Spain.
- 1999 Visiting Professor at the Department of Organic Chemistry, University of Santiago de Compostela, Spain.
- 1999-2000 Postdoctoral Researcher at the Lisa Mietner-Minerva Institute for Computational Quantum Chemistry, Hebrew University of Jerusalem, Israel. Mentor: Prof. D. Avnir.
- 1997 Postdoctoral Researcher at the Department of Physical Chemistry, University of Valencia, Spain. Mentor: Prof. J. Gálvez.
- 1993-1998 Assistant Researcher. Department of Computer-Aided Drug Design at the Center for Bioactive Chemicals, Central University of Las Villas, Cuba.
- 1990-1993 Instructor of Organic Chemistry, Department of Chemistry and Pharmacy, Central University of Las Villas, Cuba.

## **RESEARCH GRANTS**

- 2010-2012 Grant from the Engineering and Physical Sciences Research Council and the Research Councils UK Digital Economy Programme, together with Prof. D. J. Higham on the project MOLTEN: Mathematics Of Large Technological Evolving Networks. Award of £181,000.00.
- 2009 Grant “Bridging the Gap” from the University of Strathclyde and the Engineering and Physical Sciences Research Council, U.K. on the project “Water Supply Networks”. Award of £9,143.00.
- 2008-2011 Grant “New Professors Fund” from the University of Strathclyde, Glasgow, U.K. for the development of interdisciplinary researches in complex networks. Award of £25,000.00.
- 2004 Unilever UK Central Resources Limited Grant: “Development of structural alerts for chromosome aberrations and other genetic toxicological endpoints for organic compounds. Use of the TOPS-MODE approach.”

Award of 11,000.00 Euros.

- 2002-2005 FONDECYT, Chile. Grant to Motivate the International Cooperation: “QSPR models to predict physico-chemical properties of herbicides from quantum-chemical descriptors.”  
Award of \$60,000.00.
- 2001-2003 FAPESP (Fundação de Auxílio Pesquisa Estado de São Paulo) Brasil: “Synthesis of prenylated compounds with antibacterial and antimicrobial activities.”  
Award of \$10,648.40.
- 2000-2002 Ministry of Science and Technology, Spain: “Synthesis and studies of new coumarins, furocoumarins and tetracyclic derivatives of coumarins with pharmacological interest.”  
Award of 49,042.00 Euros.
- 2001 Regional Government of Galicia, Spain: “System for Molecular Design.”  
Award of 45,436.51 Euros.

## **MEMBERSHIP OF PROGRAM COMMITTEE**

Program Committee Member for ACM-SAC Conference on Bioinformatics and Computational System Biology, Riva del Garda, Italy, March 2012. Sponsored by the ACM Special Interest Group on Applied Computing (SIGAPP).

Program Committee Member for the 4th International Interdisciplinary Chaos Symposium on Chaos and Complex Systems, CCS2012, Turkey 29<sup>th</sup> April-2<sup>nd</sup> May 2012.

Program Committee Member of the GSTF's Annual International Conference on Operations Research and Statistics (ORS), Hotel Fort Canning, Singapore, 16th-17th April 2012.

Program Committee Member of the Annual International Conference on Computational Mathematics, Computational Geometry and Statistics, Hotel Fort Canning, Singapore, 30-31 January 2012.

## **INVITED LECTURES AND SEMINARS**

- 1 “Predicting toxicity from molecular structure. A topological tale”, Invited Talk at the NC3Rs/Mathematics in Medicine Study Group workshop on Mathematical Modelling and Toxicology
- 2 “Decoding Matrix Structure by Matrix Functions”, Colloquium at the Department of Mathematics and Computer Science, Emory University, Atlanta, USA, April 2011.
- 3 “Approaching Network Structure by Spectral Methods”, Mathematical Biology Seminar at the case Western Reserve University, Cleveland, Ohio, USA, April 2011.

- 4 "Communicability in Complex Networks", Seminar at Statistical and Applied Mathematical Sciences Institute, SAMSI, North Carolina, USA, April 2011.
- 5 "Spectral Analysis of Complex Networks", Invited Speaker Lecture, *The 1st International Symposium on Innovative Mathematical Modelling*, Tokyo, Japan, February, 2011.
- 6 "Patterns in Complex Networks via Spectral Analysis", Plenary Speaker Lecture, *Joint IAPR International Workshops on Structural and Syntactic Pattern Recognition (SSPR 2010) and Statistical Techniques in Pattern Recognition (SPR 2010)*, Cesme, Turkey, August 2010.  
Available at: [http://videolectures.net/ssspr2010\\_estrada\\_pcn/](http://videolectures.net/ssspr2010_estrada_pcn/)
- 7 "A Graph Theoretic Approach to Atomic Displacements in Fullerenes". Keynote Speaker Lecture, *Computers in Scientific Discovery*, University of Sheffield, Sheffield, 20/07/2010.
- 8 "Communicability and the evolution of communities in networks", Invited Lecture, *The Unexpected Link: Using Network Science to Tackle Social Problems*, Budapest, Hungary (June 17-18, 2009).
- 9 "Spectra of Complex Networks: Centrality Measures and Applications", Invited Lecture, *Applications of Physics in Financial Analysis, 7<sup>th</sup> International Conference*, Tokyo, Japan (March 1-5, 2009).
- 10 "Golden Spectral Graphs and Networks", Invited Lecture, *Spectral Graph Theory in Rio*, Rio de Janeiro, Brazil (December 1-4, 2008).
- 11 "Complex Networks: from Nature and Society to Technology", Lecture, Workshop *Complexity in the Brain*, University of Strathclyde, Glasgow (September 22, 2008).
- 12 "Centrality and Communities in Complex Socio-Economic Networks", Lecture, Tokyo Institute of Technology (May 24, 2008).
- 13 "Mathematical Characterization of Local and Global Properties in Complex Networks", Lecture, Department of Informatics, University of Tokyo (May 19, 2008).
- 14 "Protein Origami: How to Quantify the Degree of Folding of Protein Chains", Lecture, Department of Applied Physics, University of Tokyo (May 7, 2008).
- 15 "Detecting communities in Complex Networks", Lecture, Institute of Industrial Sciences, University of Tokyo, Japan (April 21, 2008).
- 16 "Complex networks: From the cell to ecosystems", Lecture, Faculty of Sciences, University of Oporto, Portugal (March 7, 2008).
- 17 "Complex networks and Biology in the XXI century", Lecture, Institute for Marine Sciences, CSIC, Vigo, Spain (March 6, 2008).
- 18 "Topological characterization of complex biological networks", Seminar, Center for Mathematics Applied to the Life Sciences, University of Strathclyde and University of Glasgow, U.K. (February 20, 2008).
- 19 "Protein Origami: The Degree of Folding of Proteins", Seminar, Bioinformatics Research Centre, University of Glasgow, U.K. (February 19, 2008).
- 20 "Topological characterization of complex biological networks", Seminar, Translational Medicine Research Collaboration, The Sir James Black Centre, University of Dundee, U.K. (February 15, 2008).
- 21 "A Novel Topological Approach to Molecular Design in Organic Chemistry", Lecture, Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria (October 30, 2007).
- 22 "From Small Molecules to "Small-Worlds", Lecture, Faculty of Experimental Sciences, University of Almería, Spain (January 26, 2007).
- 23 "The parts in the whole. The role of mathematics in the study of complex systems.", Lecture, VIII National Conference of Spanish Deans and Directors of Mathematics,

- 2006, Polytechnic University of Valencia, Valencia, Spain (November 23-25, 2006).
- 24 “How the Parts are Organized in the Whole? An Excursion to Complex Systems”, Lecture, Second Meeting of The International Academy of Mathematical Chemistry (IAMC) Dubrovnik, Croatia (June 15-17, 2006).
  - 25 “Subgraph centrality, bipartivity and spectral scaling in complex networks.”, Invited Talk, Conference on Complex Networks: Evolution and Statistical Properties, Salou, Spain (March 14-18, 2005)
  - 26 “Structural characterization of complex networks”, Lecture, VII Seminar of Discrete Mathematics, University Carlos III, Madrid, Spain (May 12-13, 2005).
  - 27 “A universal topological property of complex networks.”, Invited Talk, Nordic Workshop on Networks. NORDITA, Niels Bohr Institute, Copenhagen, Denmark (December 16-18, 2004).
  - 28 “Characterization of the Degree of Folding of Proteins”, Lecture, Faculty of Chemistry, University of Concepción, Chile (October 20, 2004).
  - 29 “Quantitative Structure-Property and Structure-Activity Relationships. A Personal View”, Lecture, Faculty of Chemistry, University of Concepcion, Chile (January 22, 2003).
  - 30 “From 2D Drug Design to 3D Characterization of the Degree of Folding of Proteins”, Lecture, Department of Chemistry, University of Campinas, Brazil (February 22, 2002).
  - 31 “Characterization of protein folding degree in lattice and real proteins.” Lecture, The Sixteenth International Course & Conference on the Interfaces among Mathematics, Chemistry & Computer Sciences, Dubrovnik, Croatia, (June 25-30, 2001).
  - 32 “Wiener number in the context of generalized topological indices”, Lecture, The Harry Wiener International Memorial Conference on the Role of Topology in Chemistry, University of Georgia, Athens, Georgia, USA (March 2001).
  - 33 “An Introduction to Bioinformatics for Mathematicians”. Invited Seminar, Institute of Mathematics, University of Santiago de Compostela, Spain (December 14, 2001).
  - 34 “Extending the molecular connectivity indices. From bond connectivity to long-range connectivity indices.”, Lecture, Symposium for the 25<sup>th</sup> Anniversary of the Connectivity Indices. 220<sup>th</sup> National Meeting of the American Chemical Society, Washington DC, USA (August 20-24, 2000).
  - 35 “Spectral Moments of the Edge adjacency Matrix. Applications to Molecular Design.”, Seminar at the Group of Combinatorics, Graph Theory and Applications, Polytechnic University of Barcelona, Spain (April 10, 1997).

## CONTRIBUTED PAPERS AND POSTER PRESENTATION

1. "From Networks to Hypernetworks", Oral communication, NETSCI 09, International Workshop and Conference on Complex Networks and their Applications, Venice, Italy (June 29-July 3, 2009). Work together with Naomichi Hatano.
2. "Proteins as Complex Networks", Lecture, IAMC, International Academy of Mathematical Chemistry, Dubrovnik, Croatia (June 10-14, 2009).
3. "Spectral Measures for Molecular Networks", Lecture, MCC 2009, International Conference Math/Chem/Comp, Dubrovnik, Croatia (June 4-9, 2009).
4. "Complex Networks and OMICS", Lecture, Symposium on Complex Networks: Biology, Ecology, Society; University of Santiago de Compostela, Spain (June 22, 2007).
5. "Complex Networks", Lecture, Second Meeting of the International Academy of Mathematical Chemistry; Dubrovnik, Croatia (June 8, 2006).
6. "Utility of Cyclodextrins for the Improvement of the Solubility of Sertaconazol", Poster, V Congress of the Spanish Society of Industrial Pharmacy, Valencia, Spain (February 6, 2001).
7. "New Tetracyclic Frameworks with Potential Antitumor Interest", Poster, XVth International Symposium on Medicinal Chemistry, Bologna, Italy (November 22, 2000).
8. "In Silico Studies for the Screening and Design of Pharmacologically Active Compounds", Poster, XVth International Symposium on Medicinal Chemistry, Bologna, Italy (November 22, 2000).
9. "New N,N-Disubstituted Piperazines as Serotonine and Dopamine Ligands", Poster, XVth International Symposium on Medicinal Chemistry, Bologna, Italy (November 22, 2000).
10. "Toss-Mode in Predicting Biological, Toxicological and ADME Parameters of Organic Compounds", Lecture, The 15th Dubrovnik International Course & Conference Math/Chem/Comp 2000, Dubrovnik, Croatia (June 24, 2000).
11. "Design, Synthesis and in Vitro Determination of the Antimicrobial Activity of New Gamma-Nitrocyclohexanones", Poster, IV Iberoamerican Meeting of Pharmaceutical and Food Sciences, La Habana, Cuba (June 30, 2000).
12. "Use of the TOPS-MODE Approach for the Classification of Capsaicin Analogues with Analgesic Activity and for Structure-Property Relationships (QSPR) Studies", Poster, IV Iberoamerican Meeting of Pharmaceutical and Food Sciences, La Habana, Cuba (June 30, 2000).
13. "Predicting Chemical Reactivity (Log K) and Octanol/Water Partition Coefficient (Lipophilicity, Log P) of Furylethylene Compounds from Graph-Theoretical Molecular Descriptors", Poster, 16<sup>th</sup> Conference of Chemistry, University of Oriente, Santiago de Cuba, Cuba, (December 10, 1999).
14. "Use of a Novel Theoretical Approach to Calculate the Fragment Contribution of a Molecule to the Biological Activity", Poster, 16<sup>th</sup> Conference of Chemistry, University of Oriente, Santiago de Cuba, Cuba, (December 10, 1999).
15. "Use of Local Spectral Moments in Drug Design", Poster, 16<sup>th</sup> Conference of Chemistry, University of Oriente, Santiago de Cuba, Cuba, (December 10, 1999).
16. "Designing Antifungal and Antibacterial Compounds by a Substructural Graph-Theoretical Approach", Poster, 16<sup>th</sup> Conference of Chemistry, University of Oriente, Santiago de Cuba, Cuba, (December 10, 1999).
17. "Piecewise Linear Regression-Discriminant Analysis (PLR-DA) in QSAR Studies", Poster, III International Congress of the Cuban Chemical Society, University of

- Oriente, Santiago de Cuba (December 4, 1998).
18. "Designing Biologically Active Compounds from a Novel Substructural Graph-Theoretical Approach", Poster, III International Congress of the Cuban Chemical Society, University of Oriente, Santiago de Cuba (December 4, 1998).
  19. "On the Nature of Topographic Indices Based on Electronic Properties of Molecules", Poster, 7th International Conference on Mathematical Chemistry and 3rd Girona Seminar on Molecular Similarity, Girona, Spain (May 31, 1997).
  20. "Generalizations of Wiener Number and other Distance-Based Graph Theoretical Invariants", Poster, 7th International Conference on Mathematical Chemistry and 3rd Girona Seminar on Molecular Similarity, Girona, Spain (May 31, 1997).
  21. "Spectral Moments of Bond Matrix. A Novel Substructural Approach to QSPR and QSAR Studies", Poster, 7th International Conference on Mathematical Chemistry and 3rd Girona Seminar on Molecular Similarity, Girona, Spain (May 31, 1997).
  22. "Theoretical Studies for the Rational Functionalization of 2-Bromo-(3-Fur-2-yl)-3-oxo-Propionamide", Poster, First Workshop on Molecular Modeling and Applications, La Habana, Cuba (March 28, 1997).
  23. "Comparative Study of the Antibiotic Activity of Gamma-Lactamic Compounds with the Use of Topological and Topographic Descriptors", Poster, First Workshop on Molecular Modeling and Applications, La Habana, Cuba (March 28, 1997).
  24. "Simulation of Antibiotics Penetration into Cerebrospinal Fluids in Bacterial Meningitis", Lecture, First International Workshop on Antibiotics, La Habana, Cuba (November 4, 1993).
  25. "Quantitative Structure-Activity Relationships (QSAR) Study of the Action Mechanism of Antibacterial Furfurylenes Derivatives", Poster, First International Workshop on Antibiotics, La Habana, Cuba (November 4, 1993).
  26. "Advances in the Registration of 1-(5-Bromofur-2-yl)-2-Bromo-2-Nitroethene in Veterinary Medicine", XIII Conference of Chemistry, University of Oriente, Santiago de Cuba, Cuba (January 25, 1990).
  27. "Quantitative Determination of Polyatomic Anions in NaCl Matrices by using IR Spectroscopy", Oral presentation, XI Conference of Chemistry and II Congress of the Cuban Chemical Society, University of Oriente, Santiago de Cuba, Cuba (January 25, 1985).

## **GRADUATE STUDENTS AND POSTDOCS SUPERVISED**

1. Enrique Molina-Pérez (Ph. D., Chemistry, University of Camagüey, Cuba, 2003).
2. Santiago Vilar (Ph. D., Pharmacy, University of Santiago de Compostela, Spain, 2006).
3. Franck Kalala-Mutombo, Ph. D. Student at the Department of Mathematics and Statistics, University of Strathclyde, 2008-2012.
4. Chanpen Phokaew, Ph. D. Student at the Department of Mathematics and Statistics, University of Strathclyde, 2008-2012.
5. Eusebio Vargas-Estrada, Ph. D. Student at the Department of Mathematics and Statistics, University of Strathclyde, 2010-2014.
6. Dr. Alan Taylor, Post Doctoral Fellow (Research Assistant) at the Department of Mathematics and Statistics, University of Strathclyde, 2010.
7. Dr. Alex Mantzaris, Post Doctoral Fellow (Research Assistant) at the Department of Mathematics and Statistics, University of Strathclyde, 2011-2013.

## PROFESSIONAL SOCIETIES

- 1 Full Member of the “*International Academy of Mathematical Chemistry*”.
- 2 Edinburg Mathematical Society
- 3 London Mathematical Society
- 4 SIAM, Society for Industrial and Applied Mathematics

## ACADEMIC SERVICE

### Membership in the Editorial Board of Journals

- 1 *Journal of Chemical Information and Computer Science*, 2001-2003.
- 2 *MATCH: Communications in Mathematical and in Computer Chemistry*.
- 3 *Current Drug Discovery Technologies*.
- 4 *Drug Design Reviews-Online*.

Reviewer for *Mathematical Reviews* of the *American Mathematical Society*.

Reviewer for: *Advances in Complex Systems*, *American Naturalist*, *Bioorganic & Medicinal Chemistry*, *Bioorganic & Medicinal Chemistry Letters*, *Centro European Journal of Chemistry*, *Chemical Physics Letters*, *Chemical Research in Toxicology*, *Chemical Reviews*, *Chirality*, *Communications in Mathematical Chemistry (MATCH)*, *Computers & Chemistry*, *Current Medicinal Chemistry*, *European Journal of Medicinal Chemistry*, *International Journal of Quantum Chemistry*, *Journal of Chemical Information and Modeling*, *Journal of Computational Chemistry*, *Journal of Computer-Aided Molecular Design*, *Journal of Medicinal Chemistry*, *Journal of Molecular Structure (Theochem)*, *Journal of Physical Organic Chemistry*, *Journal of Theoretical Biology*, *Linear Algebra and its Applications*, *Macromolecular Chemistry*, *Medicinal Research Reviews*, *Molecular Diversity*, *Molecules*, *Physical Review E*, *Physical Review Letters*, *Physics Letters A*, *SAR & QSAR in Environmental Research*, *The Journal of Physical Chemistry A*.

## PATENTS

1. Procedure for the preparation of 1-(5-bromofur-2-yl)-2-bromo-2-nitroethene and its microcide action. N. Castañedo, R. Goizueta, J. Pérez, J. González, E. Silveira, M. Cuesta, A. Martínez, E. Lugo, E. Estrada, A. C. Carta, O. Navia and M. S. Delgado. Cuban Patent 4894 (1994). European Patent Application 95500056.7. Publication number: 0 678 516 A1. Canadian Patent Application 2,147,594. Japan Patent Application 222002. U. S. Patent, application number 60008011.
2. Substituted Hydroxyacetophenon Derivatives. J. Quincoces, E. Estrada, K. Peseke, international Patent WO/2006/003010; International Application Number: PCT/EP2005/007307.

## CITATION INDICATORS

H-index<sup>1</sup>: 33  
Citations<sup>1</sup>: >3,000

2008. Ranked among the most influential scientists in Spain according to the h-index [http://es.geocities.com/indice\\_h/](http://es.geocities.com/indice_h/)
2007. Ranked as the most influential scientist in Spain in the area of Interdisciplinary Applications of Computational Sciences according to his H-index ([http://es.geocities.com/indice\\_h/computer.html](http://es.geocities.com/indice_h/computer.html))
2007. Ranked by ISI Essential Science Indicators among the *Most Cited Authors in Chemistry* (updated on January 1, 2008) in the last 10 years (from 01/01/1997 until 31/10/2007) occupying the position 5402 among 6756 chemists according to the 15.66).
2006. Ranked by ISI Essential Science Indicators among the *Most Cited Authors in Chemistry* (updated on May 1, 2007) in the last 10 years (from 01/01/1997 until 28/2/2007) occupying the position 5304 among 6365 chemists according to the number of citations (847) and the position 3382 according to citations per paper (14.60).
2005. Ranked by ISI Essential Science Indicators among the *Most Cited Authors in Chemistry* (updated on March 1, 2006) in the last 10 years (from 01/01/1995 until 31/12/2005) occupying the position 3540 among 6378 chemists according to the number of citations (1089) and the position 1878 according to citations per paper (18.78).

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<sup>1</sup> According to ISI Web of Sciences