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HIGHER EDUCATION

M.Sc., Chemistry, Central University of Las Villas, Cuba, 1990.
Honours Thesis: *Chemico-biological studies of antimicrobial 2-furylethylenes*

Ph. D., Chemistry, February 1997, Central University of Las Villas, Cuba (Prof. L. A. Montero-Cabrera). Dissertation Title: *Novel Graph-Theoretical Approaches to Molecular Design in Organic Chemistry*.

CAREER OUTLINE

2014-	Director, Institute of Complex Systems at Strathclyde, University of Strathclyde, Glasgow, U.K.
2013	Visiting Professor and Fellow, Institute of Quantitative Methods and Theory (QuanTM), Emory University, Atlanta, USA.
2008-	Full Professor and Chair in Complexity Sciences, Department of Mathematics, University of Strathclyde, Glasgow, U.K.
2008-2012	Full Professor and Chair in Complexity Sciences, Department of Mathematics and Department of Physics, 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, Coloworth, U.K.

2001-2002 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.

HONORS and AWARDS

2014 Elected member of the Academia Europeae

2014 Awarded 1964 Chair of mathematics at University of Strathclyde

2014 Royal Society Wolfson Research Merit Award "for respected scientists of outstanding achievement and potential to the UK", given by the Royal Society in 2013 for the period 2014-2018

2012 Plenary Speaker at the 2012 SIAM Annual Meeting, Minneapolis, USA, 9-13 July, 2012

2007 Award "Outstanding Scientist" given by the International Academy of

Mathematical Chemistry, Dubrovnik, Croatia

2005 Elected Full Member of the "*International Academy of Mathematical Chemistry*", Dubrovnik, Croatia

1998 National Prize of the Cuban Academy of Science, Section of Natural Science, La Habana, Cuba

VISITING POSITIONS

2013 Visiting Professor at the Department of Mathematics and Computer Sciences and Fellow of the Institute for Quantitative Theory and Methods (QuanTM), *Emory University,* Atlanta, USA

2013-2014 Visiting Professor at the Centre of Mathematical Research, Guanajuato, Mexico

2012-2013 Visiting Professor at the Centre of Mathematical Research, Guanajuato, Mexico

2011 Visiting Research Fell***ow*** of the Statistical and Applied Mathematical Sciences (SAMSI), North Carolina, USA

2008 Visiting Research Fellow of the Institute of Industrial Science, The University of Tokyo, Japan

2008 Visiting research fellow 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.

EDITORIAL WORK

Editor-in-Chief *Journal of Complex Networks* (Oxford University Press)

On the Editorial Board of:

MATCH: Communications in Mathematical and in Computer Chemistry,
Journal of Chemical Information and Computer Science, 2001-2003;

Current Drug Discovery Technologies;
Drug Design Reviews-Online;
Open Journal of Biophysics.

Governmental Experts, MAPRA Network, Animal and Plant Health, European Food Safety Authority.

Expert for Projects of the European Commission.

Reviewer of Grant Applications for The Romanian National Council for Research and Development.

Reviewer of Grant Applications for The Netherlands Organisation for Scientific Research (NWO) for Veni grants in the Innovational Research Incentives Scheme.

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).

LEADERSHIP

2014-	Director, Institute of Complex Systems at Strathclyde, University of Strathclyde, Glasgow, U.K.
2010-	Head of the Applied Analysis Group, Department of Mathematics and Statistics, University of Strathclyde.
2010-	Member of the Scientific Committee, Department of Mathematics and Statistics, University of Strathclyde.
2008-	Member of the Professorial Advisory Group, Department of Physics, University of Strathclyde.
2008-	Member of the Steering Committee, Institute of Complex Systems, University of Strathclyde.

2000-2008 Head of the Computational Chemistry and Bioinformatics Group, Department of Organic Chemistry, University of Santiago de Compostela, Spain.

1994-1998 Head of the Computer-Aided Molecular Design, Centre of Chemical Bioactive Agents, Central University of Las Villas, Cuba

1994-1998 Member of the Scientific Committee, Centre of Chemical Bioactive Agents, Central University of Las Villas, Cuba

TEACHING EXPERIENCE

Emory University

- **Combinatorics Seminar: Introduction to Network Theory** (Graduate level course attended by Mathematics, physics, Statistics and Biostatistics students).

University Strathclyde

- **Linear Algebra** (2nd year Mathematics and Physics students.)
- **Mathematics for Engineers** (1st year Engineering Students. Includes: Algebra, Geometry and Calculus)
- **Engenieering Mathematics**. **Applications** (1st Year Engineering Students. Includes: Further calculus, geometry and vectors, matrices and numerical methods)
- **Mathematical Introduction to Networks** (4th year Math students).
- **Modern Theory for Complex Networks. Dynamical Systems** (M.S. Math Students).
- **Modelling structure and dynamics in complex networks (NERC Course for** Postgraduate and professional skills development courses for environmental sciences PhD students and early career researchers)
- **Computational and Visualization Physics III** (3rd year Physics students. Includes: data analysis, Fourier transform, networks)

- I have supervised 9 students (in 4 years) for the Honours degree project in their 4th year of B.Sc Mathematics and B.Sc. Physics.

- The following students have received fellowships to work during the summer in a research project under my supervision:

  - ✓ Stephen Howorth: supervisor Ernesto Estrada; topic: Tight-binding analysis of belt-shaped carbon allotropes (Escherynes). Intern@Strathclyde, 2012.

  - ✓ Chang Xu; supervisor Ernesto Estrada; topic: Communities in Complex Networks. Intern@Strathclyde, 2011.

  - ✓ Kevin Deegan; supervisor Ernesto Estrada; topic: Ranking Problems in Complex Networks. EPSRC Vacation Bursary, 2010.

  - ✓ Yanfeng Liang; supervisor Ernesto Estrada; topic: Mathematical Study of Protein Structure and Function. Carnegie Undergraduate Vacation Scholarship, 2010.

  - ✓ Kevin Deegan; supervisor Ernesto Estrada; topic: Extension of the communicability concept based on matrix functions. Carnegie Undergraduate Vacation Scholarship, 2009.

- I have actively participated in the meetings the Department organizes for 3rd and 4th year students during a weekend in which I have given a couple of talks about general applications of mathematics in interesting areas to motivate students to continue their education beyond BSc degrees.

African Institute of Mathematical Sciences (AIMS)

- **Dynamics on Complex Networks.** (Graduate Course for Math Students).

Previous

- **Biophysics of protein folding problems** (Post graduate course. Includes: Topics in biophysics of proteins, bioinformatics)

- **Organic Chemistry I** (chemical bonding, alkanes, cycloalkanes, sterochemistry, alkenes, alkynes, substitution and elimination, radicals, aromatic compounds, nucleophilic aromatic substitution)

- **Organic Chemistry III** (nitrogen containing compounds, heterocycles, carbohydrates, stereochemistry)

- **Molecular Spectroscopy** (UV-Vis, IR, NMR, Mass spectrometry)

- **Theoretical Methods for Molecular Design** (Post graduate course).

Ph.D. THESES SUPERVISED

1. Enrique Molina-Pérez (Ph. D., Chemistry, University of Camagüey, Cuba, 2003). Currently Vice-Dean of Research at the University of Camagüey, Cuba; Member of the Editorial Board of the Cuban Journal of Chemistry.

2. Santiago Vilar (Ph. D., Pharmacy, University of Santiago de Compostela, Spain, 2006). First at the Laboratory of Biological Modeling at the National Institutes of Health (NIST) in Bethesda, Maryland and currently at the Columbia University, USA.

3. Franck Kalala-Mutombo, Ph. D. Student at the Department of Mathematics and Statistics, University of Strathclyde, 2012. Currently a Lecturer at the Mombashi University, R. D. Congo.

4. Chanpen Phokaew, Ph. D. Student at the Department of Mathematics and Statistics, University of Strathclyde, 2008-2013.

5. Eusebio Vargas-Estrada, Ph. D. Student at the Department of Mathematics and Statistics, University of Strathclyde, 2010-2014.

6. Matthew Sheering, Ph. D. Student at the Department of Mathematics and Statistics, University of Strathclyde, 2013-2017.

PUBLICATIONS

Citation indicators (from Google Scholar[1])

Number of citations: 6,955
h-index: 49

Books

B1. *A First Course in Network Theory*, E. Estrada, P. Knight, Oxford University Press, in press, **2014**.

B2. *The Structure of Complex Networks. Theory and Applications*, E. Estrada, Oxford University Press, **2011**.

[1] On 29 March 2014.

B3. *Network Science: Complexity in Nature and Technology*, Edited by E. Estrada, M. Fox, D. J. Higham and G.-L. Oppo, Springer, **2010**.

Refereed Journal Papers

P1. *Maximum walk entropy implies walk regularity*, Estrada, E., de la Peña, J.A., Linear Algebra and its Applications, 458, **2014,** 542-547.

P2. *Communicability reveals a transition to coordinated behavior in multiplex networks*, Estrada, E., Gómez-Gardeñes, J., Physical Review E, 89, **2014**, 042819.

P3. *Walk entropies in graphs*, Estrada, E., Hatano, N., de la Peña, J.A., Linear Algebra and its Applications, 443, **2014,** 235-244.

P4. *A statistical mechanics description of environmental variability in metabolic networks*, Crofts, J., Estrada, E., Journal of Mathematical Chemistry, 52, **2014**, 675-688.

P5. *Communicability in temporal networks*, Estrada, E., Physical Review E, 88, **2013**, 042811.

P6. *How peer pressure shapes consensus, leadership, and innovations in social groups*, Estrada, E. and Vargas-Estrada, E., Scientific Reports, 3, **2013**, 2905.

P7. *Integer sequences from walks in graphs*, Estrada, E., de la Peña, J.A., Notes on Number Theory and Discrete Mathematics, 19, **2013**, 78-84.

P8. *Hyperspheric embeddings of graphs and networks*, Estrada, E., Sánchez-Lirola, M.G. and de la Peña, J.A., Discrete Applied Mathematics, **2013**, in press.

P9. *Dynamic network centrality summarizes learning in human brain*, Mantzaris, A. V., Bassett, D.S., Wymbs, N.S., Estrada, E., Porter, M.A., Mucha, P.J., Grafton, S.T. and Higham, D.J., Journal of Complex Networks, 1, **2013**, 83-92.

P10. *Ranking hubs and authorities using matrix functions*, Benzi, M., Estrada, E. and Klymko, C. Linear Algebra and its Applications 438, **2013**, 2447-2474.

P11. *Atomic displacements due to spin-spin repulsion in conjugated alternant hydrocarbons*, Estrada, E. and Benzi, M. Chemical Physics Letters, 568-569, **2013**, 184-189.

P12. *Complex networks in the Euclidean space of communicability distances*, Estrada, E. Physical Review E 85, **2012**, 066122.

P13. *Distance-sum heterogeneity in graphs and complex networks*, Estrada, E. and Vargas-Estrada, E. Applied Mathematics and Computation, 218, **2012**, 10393-10405.

P14. *The communicability distance in graphs*, Estrada, E. Linear Algebra and its Applications, 436, **2012**, 4317-4328.

P15. *The physics of communicability in complex networks*, Estrada, E., Hatano, N. and Benzi, M., Physics Reports, 514, **2012**, 89-119.

P16. *Statistical mechancs of two-dimensional tilings*, Kaatz, F. H., Estrada, E., Bultheel, A. and Sharrock, N. Physica A, Statistical Mechanics and its Applications, 391, **2012**, 2957-2963.

P17. *Path Laplacian matrices. Introduction and application to the analysis of consensus in networks*, Estrada, E. Linear Algebra and its Applications, 436, **2012**, 3373-3391.

P18. *Escherynes: Novel carbon allotropes with belt shapes*, Estrada, E. and Simón-Manso, Y., Chemical Physics Letters, 548, **2012**, 80-84.

P19. *Returnability as a criterion of disequilibrium in atmospheric reactions networks*, Estrada, E., Journal of Mathematical Chemistry, 50, **2012**, 1363-1372.

P20. *Combinatorial study of the degree assortativity in networks*, Estrada, E., Physical Review E, 84, **2011**, 047101.

P21. *Epidemic spreading in networks with nonrandom long-range interactions*, Estrada, E., Kalala-Mutombo, F. and Valverde-Colmeiro, A., Physical Review E, 84, **2011**, 036110. Selected by the editor for the Virtual Journal Biological Physics Research, Volume 22, issue 7.

P22. *Communicability across evolving networks*, Grindrod, P., Higham, D.J., Parsons, M. C. and Estrada, E., Physical Review E, 83, **2011**, 046120.

P23. *Community detection based on network communicability*, Estrada, E., Chaos: An Interdisciplinary Journal of Nonlinear Science, 21, **2011**, 016103.

P24. *Quantifying network heterogeneity*, Estrada, E., Physical Review E, 82, **2010**, 066102.

P25. *Design of highly synchronizable and robust networks*, Estrada, E., Gago, S. and Caporossi, G., Automatica, 46, **2010**, 1835-1842.

P26. *Mapping directed networks*, Crofts, J.J., Estrada, E., Higham, D.H. and Taylor, A., Electronic Transactions in Numerical Analysis, 37, **2010**, 337-350.

P27. *A vibrational approach to node centrality and vulnerability in complex networks*, Estrada, E. and Hatano, N., Physica A, Statistical Mechanics and its Applications, 389 **2010**, 3648-3660.

P28. *Generalized walks-based centrality measures for complex biological networks*, Estrada, E., Journal of Theoretical Biology, 263, **2010**, 556-565.

P29. *Network properties revealed through matrix functions*, Estrada, E. and Higham, D.J., SIAM Review, 52, **2010**, 696-714.

P30. *Universality in protein residue networks*, Estrada, E., Biophysical Journal, 98, **2010**, 890-900.

P31. *Topological atomic displacements, Kirchhoff and Wiener indices of molecules*, Estrada, E. and Hatano, N., Chemical Physics Letters, 486, **2010**, 166-170.

P32. *Randić index, irregularity and complex biomolecular networks*, Estrada, E., Acta Chimica Slovenica, 57, **2010**, 597-603.

P33. *Structural contributions of substrates to their binding to P-glycoprotein. A TOPS-MODE approach*, Estrada, E., Molina, E., Nodarse, D. and Uriarte, E., Current Pharmaceutical Design, 16, **2010**, 2676-270.

P34. *Information mobility in complex networks*, Estrada, E., Physical Review E, 90, **2009**, 0326104.

P35. *Communicability graph and community structures in complex networks*, Estrada, E. and Hatano, N., Applied Mathematics and Computation, 214, **2009**, 500-511.

P36. *Returnability in complex directed networks (digraphs)*, Estrada, E. and Hatano, N., Linear Algebra and its Applications, 490, **2009**, 1886-1896.

P37. *Communicability betweenness in complex networks*, Estrada, E., Higham, D.J. and Hatano, N., Physica A, Statistical Mechanics and its Applications, 388, **2009**, 764-774.

P38. *Extensions and foundations of the continuous symmetry measure*, Estrada, E. and Carbó-Dorca, R. MATCH: Communications in Mathematical and in Computer Chemistry, 62, **2009**, 105-114.

P39. *Communicability and multipartite structure in complex networks at negative absolute temperatures*, Estrada, E., Higham, D.J. and Hatano, N., Physical Review E, 78, **2008**, 026102. Selected by the editor for the Virtual Journal Biological Physics Research, Volume 16, issue 4.

P40. *Using network centrality measures to manage landscape connectivity. A short path for assessing habitat patch importance*, Estrada, E. and Bodin, Ö., Ecological Applications, 18, **2008**, 1810-1825.

P41. *"Clumpiness" mixing in complex networks*, Estrada, E. and Hatano, N., Journal of Statistical Mechanics: Theory and Experiment **2008**, P03008.

P42. *Communicability in complex networks*, Estrada, E. and Hatano, N., Physical Review E, 77, **2008**, 036111. Selected by the editor for the Virtual Journal Biological Physics Research, Volume 15, issue 6.

P43. *The complex networks of Earth minerals and chemical elements*, Estrada, E., MATCH: Communications in Mathematical and in Computer Chemistry, 59, **2008**, 605-624.

P44. *Atom-Bond Connectivity and the energetic of branched alkanes*, Estrada, E., Chemical Physics Letters, 463, **2008**, 422-425.

P45. *GTI-Space: The space of generalized topological indices*, Estrada, E. and Matamala, A. R., Journal of Mathematical Chemistry, 43, **2008**, 508-517.

P46. *Quantum-chemical foundations of the topological sub-structural molecular design*, Estrada, E., Journal of Physical Chemistry A, 112, **2008**, 5208-5217.

P47. *Quantitative structure-antibacterial activity relationship modeling using a combination of piecewise linear regression-discriminant analysis (I): Quantum chemical, topographic, and topological descriptors*, Molina, E., Estrada, E., Nodarse, D., Torres, L.A., González, H. and Uriarte, E., International Journal of Quantum Chemistry, 108, **2008**, 1856-1871.

P48. *How the parts organize in the whole? A top-down view of molecular descriptors and properties for QSAR and drug design*, Estrada, E., Mini Reviews in Medicinal Chemistry, 8, **2008**, 213-221.

P49. *Statistical-mechanical approach to subgraph centrality in complex networks*, Estrada, E. and Hatano, N., Chemical Physics Letters, 439, **2007**, 247-251.

P50. *Graphs (networks) with golden spectral ratio*, Estrada, E., Chaos, Solitons & Fractals, 33, **2007**, 1168-1182.

P51. *Topological structural classes of complex networks*, Estrada, E., Physical Review E 75, **2007**, 016103. Selected by the editor for the Virtual Journal Biological Physics Research, Volume 13, issue 3.

P52. *Characterization of topological keystone species. Local, global and "meso-scale" centralities in food webs*, Estrada, E., Ecological Complexity 4, **2007**, 48-57.

P53. *Functional centrality in graphs*, Rodríguez, J.A., Estrada, E. and Gutiérrez A., Linear and Multilinear Algebra, 55, **2007**, 293-302.

P54. *Food web robustness to biodiversity loss. The roles of connectance, expansibility and degree distribution*, Estrada, E., Journal of Theoretical Biology, 244, **2007**, 296-307.

P55. *On a graph-spectrum-based structure descriptor*, Gutman, I., Estrada, E. and Rodríguez-Velázquez, J.A., Croatica Chemica Acta, 80, **2007**, 151-154.

P56. *Generalized topological indices. Modeling gas-phase rate coefficients of atmospheric relevance*, Estrada, E. and Matamala, A., Journal of Chemical Information & Modeling, 47, **2007**, 794-804.

P57. *A tight-binding "Dihedral Orbitals" approach to electronic communicability in protein chains*, Estrada, E. and Hatano, N., Chemical Physics Letters, 449, **2007**, 216-220.

P58. *A tight-binding "Dihedral Orbitals" approach to the degree of folding of macromolecular chains*, Estrada, E., Journal of Physical Chemistry B, 111, **2007**, 13611-13618.

P59. *Point scattering: a new geometric invariant with applications from (nano)clusters to biomolecules*, Estrada, E., Journal of Computational Chemistry, 28, **2007**, 767-777.

P60. *Network robustness. The interplay of expansibility and degree distribution*, Estrada, E., European Physical Journal B, 52, **2006**, 563-574.

P61. *Subgraph centrality and clustering in complex hyper-networks*, Estrada, E. and Rodríguez-Velázquez, J.A., Physica A, Statistical Mechanics and its Applications, 364, **2006**, 581-594.

P62. *Spectral scaling and good expansion properties in complex networks*, Estrada, E., Europhysics Letters, 73, **2006**, 649-655.

P63. *On the dimensionality of aromaticity criteria*, Estrada, E., MATCH: Communications in Mathematical and in Computer Chemistry, 56, **2006**, 331-344.

P64. *Atomic branching in molecules*, Estrada, E., Rodríguez-Velázquez, J.A. and Randić, M., International Journal of Quantum Chemistry, 106, **2006**, 823-832.

P65. *Predicting infinite dilution activity coefficients of organic compounds in water by quantum-connectivity descriptors*, Estrada, E., Díaz, G.A. and Delgado, E., Journal of Computer-Aided Molecular Design, 20, **2006**, 539-548.

P66. *Rational design and first principles studies toward the discovery of a small and versatile new type of proton sponge*, Estrada, E. and Simón-Manso, Y., Angewandte Chemie, International Edition, 45, **2006**, 1719-1721.

P67. *Automatic extraction of structural alerts for predicting chromosome aberrations of organic compounds*, Estrada, E. and Molina, E., Journal of Molecular Graphics and Modelling, 25, **2006**, 275-288.

P68. *Synthesis of compounds with antiproliferative activity as analogues of prenylated natural products existing in Brazilian propolis*, Pisco, L., Kordian, M., Peseke, K., Feist, H., Michalik, D., Estrada, E., Carvalho, J. and Quincoces, J., European Journal of Medicinal Chemistry, 41, **2006**, 401-407.

P69. *Protein bipartivity and essentiality in the yeast protein-protein interaction network*, Estrada, E., Journal of Proteome Research, 5, **2006**, 2177-2184.

P70. *Virtual identification of essential proteins within the protein interaction network of yeast*, Estrada, E., Proteomics, 6, **2006**, 35-40.

P71. *An integrated in silico analysis of drug-binding to human serum albumin*, Estrada, E., Uriarte, E., Molina, E., Simón-Manso, Y. and Milne, G.W.A., Journal of Chemical Information and Modeling, 46, **2006**, 2709-2724.

P72. *Effect of protein folding on the stability of protein-ligand complexes*, Estrada, E., Uriarte, E. and Vilar, S., Journal of Proteome Research, 5, **2006**, 105-111.

P73. *Spectral measures of bipartitivity in complex networks*, Estrada, E. and Rodríguez-Velázquez, J.A. Physical Review E, 72, **2005**, 046105. Selected by the editor for the Virtual Journal Biological Physics Research, Volume 10, issue 8.

P74. *Subgraph centrality in complex networks*, Estrada, E. and Rodríguez-Velázquez, J.A., Physical Review E, 71, **2005**, 056103. Selected by the editor for the Virtual Journal Biological Physics Research, Volume 9, issue 10.

P75. *Folding degree of azurins and pseudoazurins. Implications on structure and function*, Estrada, E. and Uriarte, E., Computational Biology and Chemistry, 29, **2005**, 345-353.

P76. *Order from chaos: Observing hormesis at the proteome level*, Randić, M. and Estrada, E., Journal of Proteome Research, 4, **2005**, 2133-2136.

P77. *GTI-Simplex: A unified approach to optimize QSPR models*, Matamala, A.R. and Estrada, E., Journal of Physical Chemistry A, 109, **2005**, 9890-9895.

P78. *Generalised topological indices. Methodology and physico-chemical interpretation*, Matamala, A.R. and Estrada, E., Chemical Physics Letters, 410, **2005**, 343-347.

P79. *In silico studies toward the discovery of new anti-HIV nucleoside compounds through the use of TOPS-MODE and 2D/3D connectivity indices. 2. Purine derivatives*, Vilar, S., Estrada, E., Uriarte, E., Santana, L. and Gutierrez, Y., Journal of Chemical Information and Modeling, 45, **2005**, 502-514.

P80. *A protein folding degree measure and its dependence on crystal packing, protein size, secondary structure, and domain structural class*, Estrada, E., Journal of Chemical Information and Computer Sciences, 44, **2004**, 1238-1250.

P81. *Characterisation of the amino-acids contributions to the folding degree of proteins*, Estrada, E., Proteins: Structure, Function and Bioinformatics, 54, **2004**, 727-737.

P82. *Three-dimensional generalized graph matrix, Harary descriptors and a generalized interatomic Lennard-Jones potential*, Estrada, E., Journal of Physical Chemistry A, 108, **2004**, 5468-5473.

P83. *Ranking of hair dye substances according to predicted sensitisation potency: quantitative structure-activity relationships*, Søsted, H., Basketter, D.A., Estrada, E., Johansen, J.D. and Patlewicz, G.Y., Contact Dermatitis, 51, **2004**, 241-254.

P84. *A modelling assessment of the atmospheric fate of volatile methyl siloxanes and their reaction products*, Whelan, M.J., Estrada, E. and van Egmond, R., Chemosphere, 57, **2004**, 1427-1437.

P85. *Quantum-connectivity descriptors in modeling solubility of environmentally important organic compounds*, Estrada, E., Delgado, E.J., Alderete, J.B. and Jaña, G.A., Journal of Computational Chemistry, 25, **2004**, 1787-1796.

P86. *On the usefulness of graph-theoretic descriptors in predicting theoretical parameters. Phototoxicity of polycyclic aromatic hydrocarbons (PAHs)*, Estrada, E. and Patlewicz, G., Croatica Chemica Acta, 77, **2004**, 203-211.

P87. *From knowledge generation to knowledge archive. A general strategy using TOPS-MODE with DEREK to formulate new alerts for skin sensitisation*, Estrada, E., Patlewicz, G. and Gutierrez, Y., Journal of Chemical Information and Computer Sciences, 44, **2004**, 688-698.

P88. *Creating molecular diversity from antioxidants in Brazilian propolis. Combination of TOPS-MODE QSAR and Virtual structure generation*, Estrada, E., Quincoces, J. and Patlewicz, G., Molecular Diversity, 8, **2004**, 21-33.

P89. *Application of a novel graph theoretic folding degree index to the study of steroid-DB3 binding affinity*, Estrada, E., Computational Biology & Chemistry, 27, **2003**, 305-313.

P90. *Continuous symmetry numbers and entropy*, Estrada, E. and Avnir, D., Journal of the American Chemical Society, 125, **2003**, 4368-4375.

P91. *Generalized graph matrix, graph geometry, quantum chemistry and the optimal description of physicochemical properties*, Estrada, E., Journal of Physical Chemistry A, 107, **2003**, 7482-7489.

P92. *What are the limits of applicability for graph theoretic descriptors in QSPR/QSAR? Modeling dipole moments of aromatic compounds with TOPS-MODE* descriptors, Estrada, E. and Gonzalez, H., Journal of Chemical Information and Computer Sciences, 43, **2003**, 75-84.

P93. *From molecular graphs to drugs. A review on the use of topological indices in drug design and discovery*, Estrada, E., Patlewicz, G. and Uriarte, E., Indian Journal of Chemistry, 42A, **2003**, 1315-1329.

P94. *Computer-aided knowledge generation for understanding skin sensitization mechanisms. The TOPS-MODE approach*, Estrada, E, Patlewicz, G., Chamberlain, M., Basketter, D. and Larbey, S., Chemical Research in Toxicology, 16, **2003**, 1226-1235.

P95. *Quantitative structure-toxicity relationships using TOPS-MODE. 3. Structural factors influencing the permeability of commercial solvents through living human skin*, Estrada, E., Uriarte, E., Gutierrez, Y. and Gonzalez, H., SAR and QSAR in Environmental Research, 14, **2003**, 145-163.

P96. *Characterization of the folding degree of proteins*, Estrada, E., Bioinformatics, 18, **2002**, 697-704.

P97. *Physicochemical interpretation of molecular connectivity indices*, Estrada, E., Journal of Physical Chemistry A, 106, **2002**, 9085-9091.

P98. *In silico studies toward the discovery of new anti-HIV nucleoside compounds with the use of TOPS-MODE and 2D/3D connectivity indices. 1. Pyrimidyl derivatives*, Estrada, E., Vilar, S., Uriarte, E. and Gutierrez, Y., Journal of Chemical Information and Computer Sciences, 42, **2002**, 1194-1203.

P99. *Effect of cyclodextrins on the solubility and antimycotic activity of sertaconazole: experimental and computational studies*, Perdomo-López, I., Rodríguez-Pérez, A.I., Yzquierdo-Peiró, J.M., White, A., Estrada, E., Villa, T.G. and Torres-Labandeira, J.J. Journal of Pharmaceutical Sciences, 91, **2002**, 2408-2415.

P100. *Utility of nuclear magnetic resonance spectroscopy to characterize the structure of dexamethasone sodium phosphate inclusion complexes with cyclodextrins in solution and to analyze potential competitive effects*, Echezarreta-Lopez, M.M., Perdomo-Lopez, I., Estrada, E., Vila-Jato, J.L. and Torres-Labandeira, J.J., Journal of Pharmaceutical Sciences, 91, **2002**, 1536-1547.

P101. *The Balaban J index in the multidimensional space of generalized topological indices. Generalizations and QSPR improvements*, Estrada, E. and Gutierrez , Y., MATCH: Communications in Mathematical and in Computer Chemistry, 44, **2001**, 155-167.

P102. *Generalization of topological indices*, Estrada, E., Chemical Physics Letters, 336, **2001**, 248-252.

P103. *Novel local (fragment-based) topological molecular descriptors for QSPR/QSAR and molecular design*, Estrada, E. and Molina, E., Journal of Molecular Graphics and Modelling, 20, **2001**, 54-74.

P104. *3D connectivity indices in QSPR/QSAR*, Estrada, E. and Molina, E., Journal of Chemical Information and Computer Science, 41, **2001**, 791-797.

P105. *Can 3D structural parameters be predicted from 2D (topological) molecular descriptors?*, Estrada, E., Molina, E. and Perdomo-López, I., Journal of Chemical Information and Computer Sciences, 41, **2001**, 1015-1021.

P106. *Quantitative structure-toxicity relationships using TOPS-MODE. 2. Neurotoxicity of a non-congeneric series of solvents*, Estrada, E., Molina, E. and Uriarte, E., SAR and QSAR in Environmental Research, 12, **2001**, 445-459.

P107. *Quantitative structure-toxicity relationships using TOPS-MODE. 1. Nitrobenzene toxicity to Tetrahymena pyriformis*, Estrada, E. and Uriarte, E., SAR and QSAR in Environmental Research, 12, **2001**, 309-324.

P108. *Combination of 2D, 3D-connectivity and quantum chemical descriptors in QSPR. Complexation of α- and β-cyclodextrin with benzene derivatives*, Estrada, E., Perdomo-López, I. and Torres-Labandeira, J.J., Journal of Chemical Information and Computer Sciences, 41, **2001**, 1561-1568.

P109. *Recent advances on the role of topological indices in drug discovery research*, Estrada, E. and Uriarte, E., Current Medicinal Chemistry, 8, **2001**, 1699-1714.

P110. *Improvement of water solubility of sulfamethizole through its complexation with β- and hydroxypropyl-β-cyclodextrin. Characterization of the interaction in solution and in solid state*, Pose-Vilarnovo, B., Perdomo-Lopez, I., Echezarreta-Lopez, M., Schroth-Pardo, P., Estrada, E. and Torres-Labandeira, J.J., European Journal of Pharmaceutical Science, 13, **2001**, 325-331.

P111. *Modeling diamagnetic and magneto-optic properties of organic compounds with the TOSS-MODE approach*, Estrada, E., Gutiérrez, Y. and González, H., Journal of Chemical Information and Computer Sciences, 40, **2000**, 1386-1399.

P112. *Connectivity-, Wiener- and Harary-type indices of dendrimers*, Diudea, M., Kiss, A. A., Estrada, E. and Guevara, N., Croatica Chemica Acta, 73, **2000**, 367-381.

P113. *A computer-based approach to describe the Carbon-13 NMR chemical shifts of alkanes by the generalized spectral moments of iterated line graphs*, Estrada, E., Computers & Chemistry, 24, **2000**, 193-201.

P114. *Characterization of 3D molecular structure*, Estrada, E., Chemical Physics Letters, 319, **2000**, 713-718.

P115. *Molecular modeling (MM2 and PM3) and experimental (NMR and thermal analysis) studies on the inclusion complex of salbutamol and β-cyclodextrin*, Estrada, E., Perdomo-Lopez, I. and Torres-Labandeira, J.J., The Journal of Organic Chemistry, 65, **2000**, 8510-8517.

P116. *In Silico studies for the rational discovery of anticonvulsant compounds*, Estrada, E. and Peña, A., Bioorganic and Medicinal Chemistry, 8, **2000**, 2755-2770.

P117. *Synthesis, X-ray molecular structure and semiempirical calculations of a new heteroarylpiperazine derivative*, Estrada, E., González, J.C., Santana, L., Uriarte, E. and Castiñeiras, A., Structural Chemistry, 11, **2000**, 249-256.

P118. *A novel approach for the virtual screening and rational design of anticancer compounds*, Estrada, E., Uriarte, E., Montero, A., Teijeira, M., Santana, L. and De Clercq, E., Journal of Medicinal Chemistry, 43, **2000**, 1975-1985.

P119. *On the Topological Sub-Structural Molecular Design (TOSS-MODE) in QSPR/QSAR and drug design research*, Estrada, E., SAR & QSAR in Environmental Research, 11, **2000**, 55-73.

P120. *On the edge-connectivity indices in QSPR/QSAR Studies. 2. Accounting for long-range bond contributions*, Estrada, E., Journal of Chemical Information and Computer Sciences, 39, **1999**, 1042-1048.

P121. *On the edge-connectivity indices in QSPR/QSAR studies. 1. Comparison to other topological indices in QSPR studies*, Estrada, E. and Rodríguez, L., Journal of Chemical Information and Computer Sciences, 39, **1999**, 1037-1041.

P122. *Connectivity polynomial and long-range contributions in the molecular connectivity model*, Estrada, E., Chemical Physics Letters, 312, **1999**, 556-560.

P123. *Some properties of the Wiener polynomial of trees*, Gutman, I., Estrada, E. and Ivanciuc, O., Graph Theory Notes. New York XXXVI, **1999**, 7-13.

P124. *Generalized spectral moments of the iterated line graphs sequence. A novel approach to QSPR studies*, Estrada, E., Journal of Chemical Information and Computer Science, 39, **1999**, 90-95.

P125. *Modeling chromatographic parameters by a novel graph theoretical sub-structural approach*, Estrada, E. and Gutierrez, Y., Journal of Chromatography A, 858, **1999**, 187-199.

P126. *Theoretical and experimental study on the structure of 1-(5-X-fur-2-yl)-2-nitro-2-Y-ethylenes*, Estrada, E., Gómez, M., Castañedo and N., Pérez, C., Journal of Molecular Structure (THEOCHEM), 468, **1999**, 193-200.

P127. *Molecular connectivity indices of iterated line graphs. A new source of descriptors for QSPR and QSAR*. Estrada, E., Guevara, N., Gutman, I. and Rodríguez, L., SAR & QSAR in Environmental Research, 9, **1998**, 229-240.

P128. *Extended Wiener indices. A new set of descriptors for quantitative structure-property studies*, Estrada, E., Ivanciuc, O., Gutman, I., Gutierrez, A. and Rodríguez, L., New Journal of Chemistry, 22, **1998**, 819-823.

P129. *Extension of edge connectivity index. Relationships to line graph vertex connectivity indices*, Estrada, E., Guevara, N. and Gutman, I., Journal of Chemical Information and Computer Science, 38, **1998**, 428-431.

P130. *Modelling the diamagnetic susceptibilities of organic compounds by a substructural graph theoretical approach*, Estrada, E., Journal of Chemical Society. Faraday Transactions, 94, **1998**, 1407-1411.

P131. *Spectral moments of edge adjacency matrix in molecular graphs. 3. Molecules containing cycles*, Estrada, E., Journal of Chemical Information and Computer Science, 38, **1998**, 23-27.

P132. *Approximating total π-electron energy in terms of spectral moments. A quantitative approach*, Gutman, I., Marković, S., Vesović, A. and Estrada, E., Journal of the Serbian Chemical Society, 63, **1998**, 639-646.

P133. *An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes*, Estrada, E., Torres, L., Rodríguez, L. and Gutman, I., Indian Journal of Chemistry, 37A, **1998**, 849-855.

P134. *The line graph model. Predicting physico-chemical properties of alkanes*, Gutman, I., Popović, L., Estrada, E. and Bertz, S. H., Models in Chemistry, 135, **1998**, 147-155.

P135. *Designing sedative/hypnotic compounds from a novel substructural graph-theoretical approach*, Estrada, E., Peña, A. and García-Domenech, R., Journal of Computer-Aided Molecular Design, 12, **1998**, 583-595.

P136. *Structure-mutagenicity relationships in 2-furylethylene derivatives. A molecular orbital study of the role of nitro groups*, Estrada, E, Mutation Research, 420, **1998**, 67-75.

P137. *Matrix algebraic manipulations of molecular graphs. 2. Harary- and MTI-like molecular descriptors*, Estrada, E. and Rodríguez, L., MATCH: Communications in Mathematical and in Computer Chemistry, 35, **199**7, 157-167.

P138. *Matrix algebraic manipulations of molecular graphs. 1. Graph theoretical invariants based on distances and adjacency matrices*, Estrada, E., Rodríguez, L. and Gutiérrez, A., MATCH: Communications in Mathematical and in Computer Chemistry, 35, **1997**, 145-156.

P139. *Spectral moments of edge adjacency matrix in molecular graphs. 2. Molecules containing heteroatoms and QSAR applications*, Estrada, E., Journal of Chemical Information and Computer Science, 37, **1997**, 320-328.

P140. *Application of line graphs in physical chemistry. Predicting the surface tensions of alkanes*, Gutman, I., Popović, L., Mishra, B. K., Kuanar, M., Estrada, E. and Guevara, N., Journal of the Serbian Chemical Society, 62, **1997**, 1025-1029.

P141. *Decomposition of the Wiener number into contributions coming from homodistant pairs of vertices. Definition and a QSAR application*, Estrada, E. and Rodríguez, L., Journal of the Serbian Chemical Society, 62, **1997**, 199-206.

P142. *Topological indices based on distances among edges in molecular graphs*, Estrada, E. and Gutman, I., Journal of Chemical Information and Computer Science, 36, **1996**, 850-853.

P143. *Spectral moments of edge adjacency matrix in molecular graphs. 1. Definition and applications to the prediction of physical properties of alkanes*, Estrada, E., Journal of Chemical Information and Computer Science, 36, **1996**, 844-849.

P144. *Topological indices based on the line graph of the molecular graph*, Gutman, I. and Estrada, E., Journal of Chemical Information and Computer Science, 36, **1996**, 541-543.

P145. *Edge adjacency relationships and molecular topographic descriptors. Definition and QSAR applications*, Estrada, E. and Ramírez, A., Journal of Chemical Information and Computer Science, 36, **1996**, 837-843.

P146. *Graph theoretical invariant of Randić revisited*, Estrada, E., Journal of Chemical Information and Computer Science, 35, **1995**, 1022-1025.

P147. *Three-dimensional descriptors based on electron charge density weighted graphs*, Estrada, E., Journal of Chemical Information and Computer Science, 35, **1995**, 708-713.

P148. *Edge adjacency relationships in molecular graphs containing heteroatoms: A new topological index related to molar volume*, Estrada, E., Journal of Chemical Information and Computer Science, 35, **1995**, 701-707.

P149. *Edge adjacency relationships and a novel topological index related to molecular volume*, Estrada, E., Journal of Chemical Information and Computer Science, 35, **1995**, 31-33.

P150. *A QSAR study of quinolones based on electrotopological state index for atoms*, Llorente, B., Rivero, N., Carrasco, R., Martínez, R. S. and Estrada, E., Quantitative Structure-Activity Relationships, 13, **1994**, 419-425.

P151. *Bond order weighted graphs in molecules as structure-property indices*, Estrada, E. and Montero, L. A., Molecular Engineering, 2, **1993**, 363-373.

Refereed Book Chapters

Bc1. *Introduction to Complex Networks. Structure and Dynamics*, by Estrada, E., *Evolutionary Equations with Applications to Natural Sciences* edited by J. Banasiak, M. Mokhtar-Kharroubi, , *Lecture Notes in Mathematics*, Springer, **2014**.

Bc2. *Graphs and Network Theory*, by Estrada, E., *Mathematical Tools for Physicists. 2nd Edition*, edited by M. Grinfeld, John Wiley & Sons, **2013**.

Bc3. *Chemical Graph Theory* by Estrada, E. and Bonchev, D., *Handbook of Graph Theory, Second Edition*, edited by J. L. Gross, J. Yellen and P. Zhang, Chapman and Hall/CRC, **2013**.

Bc4. *A Graph Theoretic Approach to Atomic Displacements in Fullerenes*, by Estrada, E., Hatano, N. and Matamala, A.R., Chapter 9X, pages 171-185, *The Mathematics and Topology of Fullerenes (Carbon Materials: Chemistry and Physics)*, edited by F. Cataldo, A. Graovac and O. Ori, Springer, **2011 (**with Foreword by H. Kroto, Nobel Prize Winner**)**.

Bc5. *Resistance distance, information centrality, node vulnerability and vibrations in complex networks*, by Estrada, E. and Hatano, N., Chapter 2, pages 13-29, *Complex Networks across the Natural and Technological Sciences*, edited by E. Estrada, D. J. Higham, M. Fox and G.-L. Oppo, Springer, **2010**.

Bc6. *Communicability and Communities in Complex Socio-Economic Networks*, by Estrada, E. and Hatano, N., Chapter 14, pages 271-288, *Econophysics Approaches to Large-Scale Business Data and Financial Crisis*, edited by M.Takayasu, T.Watanabe and H.Takayasu, Springer, **2010**.

Bc7. *Generalized Graph Theoretic Indices in Chemistry* by Estrada, E. and Matamala, A.R. Chapter 11, pages 217-230, *Novel Molecular Descriptors. Theory and Applications II. Mathematical Chemistry Monographs No. 9*, edited by I. Gutman and B. Furtula, University of Kragujevac, **2010**.

Bc8. *Topological Atomic Displacement and Resistance Distance in Molecules*, by Estrada, E. and Hatano, N., Chapter 1, pages 3-28, *Novel Molecular Descriptors. Theory and Applications I. Mathematical Chemistry Monographs No. 8*, edited by I. Gutman and B. Furtula, University of Kragujevac, **2010**.

Bc9. *Spectral Theory of Networks: From Biomolecular to Ecological Systems*, by Estrada, E., Chapter 4, pages 55-84, *Analysis of Complex Networks: From Biology to Linguistics*, edited by M. Dehmer, Wiley-VCH, **2009**.

Bc10. *Modeling solubility in water of environmentally important organic compounds*, by Estrada, E., Delgado, E. and Simón-Manso, Y. Chapter 2, pages 17-31, *Thermodynamics, Solubility and Environmental Issues*, edited by Trevor M. Letcher, Elsevier, **2007**.

Bc11. *Wiener number in the context of generalized topological indices*, by Estrada, E., Chapter 7, pages 181-202, *Topology in Chemistry*, edited by D. Rouvray and R. B. King, Horwood, **2001**.

Bc12. *QSPR/QSAR by Graph-Theoretical descriptors Beyond the Frontiers*, by Estrada, E. and Molina, E. Chapter 5, pages 83-107, *QSAR/QSPR Studies by Molecular Descriptors*, edited by M. Diudea, Nova Science, **2001**.

Bc13. *Novel Strategies in the Search of Topological Indices*, by Estrada, E, Chapter 9, pages 503-553, *Topological Indices and Related Descriptors in QSAR and QSPR*, edited by J. Devillers and A. T. Balaban, Gordon and Breach, **1999.**

Patents

Pa1. Substituted Hydroxyacetophenon Derivatives. J. Quincoces, E. Estrada, K. Peseke, international Patent WO/2006/003010; International Application Number: PCT/EP2005/007307.

Pa2. 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.

SCHOOLS AND SIMPOSIA ORGANISED

2014 Co-organiser of the International Summer School on Complex Networks, Bertinoro, Italy

2009 Co-director of the programme Complex Networks across the Natural and Technological Sciences, Scottish Universities Insight Institute, Glasgow, U.K.

2007 Organiser of the Workshop on Complex Networks across Disciplines, University of Santiago de Compostela, Spain

PRINCIPAL INVITED LECTURES

2015 Plenary Speaker at NetSci-X 2015 in Rio de Janeiro

2014 Plenary Speaker at the European Conference on Complex Systems, Lucca, Italy,

2013 Invited Speaker at The 36th German Conference on Pattern Recognition (GCPR 2014), Münster, Germany

2013 "How to navigate in a complex world", Invited "Science Talks" at the Faculty of Science, Kennesaw State University, Atlanta, USA

2012 Plenary Speaker at 4th International Interdisciplinary Chaos Symposium on Chaos and Complex Systems, Antalya, Turkey

2012 "Complex networks: A tour'd horizon", Plenary Speaker at 2012 SIAM Annual Meeting, Minneapolis, USA

2012 Invited speaker at the conference "Applications of Graph Spectra in Computer Sciences", CRM Barcelona, Spain

2012 "Communicability in complex networks: Quantum vs. classical approaches" invited talk at the meeting "Function Prediction in Complex Networks", Kavli Royal Society International Scientific Centre

2011 Plenary Speaker at *The 1st International Symposium on Innovative Mathematical Modelling*, Tokyo, Japan

2010 Plenary Speaker at *Joint IAPR International Workshops on Structural and Syntactic Pattern Recognition (SSPR 2010) and Statistical Techniques in Pattern Recognition (SPR 2010)*, Cesme, Turkey

2010 "A Graph Theoretic Approach to Atomic Displacements in Fullerenes". Keynote Speaker Lecture, *Computers in Scientific Discovery*, University of Sheffield, Sheffield

2009 "Communicability and the evolution of communities in networks", Invited Lecture, *The Unexpected Link: Using Network Science to Tackle Social Problems*, Budapest, Hungary

2009 "Spectra of Complex Networks: Centrality Measures and Applications", Invited Lecture, *Applications of Physics in Financial Analysis, 7th International Conference*, Tokyo, Japan

2008 "Golden Spectral Graphs and Networks", Invited Lecture, *Spectral Graph Theory in Rio*, Rio de Janeiro, Brazil

2005 "Subgraph centrality, bipartivity and spectral scaling in complex networks.", Invited Talk, Conference on Complex Networks: Evolution and Statistical Properties, Salou, Spain

2004 "A universal topological property of complex networks.", Invited Talk, Nordic Workshop on Networks. NORDITA, Niels Bohr Institute, Copenhagen, Denmark

2001 "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

2001 "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

2000 "Extending the molecular connectivity indices. From bond connectivity to long-range connectivity indices.", Lecture, Symposium for the 25th Anniversary of the Connectivity Indices. 220th National Meeting of the American Chemical Society, Washington DC, USA

INVITED LECTURES AT INSTITUTIONS/SOCIETIES

2012 "Communicability in complex networks" invited talk at the Inaugural Sesion of the SIAM Students Chapter, University of Edinburgh

2012 "An Invitation to Complex Networks" invited talk at the Inaugural Sesion of the SIAM Students Chapter, University of Manchester

2011 "Complex Networks: Interdisciplinary Research" invited talk at the Inaugural Sesion of the SIAM Students Chapter, University of Strathclyde, Glasgow

2011 "Predicting toxicity from molecular structure. A topological tale", Invited Talk at the NC3Rs/Mathematics in Medicine Study Group workshop on Mathematical Modelling and Toxicology

2008 "Complex Networks: from Nature and Society to Technology", Lecture,

Workshop *Complexity in the Brain*, University of Strathclyde, Glasgow

2008 "Centrality and Communities in Complex Socio-Economic Networks", Lecture, Tokyo Institute of Technology

2008 "Protein Origami: How to Quantify the Degree of Folding of Protein Chains", Lecture, Department of Applied Physics, University of Tokyo

2008 "Detecting communities in Complex Networks", Lecture, Institute of Industrial Sciences, University of Tokyo, Japan

2008 "Complex networks: From the cell to ecosystems", Lecture, Faculty of Sciences, University of Oporto, Portugal

2008 "Complex networks and Biology in the XXI century", Lecture, Institute for Marine Sciences, CSIC, Vigo, Spain

2007 "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

2007 "From Small Molecules to "Small-Worlds", Lecture, Faculty of Experimental Sciences, University of Almería, Spain

2006 "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

2006 "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

2005 "Structural characterization of complex networks", Lecture, VII Seminar of Discrete Mathematics, University Carlos III, Madrid, Spain

2004 "Characterization of the Degree of Folding of Proteins", Lecture, Faculty of Chemistry, University of Concepción, Chile

2003 "Quantitative Structure-Property and Structure-Activity Relationships. A Personal View", Lecture, Faculty of Chemistry, University of Concepcion, Chile

2002 "From 2D Drug Design to 3D Characterization of the Degree of Folding of Proteins", Lecture, Department of Chemistry, University of Campinas, Brazil

PRINCIPAL COLLOQUIA AND SEMINARS

1 "Communicability in complex networks. Theory and Applications", Seminar at the Department of Actuarial Mathematics, Herriot-Watts University, Edinburgh, U.K., February 2014.

2 "Path Laplacian Matrices. Theory and Applications", Seminar at GERAD, University of Montreal, Canada, November 2013.

3 "Communicability and Information Diffusion on Complex Networks", Colloquium at the Department of Mathematics, Dartmouth College, Hanover, USA, November 2013.

4 "Communicability and Information Diffusion on Complex Networks", Seminar at the Laboratory for the Modeling of Biological and Socio-Technical Systems, Northeastern University, Boston, USA, November 2013.

5 "How Peer Pressure Shapes Consensus in Social Groups", Talk presented at the Computational Social Science Workshop organised by Georgia Institute of Technology and Emory University, November 2013.

6 "Golden spectral graphs", Seminar at the Department of Mathematics and Computer Sciences, Emory University, Atlanta, USA, October 2013.

7 "Communicability in Social Networks", Political Sciences Colloquium at the Emory University, Atlanta, USA, October 2013.

8 "How not to get lost when navigating through a city, the Internet or the brain?" Seminar at the Network Research Group, Swansea University, Wales, UK, 25th June 2013.

9 "Networks on Hyperspheres", Colloquium at the Centre of Mathematical Researches, CIMAT, Guanajuato, Mexico, June 2012.

10 "Communicability in complex networks", Colloquium at the Centre of Mathematical Researches, CIMAT, Guanajuato, Mexico, February 2012.

11 "Communicability in complex networks", seminar at the Department of Mathematical Engineering, Universite Catholique de Louvain, Louvain-la-Neuve, 2nd December 2011.

12 "Path Laplacian matrices. Theory and Applications", seminar at the Applied Analysis group, Department of Mathematics and Statistics, University of Strathclyde, Glasgow, 24th November 2011.

13 "Communicability and subgraph centrality in complex networks", seminar at Department of Physics, University of Catania, Sicily, Italy, 22nd November 2011.

14 "Communicability in complex networks", seminar at Bristol Centre for Complexity Sciences, Dept. of Engineering Mathematics & School of Biological Sciences, 9th November 2011.

15 "Decoding Matrix Structure by Matrix Functions", Colloquium at the Department of Mathematics and Computer Science, Emory University, Atlanta, USA, April 2011.

16 "Approaching Network Structure by Spectral Methods", Mathematical Biology Seminar at the case Western Reserve University, Cleveland, Ohio, USA, April 2011.

17 "Communicability in Complex Networks", Seminar at Statistical and Applied Mathematical Sciences Institute, SAMSI, North Carolina, USA, April 2011.

18 "An excursion through the world of complex networks guided by matrix theory", Seminar at the Computational Mathematics and Applications Group, Rutherford Appleton Laboratory, Oxford, UK, 21st January 2010.

19 "Introduction to Complex Networks I. Network Science Tutorial for non-specialists." Workshop Complex Networks across the Natural and Technological Sciences. Institute for Advanced Studies. Glasgow. 19th-23th January, 2009.

20 "Introduction to Complex Networks II. Modern Concepts, Algorithms and Applications. Network Science Tutorial for non-specialists." Workshop Complex Networks across the Natural and Technological Sciences. Institute for Advanced Studies. Glasgow. 19th-23th January, 2009.

21 "Joining the Dots", Public Lecture at the Workshop: Complex Networks across the Natural and Technological Sciences. Institute for Advanced Studies. Glasgow. 19th-23th January, 2009.

22 "Introduction to Network Theory", PhD Workshop in Modelling Skills. Institute for Advanced Studies. Glasgow. 5th-6th November 2009.

23 "Golden Spectral Graphs and Networks". Lecture at the Workshop Complex Networks across the Natural and Technological Sciences. Institute for Advanced Studies. Glasgow. 19th-23th January, 2009.

24 "Information Mobility in Complex Networks". Workshop Applications of Complex Networks, Institute for Advanced Studies, Glasgow, 25th-29th May, 2009.

25 "Modelling Complex Networks through Matrix Functions". Centre for Interdisciplinary Computational and Dynamical Analysis (CICADA), university of Manchester. 11 - 14 January 2009

26 "Communicability and Community Structure in Complex Network". BBSRC MATSYB network I2M: Immunology, Imaging and Modelling. School of Mathematics, University of Leeds. 2nd April, 2009.

27 "Centrality and Communicability in Complex Networks". Department of Computing Sciences and Mathematics, University of Stirling. 14th April 2009.

28 "Mathematical Characterization of Local and Global Properties in Complex Networks", Lecture, Department of Informatics, University of Tokyo (May 19, 2008).

29 "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).

30 "Protein Origami: The Degree of Folding of Proteins", Seminar, Bioinformatics Research Centre, University of Glasgow, U.K. (February 19, 2008).

31 "Topological characterization of complex biological networks", Seminar, Translational Medicine Research Collaboration, The Sir James Black Centre, University of Dundee, U.K. (February 15, 2008).

32 "An Introduction to Bioinformatics for Mathematicians". Invited Seminar, Institute of Mathematics, University of Santiago de Compostela, Spain (December 14, 2001).

33 "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).

PRINCIPAL 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. "Matrix Functions for the Analysis of Complex Networks". Minisymposium Function of Matrices. SIAM Conference on Applied Linear Algebra. Monterey, CA. 26-29 October, 2009.

3. "Proteins as Complex Networks", Lecture, IAMC, International Academy of Mathematical Chemistry, Dubrovnik, Croatia (June 10-14, 2009).

4. "Spectral Measures for Molecular Networks", Lecture, MCC 2009, International Conference Math/Chem/Comp, Dubrovnik, Croatia (June 4-9, 2009).

5. "Complex Networks and OMICS", Lecture, Symposium on Complex Networks: Biology, Ecology, Society; University of Santiago de Compostela, Spain (June 22, 2007).

6. "Complex Networks", Lecture, Second Meeting of the International Academy of

Mathematical Chemistry; Dubrovnik, Croatia (June 8, 2006).

7. "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).

8. "New Tetracyclic Frameworks with Potential Antitumor Interest", Poster, XVIth International Symposium on Medicinal Chemistry, Bologna, Italy (November 22, 2000).

9. "In Silico Studies for the Screening and Design of Pharmacologically Active Compounds", Poster, XVIth International Symposium on Medicinal Chemistry, Bologna, Italy (November 22, 2000).

10. "New N,N-Disubstituted Piperazines as Serotonine and Dopamine Ligands", Poster, XVIth International Symposium on Medicinal Chemistry, Bologna, Italy (November 22, 2000).

11. "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).

12. "Design, Synthesis and in Vitro Determination of the Antimicrobian Activity of New Gamma-Nitrocyclohexanones", Poster, IV Iberoamerican Meeting of Pharmaceutical and Food Sciences, La Habana, Cuba (June 30, 2000).

13. "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).

14. "Predicting Chemical Reactivity (Log K) and Octanol/Water Partition Coefficient (Lipophilicty, Log P) of Furylethylene Compounds from Graph-Theoretical Molecular Descriptors", Poster, 16th Conference of Chemistry, University of Oriente, Santiago de Cuba, Cuba, (December 10, 1999).

15. "Use of a Novel Theoretical Approach to Calculate the Fragment Contribution of a Molecule to the Biological Activity", Poster, 16th Conference of Chemistry, University of Oriente, Santiago de Cuba, Cuba, (December 10, 1999).

16. "Use of Local Spectral Moments in Drug Design", Poster, 16th Conference of Chemistry, University of Oriente, Santiago de Cuba, Cuba, (December 10, 1999).

17. "Designing Antifungal and Antibacterial Compounds by a Substructural Graph-Theoreical Approach", Poster, 16th Conference of Chemistry, University of Oriente, Santiago de Cuba, Cuba, (December 10, 1999).

18. "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).

19. "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).

20. "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).

21. "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).

22. "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).

23. "Theoretical Studies for the Racional Functionalization of 2-Bromo-(3-Fur-2-yl)-3-oxo-Propyonamide", Poster, First Workshop on Molecular Modeling and Applications, La Habana, Cuba (March 28, 1997).

24. "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).

25. "Simulation of Antibiotics Penetration into Cerebrospinal Fluids in Bacterial Meningitis", Lecture, First International Workshop on Antibiotics, La Habana, Cuba (November 4, 1993).

26. “Quantitative Structure-Activity Relationships (QSAR) Study of the Action Mechanism of Antibacterial Furylethylenes Derivatives”, Poster, First International Workshop on Antibiotics, La Habana, Cuba (November 4, 1993).

27. “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).

28. “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).

RESEARCH GRANTS

2014-2018 Wolfson Research Mertit Award, Royal Society of London for "Physico-mathematical modelling of communication patterns in complex networks".
Award of £75,000.00.

2013-2015 Grant from Engineering and Physical Sciences Research Council (EPRSC) and the Weir Group "Modelling Complex Networks of Fractures in Rocks of Petrophysical Interest".
Award of £36,000.00.

2012 Grant from the Scottish Funding Council for developing a join research project with the company Isochron on business forecasting using network techniques.
Award of £5,000.00.

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 Engineering and Physical Sciences Research Council (EPRSC), 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.