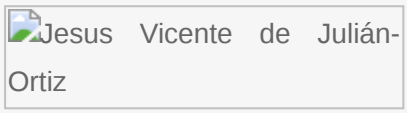
Jesus Vicente de Julián-Ortiz

Subjects: Chemistry, Physical

Contributor: Jesus Vicente de Julián-Ortiz

Chirality | Computational Chemistry | Medicinal Chemistry

Basic Information



Name: Jesus Vicente de Julián-Ortiz (Apr 1963–)

Birth Location:	Mislata, Valencia, Spain
Titles:	Scientist Professor
Affiliation:	Unknown
Honor:	Unknown

1. Brief Introduction

Bachelor of Chemical Sciences in the specialty of Biochemistry. He did the doctorate program in Organic Synthesis and Fine Chemistry. Doctor of Pharmacy. His initial research focused on the design, synthesis and microbiological tests of new potential drugs against Herpes simplex virus type 1, as well as the design of new potential antimycobacterial agents, including the corresponding activity tests in cell cultures. All this university activity was carried out at the University of Valencia. He has experience in the bioinformatics business world for having worked as a scientific consultant and for having created his own QSAR and custom software company, MOLware SL, for whose activity he implemented all the specific software personally. He worked at the CSIC Institute of Chemical Technology in the group of Prof. Avelino Corma in Molecular Design of agents directing the synthesis of zeolitic catalysts within the framework of a project with the multinational Exxon.

He was selected by the INNCORPORA program and completed the Executive Master in Innovation from the School of Industrial Organization, financed by said call. He has been editor of research projects at the Foundation Center for Innovation and Technological Demonstration. He has been selected by the Torres-Quevedo program to carry out a project on the design of bioactive peptides. He is an assistant professor in the Department of Physical Chemistry at the University of Valencia. He has contributed four patents, more than 90 articles in journals and book

chapters, including Chemical Reviews, the magazine with the highest impact index worldwide in Chemistry. He has co-edited the book 'Physical Chemistry for Chemists and Chemical Engineers: Multidisciplinary Research Perspectives'. He has participated in 12 national projects and in 6 European ones. He has advised, among other companies, ProtoQSAR 2000 SL, an outsourcing company for computational prediction services, MolDrug AI Systems SL, a drug design company and EQA, a certification consultant for Research, Development and Innovation projects.

He has been considered as a pioneer in the field of the topological characterization of the chemical chirality. His scientific interests has included molecular modeling, predicting the pharmacological properties of new compounds, drug design, and virtual combinatorial chemistry, the application of the graph-theoretical indices to the construction of chemical structures (inverse QSAR), the modeling of crystalline media and the factors that influence the synthesis of the different zeolite structures, the obtaining of mathematical models able to generalize and the desing of drug release systems.

2. Notable Contributions

Application of Neural Networks to Quantitative Structure-Activity Relationships (QSAR): Jesus Vicente de Julián-Ortiz made significant contributions to the field of QSAR by being a pioneer in the application of neural networks to quantitative relationships between the chemical structure of compounds and their biological activity[1]. This approach allows for the prediction and optimization of pharmacological properties of new compounds, aiding in the design of potential drugs with improved activity and efficacy.

Development of Topological Indices for Chirality: De Julián-Ortiz contributed to the development of topological indices that accounted for chirality, providing a unique perspective on the characterization of chemical chirality [2].

Application of Molecular Connectivity to Polymers: Garcia-Domenech and de Julián-Ortiz explored the prediction of properties of linear polymers by utilizing graph-theoretical indices based on molecular connectivity[3]. This work provided insights into the relationship between the structural features of polymers and their physical properties, such as indices of refraction and glass transition temperatures.

Advancement in Virtual Combinatorial Synthesis and Screening: De Julián-Ortiz, along with collaborators, made significant contributions to the field of virtual combinatorial synthesis and screening[4]. Their work involved the development and application of computational methods to generate and evaluate large virtual libraries of compounds for drug discovery purposes. This approach allowed for efficient screening of potential anti-herpes compounds[4], as well as the identification of new agents active against Mycobacterium avium complex[9] and antimalarial drugs[10].

3. Principal Work

One of the principal works of Jesus Vicente de Julián-Ortiz is the development of methods for the design of drugs based on structural invariants. These structural invariants are molecular descriptors that remain constant despite conformational changes in the molecule[5][6][7][8][9][10].

By focusing on these invariants, de Julián-Ortiz aimed to design drugs with improved properties and reduced side effects. This research involved the application of various computational and molecular modeling techniques, including neural networks, topological indices, and virtual screening.

Additionally, de Julián-Ortiz has contributed significantly to the field of chemical graph theory, exploring new trends and approaches[5][6]. He has also made important contributions to the topological approach to analgesia and drug design[6][7], as well as the development of pharmacological distribution diagrams for de novo drug design[8].

Throughout his career, de Julián-Ortiz has published numerous articles in prestigious journals, including the Journal of Chemical Information and Computer Sciences, Journal of Molecular Graphics and Modelling, Journal of Medicinal Chemistry, Chemical Reviews, and Journal of Antimicrobial Chemotherapy. He has also participated in national and European research projects and provided guidance and expertise to various companies in computational prediction services, drug design, and certification consultancy.

References

1. García-Domenech, R., De Julián-Ortiz, J.V. Antimicrobial activity characterization in a heterogeneous group of compounds. *Journal of Chemical Information and Computer Sciences* **1998**, *38*, 445, 10.1021/ci9702454.
2. de Julián-Ortiz, J.V., De Gregorio Alapont, C., Ríos-Santamarina, I., García-Doménech, R., Gálvez, J. Prediction of properties of chiral compounds by molecular topology. *Journal of Molecular Graphics and Modelling* **1998**, *16*, 14, 10.1016/S1093-3263(98)00013-8.
3. García-Domenech, R., de Julián-Ortiz, J.V. Prediction of indices of refraction and glass transition temperatures of linear polymers by using graph theoretical indices. *Journal of Physical Chemistry B* **2002**, *106*, 1501, 10.1021/jp012360u.
4. de Julián-Ortiz, J.V., Gálvez, J., Muñoz-Collado, C., García-Domenech, R., Gimeno-Cardona, C. Virtual combinatorial syntheses and computational screening of new potential anti-herpes compounds. *Journal of Medicinal Chemistry* **1999**, *42*, 3308, 10.1021/jm981132u.
5. García-Domenech, R., Gálvez, J., de Julián-Ortiz, J. V., Pogliani, L. Some new trends in chemical graph theory. *Chemical Reviews* **2008**, *108*, 1127, 10.1021/cr0780006.

6. Gálvez, J., Garcia-Domenech, R., De Julián-Ortiz, V., Soler, R. Topological Approach to Analgesia. *Journal of Chemical Information and Computer Sciences* **1994**, *34*, 1198, 10.1021/ci00021a030.
7. Gálvez, J., García-Domenech, R., de Julián-Ortiz, J.V., Soler, R. Topological Approach to Drug Design. *Journal of Chemical Information and Computer Sciences* **1995**, *35*, 272, 10.1021/ci00024a017.
8. Gálvez, J., García-Domenech, R., de Gregorio Alapont, C., de Julián-Ortiz, J.V., Popa, L. Pharmacological distribution diagrams: A tool for de novo drug design. *Journal of Molecular Graphics* **1996**, *14*, 272, 10.1016/S0263-7855(96)00081-1.
9. García-García, Á., Gálvez, J., de Julián-Ortiz, J. V., García-Domenech, R., Muñoz, C., Guna, R., Borrás, R. New agents active against Mycobacterium avium complex selected by molecular topology: A virtual screening method. *Journal of Antimicrobial Chemotherapy* **2004**, *53*, 65, 10.1093/jac/dkh014.
10. Mahmoudi, N., de Julián-Ortiz, J.-V., Ciceron, Galvez, J., Mazier, D., Danis, M., L., Derouin, F., García-Domenech, R. Identification of new antimalarial drugs by linear discriminant analysis and topological virtual screening. *Journal of Antimicrobial Chemotherapy* **2006**, *57*, 489, 10.1093/jac/dki470.