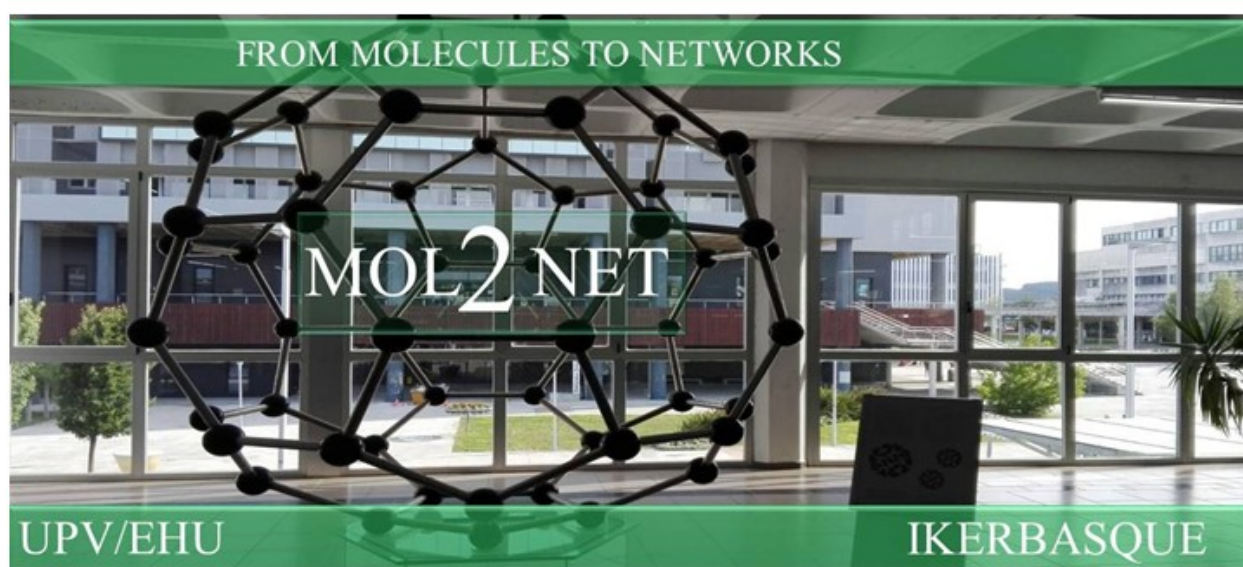


MOL2NET: FROM MOLECULES TO NETWORKS (PROCEEDINGS BOOK), Vol. 5.



sciforum

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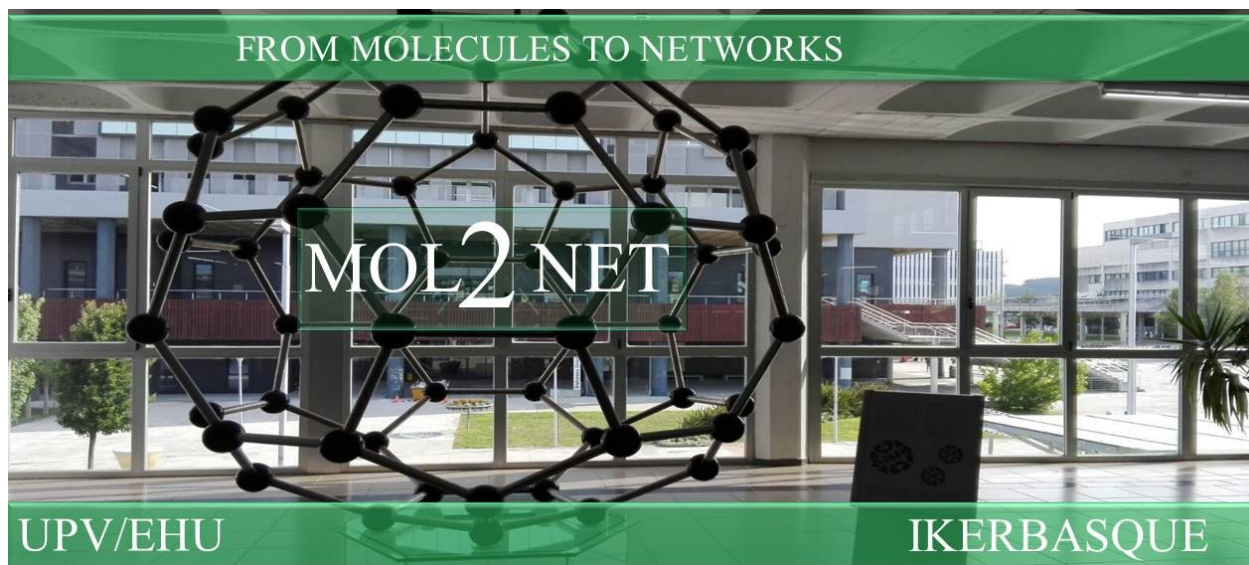
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Organic Chemistry, Chemical Synthesis, Medicinal Chemistry, Physical Chemistry, Pharmaceutical Law, Pharmaceutical Sciences, Applied Physics, Nanotechnology, Materials Science, Polymers, Applied Mathematics, Complex Networks, Data Analysis, Big Data Analytics, Computational Chemistry, Computational Biology, Artificial Intelligence, Machine Learning, Statistics, Bioinformatics, Cheminformatics, Biomedical Sciences, Image Analysis, Bioethics, Data Protection, Gene Edition, OMICS

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Welcome From Chairs

Dear colleagues worldwide, we are glad to invite you to MOL2NET-05, International Conference on Multidisciplinary Sciences, ISSN: 2624-5078, MDPI SciForum, Basel, Switzerland, 2019. MOL2NET is a **year-round conference series** with multiple **associated workshops worldwide** running and open to submissions almost all the year, please read [[Workshops Schedule](#)]. The **topics of interest** include, but are not limited to, **Chemistry (All areas), Mathematics (Applied), Physics (Applied), Materials Science, Nanotechnology, Biology and Life Sciences (All areas), Medicine, Biomedical Engineering, Education**, along with **Computer Sciences, Data Analysis, Statistics, Artificial Intelligence, Deep Learning, Bioinformatics, Systems Biology, and Complex Networks Sciences**. We suggest you to **download** the [[MOL2NET Template.doc](#)] of [[USEDAT Template.doc](#)] to write your communications for conference or training school workshops. Whoever, some other workshops of the series have their custom templates. Please, **read carefully** the [[Instructions to authors](#)] about publication model, copyright, authors responsibilities, *etc.*

Headquarters and Supporters

MOL2NET runs both online and/or in person workshops in **host universities worldwide** and at the [SciForum](#) platform maintained by the editorial [MDPI](#), Basel, Switzerland. The Scientific Headquarters (HQs) of this conference series are in the [Faculty of Science and Technology, University of Basque Country \(UPV/EHU\)](#), Biscay. However, the idea of this multidisciplinary conference emerged from the melting pot formed as the result of multiple collaborations of professors from many centers worldwide. Locally, the founders and strongest supporters of the conference are professors endowed by [IKERBASQUE, Basque Foundation for Sciences](#), professors from the two departments [Department of Organic Chemistry I](#) and [Department of Organic Chemistry II](#) of the [University of Basque Country \(UPV/EHU\)](#), and professors from the [Department of Computer Sciences](#) of the [University of Coruña \(UDC\)](#).

Internationally, professors from [Dept of Biological Chemistry & Molecular Pharmacology \(BCMP\), Harvard Medical School, USA](#); the [Center for the Study of Biological Complexity](#) of the [Virginia Commonwealth University \(VCU\)](#), USA; the [Natural Resources Research Institute](#), of the [University of Minnesota](#), USA; [CNRS-Université Paris-Sud](#), Paris, France, and other institutions are also founders and/or supporters of this conference, please see full committees lists [[Honor Committee](#)] [[Co-Chairs Committee](#)] [[Scientific Committee \(Abroad\)](#)] [[Scientific Committee \(Local\)](#)] and [[MOL2NET-IKERBASQUE Staff](#)].

Conference Lemma

The acronym [MOL2NET](#) summarizes the running title of this conference: **[FROM MOLECULES TO NETWORKS](#)**. This lemma is inspired by the possibility of spreading the knowledge about multiple topics by promoting multidisciplinary collaborations in science with conferences including topics ranging from quantum world to large social networks. In this sense, the spirit of this conference is in consonance with the lemma **EMAN TA ZABAL ZAZU** (Give and extend knowledge). This anthem from the 19th century is written in [Basque language \(Euskera\)](#) and is used now a days as the official motto of the [University of Basque Country \(UPV/EHU\)](#).

USEDAT Summer School

The professors, researchers, and students interested on this workshop are also welcome to participate in the international network USEDAT: USA-Europe Data Analysis Training Summer School. USEDAT is a Multi-center Trans-Atlantic initiative offering hands-on training in Data Analysis, Machine Learning, Bioinformatics, Cheminformatics, etc., directed to researchers and students worldwide. The initiative joins various sister summer schools, workshops, boot camps, hands-on training courses, and/or capstone courses involving Miami Dade College (MDC), Saint Thomas University (STU), and West Coast University (WCU) Miami, University of Coruña (UDC), University of the Basque Country (UPV/EHU), Ikerbasque, Basque Foundation for Science, and other centers. Almost all USEDAT schools have one workshop published by the MOL2NET Conference series.

The students of the school can visit one or more of the universities to receive personalized training. It included in introduction to experimental techniques (NMR, EEG, MS, HPLC, 2DGE, etc.) for data acquisition and/or computational algorithms (ML, AI, ANN, SVM, LDA, Deep Learning, SQL, Python, etc.) for data analysis in Chemistry (All), Biotechnology, Nanotechnology, Biomedical Engineering, etc.

Enrollment is free of cost in most of the workshops however typical USEDAT students/professors obtain financial support (to cover traveling, living, and insurance costs) from institutions like MSCA Europe Commission, EMBL-EBI United Kingdom, FCT Portugal, NSF China, COLCIENCIAS Colombia, SENESCYT Ecuador, CONACYT, DELFIN Program México, and PANELFIT H2020 Europe Commission Projects, etc. Please, see more details visiting the page of USEDAT in the menu of MOL2NET conference (left panel of this page) as well as our pages in [\[USEDAT Researchgate\]](#) and [\[USEDAT Facebook\]](#) social networks. If you are interested to enroll in one of the courses do not hesitate to contact directly USEDAT coordinator by email or join our Whatsapp group for enrollment, classmates chat, rooming, travel tips, etc.

Contents Veracity & Authors Liability

MOL2NET conference is an online platform for early publication of preliminary results. In this sense, most of MOL2NET workshops do not preform peer-review of materials to be published by external referees. Consequently, the modality of publication is ore similar to a pre-print server where authors can post early versions of their results to obtain feedback from the community. In addition, authors can upload also short communications with post-publication discussion of results already published in other media. In all cases, **the authors are personally responsible**, to perform a **similarity checking** , ensure **veracity of contents**, and carry out a **proper citation of previous works**.

In concordance, the members of MOL2NET **committee are not responsible of aspects** like veracity, similarity, copyright, etc. in this publishing modality. Consequently, the opinions expressed on the communications are not necessarily coincident to the opinions of the members of the committees. In this sense, we strongly recommend the authors to **use online text-similarity checking services**, such as Turnitin, etc., if possible. These tools may help authors to **avoid any form of plagiarism or copyright violation**. The authors may be requested to modify the communication (re-write their texts) previous or posterior to publication in the case that high similarity, veracity, or other problems are detected and reported to the committee. In these cases, the manuscript could be put on standby or withdrawn temporarily until the authors

re-submit the proper version. The authors are also allowed to submit short reviews, comments, letters, or discussions of papers already published if they guarantee sufficient difference to previous public contents.

Sessions & Workshops

You can participate both online or in person (face-to-face) in some of the workshops we organize in different universities worldwide (see sessions in the conference menu). Publication of all communications of the workshops will be online via the platform SciForum. We welcome proposals for organization of workshops in different universities. Please, do not hesitate to contact conference chairperson and/or scientific committee presidents. See also a list of workshops running this year.

Sessions

[01. USEDAT-07: USA-Europe Data Analysis Training School, UPV/EHU, Bilbao-MDC, Miami, USA, 2019](#)

[02. USINEWS-03: US-IN-EU Worldwide Science Workshop Series, UMN, Duluth, USA, 2019](#)

[03. IWIMSM-03: Iberoamerican Workshop on Model. and Simulation Methods, Valencia, Spain, 2019](#)

[04. ICWM-01: I International Conference and Workshop: Microbiota, UDC, Coruña, Spain, 2019](#)

[05. CHEMINFOUNC-01: Chemoinformatics Workshop, UNC Chape Hill, USA, 2019](#)

[06. NANOMATJND-01: JSU-NDSU Nanotech. & Materials Science Workshop, Jackson & Fargo, USA, 2019](#)

[07. EJIBCE-03: Structural Computational Biology, Lisboa, Portugal, 2019](#)

[08. MODEC-04: Nat. Prod. & Agro-Indust. Proc. in Amazon, UEA, Puyo, Ecuador, 2019](#)

[09. LAWSCI-03: PANELFIT H2020 Law & Tech. Challenges, UPV/EHU, Bilbao, Spain, 2019](#)

[10. UDLABIOTECH-01: I International Biotechnology Congress, UDLA, Quito, Ecuador, 2019](#)

MOL2NET Steps for Participation

- (0) Register, Sign in/Login, to Sciforum platform [[Sciforum login](#)]
- (1) Submit the title and abstract, select a section or workshop (do not upload paper here) [[Submit New Abstract](#)]
- (2) Wait for Sciforum abstract acceptance email, follow the link, and/or login to upload paper, doc and pdf format
- (3) Download template doc to prepare your communication, for general sessions: [[MOL2NET 2019 Template.doc](#)], or use the for other workshops: [[BioChemPhys Template](#)], [[WRSAMC template](#)], [[MODEC 2019 Template.doc](#)], [[AWP-04 Template](#)]
- (4) Wait for paper acceptance and publication emails (follow link to proofread your paper) (Asap after upload)
- (5) Communicate with chairpersons if corrections are necessary, including past editions (All the year)
- (6) Log in to post comments, questions, or answers in a section or one of the workshops
- (7) Contact chairpersons if you need attendance certificate for conference and/or workshops (All the year).

Conference, School, and Workshops Schedule

General Schedule: [MOL2NET](#) International Conference Series on Multidisciplinary Sciences, MDPI Sciforum, Basel, Switzerland has online and/or in person workshops (>10) associated. The conference usually **runs online** at the online platform [SciForum](#) maintained by the editorial [MDPI](#), Basel, Switzerland. The **platform is open on a year-round basis** almost all the days of the year in course. We have this modality for practical reasons; *e.g.*, accommodation of many workshops in different dates along the year, flexible reception of communications, *etc.*

Submission and Publication of communications: As we mentioned before, in the practice, the online platform is open at the beginning of the year in course and continue open all the year for submissions of communications. However, the associated workshops may open in different dates along the year (see specific workshop pages). Submission of papers to all workshops is open until the last days of the year in course or the first days of the following. The **publication of communications** is continuous all the year upon acceptance.

Schedule for for MOL2NET Workshops Online participation: You can participate online in all MOL2NET workshops all the year uploading your communication directly by Sciforum platform. In addition, after publication of papers is closed we open the online platform for online participation. The authors will be able to post online comments and/or answers to comments in this workshop/section and also in the other general sections and/or >10 international workshops of the MOL2NET conference (many of them also run both online and in person). The participants are entitled to receive participation certificates for MOL2NET conference and all the workshops they participate upon request to the respective chairpersons. See committees of MOL2NET and each workshop.

Schedule for MOL2NET Workshops in Person Participation: Many of the workshops associated to MOL2NET are going to be held also *in person (face-to-face)* in different universities of USA, Spain, Italy, Mexico, Chile, etc. This in person workshops have specific

schedules in parallel to their online versions. Please, go to the homepages of these workshops and/or contact their chairpersons for further details.

Schedule for USEDAT Summer School participation: The schedule of the different USEDAT courses varies in different universities along the year, even when many of them are in summer season, some of them run all the year. If you are interested to enroll in one of the courses do not hesitate to contact directly USEDAT coordinator at: usedat.chair@gmail.com

Note for participants: MOL2NET conference runs both online (general sections) and/or in person (associated workshops). No physical presence is needed for online participation saving traveling costs. We accept experimental works, theoretical works, or experimental-theoretic works in the areas mentioned. Proceedings will be Published Online, Open Access, and **Totally Free of Charges** (no cost). For details about in person (face-to-face) participation on associated workshops contact the respective members of the local committees. USEDAT School workshop also runs online however most of the hand-on training courses run in person.

Types of Communications

Before to submit your communication recommend to download and use the [\[Template File\]](#) to write your communication; we strongly recommend you to read carefully the following information about publication model, copyright, authors responsibilities, *etc* Firstly, be aware that the works published here belongs to two main modalities preliminary communications or comments on previous works.

Research Preprints. These are short communications of unpublished results but they are not post-print journal papers. In this sense, committee and/or external reviewers check only scope and apparent scientific soundness. They have the same editorial process than for an online [Preprint](#) service. Therefore, all works receive doi number and are indexed in databases (GoogleScholar, Publons, *etc.*). The works may receive also comments from registered participants (public post-publication review). The authors are encouraged to submit their works to a peer-reviewed scientific journals of MDPI or other editorials during or after finalization of the conference, as per [SciForum copyright rules](#).

Research Highlights. These short communications are comments on already published papers. They are short notes to comment about the more interesting points, highlights, *etc.* of works previously published by the authors or other groups. In this case, committee and/or external reviewers check also only scope and apparent scientific soundness. The works may receive also comments from registered participants (public post-publication review).

Authors Liability

In all cases, **it is responsibility of authors**, to perform a **similarity checking**, ensure **veracity of contents**, and carry out a **proper citation of previous works**. The **committee is not responsible of the previous aspects** in this publishing modality. Consequently, the opinions expressed on the communications are not necessarily coincident to the opinions of the members of the committees. In this sense, we strongly recommend the authors to **use online text-**

similarity checking services, such as Turnitin, etc., if possible. These tools may help authors to **avoid any form of plagiarism or copyright violation**. The authors may be requested to modify the communication (re-write their texts) in the case that high similarity is detected and reported to the committee. In these cases, the manuscript could be put on standby or withdrawn temporarily until the authors re-submit the proper version. The authors are also allowed to submit short reviews, comments, letters, or discussions of papers already published if they guarantee sufficient difference to previous public contents.

MDPI Journals Issues (Edited by MOL2NET Committee Members)

In parallel, the members of committees and/or authors are encouraged to edit special issues for different journals of the editorial MDPI (<http://www.mdpi.com/>). The special issue is now in call for papers, submissions are welcome in *a posteriori*, in parallel, or totally independently from the conference. Manuscripts should be submitted online at www.mdpi.com by [registering](#) and [logging in to this website](#). In order to send a proposal of associated workshop and/or special issue contact the chairperson of the conference Prof. [González-Díaz H.](#) IIKERBASQUE Prof., University of the Basque Country (UPV/EHU), Biscay, **Basque Country, Spain**. Email: mol2net.chair@gmail.com. Please, check the list of past and present special issues associated to our conference at follows. Please, click the following link [\[MOL2NET MDPI JCR Special issues\]](#) to see all past and present JCR journal issues (Impact Factor IF = 2-5 range) associated to our conference.

Call for Collaborators, Editors, Chairpersons, and Sponsors

We welcome indirect nominations and/or personal applications for a position in some of the following modalities, or other modalities of collaboration: (1) Committee membership (nomination or personal application for membership in honor, steering, or scientific committees). (2) Guest-Editor of JCR MDPI journal issue (help to propose, editing, announce your special issue in one of the MDPI journals). (3) Chairperson of workshop (publishing an online or in person workshop of your institution with you as chairperson). (4) Sponsor of conference (including logo, description, flyer, and link to homepage of your institution). (5) Speaker (publication of video conferences with cover poster, issn, isbn, and doi number). We sincerely invite you to join MOL2NET Conference Series or one of the worldwide associated workshops; please, sent a direct email to the chairperson.

MOL2NET - MDPI Journals Issues

MOL2NET - MDPI Journals Issues (Organized by MOL2NET Committee Members)

In parallel, the members of committees and/or authors are encouraged to edit special issues for different journals of the editorial MDPI (<http://www.mdpi.com/>). The special issue is now in call for papers, submissions are welcome in *a posteriori*, in parallel, or totally independently from the conference. Manuscripts should be submitted online at www.mdpi.com by [registering](#) and [logging in to this website](#). In order to send a proposal of associated workshop and/or special issue contact the chairperson of the conference Prof. [González-Díaz H.](#) IIKERBASQUE Prof., University of the Basque Country (UPV/EHU), Biscay, **Basque Country, Spain**. Email: mol2net.chair@gmail.com. Please, check the following list of past and present special issues associated to our conference:



pharmaceutics

01. Pharmaceutics (Call For Papers): Special Issue: [Nanosystems as Drug Delivery Carrier: From Nature to the Medication](#). Journal: [Pharmaceutics](#) (ISSN 1999-4923), JCR IF = 4.773. Topics: drug delivery systems, cyclodextrin, nanomedicine, active drugs, bioavailability. Editor: [Prof. Eduardo Sobarzo-Sanchez](#), Email: eduardo.sobarzo@ucentral.cl, Instituto de Investigación e Innovación en Salud, Facultad de Ciencias de la Salud, Universidad Central de Chile, **Chile**.



biomolecules

02. Biomolecules (Call For Papers): Special Issue: [Big Data Analysis in Biomolecular Research, Bioinformatics, and Systems Biology with Complex Networks and Multi-Label Machine Learning Models](#). Journal: [Biomolecules](#) (ISSN 2218-273X). JCR IF = 4.694. Section: Bioinformatics and Systems Biology. Topics: Cheminformatics; Bioinformatics; Machine Learning; Complex Networks; Drug Discovery, Databases, Big Data, Systems Biology. Guest Editor: [Prof. Humbert González-Díaz](#), Email: mol2net.chair@gmail.com, Department of Organic Chemistry II, University of the Basque Country (UPV/EHU) and Ikerbasque - Basque Foundation for Science, 48011 Bilbao, Biscay, **Spain**. Submissions until: **31 July 2020**.

03. Biomolecules (Call For Papers): Special Issue: [Relevant Biomolecules for Germ Cells and Fertilization](#). Journal: [Biomolecules](#) (ISSN 2218-273X). JCR IF = 4.694. Topics: Germ cells, Gamete quality, Cryopreservation, Biomarkers, Antioxidants. Guest Editors: Prof. [Vanessa](#)

Robles, Email: robles.vanesa@gmail.com, **MODCELL Group**, Department of Molecular Biology, Universidad de León, 24071 León, Spain. Dr. **Marta F. Riesco**, Spanish Institute of Oceanography (IEO), Santander, 39012, Spain, Dr. **David G. Valcarce**, Spanish Institute of Oceanography (IEO), Santander, 39012, Spain. Submissions until: **15 February 2020**.



International Journal of *Molecular Sciences*

04. IJMS (Call For Papers): Special Issue: [QSAR and Chemoinformatics Tools for Modeling](#). Journal: [International Journal of Molecular Sciences](#) IJMS (ISSN 1422-0067), **JCR IF = 4.183**. Topics: Chemometrics, QSAR/QSPR, Multi-criteria decision making, Molecular descriptors, Software development, Editor: [Prof. Roberto Todeschini](#), Email: roberto.todeschini@unimib.it, University of Milano-Bicocca, Italy.

05. IJMS (Published): Special issue entitled: [Molecular Recognition of Carbohydrates](#). Journal: [International Journal of Molecular Sciences](#) IJMS (ISSN 1422-0067), **JCR IF = 3.257**. Topics: Carbohydrates, Molecular recognition, NMR, Drug and Molecular probe design. Editors: [Prof. Francisco Javier Cañada](#), Chemical and Physical Biology, Centro de Investigaciones Biológicas, CIB-CSIC, Ramiro de Maeztu 9, 28040 Madrid, Spain, [Website 1](#) | [Website 2](#) | [E-Mail, Prof. Dr. Jesus Jimenez-Barbero](#), [Website](#) | [E-Mail](#), (MOL2NET Honor Comm.), CIC bioGUNE, Bizkaia Technology Park, Building 800, 48160 Derio, Spain; Ikerbasque, Basque Foundation for Science, Maria López de Haro 3, 48013 Bilbao, Spain.

06. IJMS (Published): Special issue entitled: [Data Analysis in Molecular Sciences](#). Journal: [International Journal of Molecular Sciences](#) IJMS (ISSN 1422-0067), **JCR IF = 3.257**. Topics: Cheminformatics, Computational Chemistry, Bioinformatics, Data Analysis, Proteomics, Biological Networks, Editors: [Prof. Humbert González-Díaz](#), University of the Basque Country UPV/EHU, Biscay, Spain. [Prof. Roberto Todeschini](#), University of Milano-Bicocca, Italy, [Prof. Alejandro Pazos Sierra](#), University of Coruña UDC, Spain, [Prof. Sonia Arrasate](#), University of the Basque Country (UPV/EHU), Biscay, **Basque Country, Spain**.

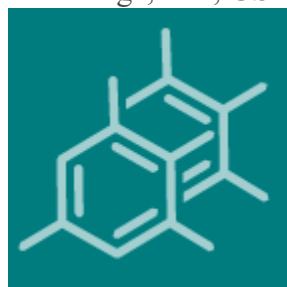


nanomaterials

07. Nanomaterials (Call For Papers): Special Issue: [Computational Nanomaterials Design: Databases, Machine Learning, Artificial Intelligence, and Big Data Analysis](#). Journal [Nanomaterials](#) (ISSN 2079-4991), **JCR IF = 4.034**. Editors: [Prof. Humbert González-Díaz](#), UPV/EHU, Leioa, Bilbao, Basque Country, Spain.

08. Nanomaterials (Published): Special Issue: [Experimental Nanosciences, Computational](#)

Chemistry, and Data Analysis. Journal Nanomaterials (ISSN 2079-4991), JCR IF = 3.55. Editors: **Prof. Humbert González-Díaz**, UPV/EHU, Basque Country, Spain, **Prof. Dr. H. Kušić**, UZ, Croatia, **Prof. B. Rasulev**, NDSU, USA, **Dr. Shameer Khader**, Philips, Cambridge, MA, USA.



molecules

09. Molecules (Call For Papers): Special Issue: **Cheminformatics, Past, Present, and Future: From Chemistry to Nanotechnology and Complex Systems.** Journal: Molecules (ISSN 1420-3049), JCR IF = 3.06. Last Date: 2020-Jul-31. Topics: Chemoinformatics, Multi-label classification, Quantum Mechanics, Molecular Mechanics (QM/MM), Molecular Docking, Big Data, Natural Computing, Quantum Computing, Artificial Neural Networks (ANN), Machine Learning, Data Analysis, Chemical Reactivity, Catalysis, Bioinformatics, Complex Biosystems, Protein Networks, Gene Regulatory Networks, Metabolic Networks, Computational Materials and Nano-sciences, Cheminformatics Regulatory issues, GDPR and Data Protection, OECD/REACH Regulation. Editors: **Prof. Humbert González-Díaz**, Current Affiliation: IKERBASQUE Professor, Dept. of Organic Chemistry II, University of the Basque Country UPV/EHU, 48940, Leioa, Biscay, Basque Country, Spain. Email: mol2net.chair@gmail.com. **Prof. Alejandro Pazos Sierra**, Chair and Director of Department of Computer Science and Information Technology, University of Coruña (UDC), Coruña, Spain. **Dr. Aliuska Duardo-Sanchez**, Chair in Law & The Human Genome Research Group, PANELFIT H2020, Project Manager & EDC Board Coordinator, Europe Commission. Lecturer Criminal Law, Faculty of Law, University of The Basque Country UPV/EHU, Leioa (Great Bilbao), Biscay, Basque Country, Spain.

10. Molecules (Call For Papers): Special Issue: **Recent Advances in Computational Drug Discovery: From In Silico Screening to Multiscale De Novo Drug Design.** Journal: Molecules (ISSN 1420-3049), JCR IF = 3.06. Last Date: 2020-Jan-31. Topics: Multi-Scale De Novo Drug Design, Multi-Scale Models, QSAR-Based Approaches, Chemoinformatics, Bioinformatics, Big Data and Data Mining, Computer-Aided Drug Discovery, and Virtual Screening. Editor: **Prof. Alejandro Speck-Planche**, Email: alejspivanovich@gmail.com, Department of Chemistry (Institute of Pharmacy), I.M. Sechenov First Moscow State Medical University, Moscow, Russian Federation.

11. Molecules (Call For Papers): Special Issue: **Computational Methods for Drug Discovery and Design.** Journal: Molecules (ISSN 1420-3049), JCR IF = 3.098. Last Date: 2019-Dec-30. Topics: molecular modeling; molecular simulations; computational biochemistry; computer-aided drug design; protein kinase inhibitors. Editor: **Prof. Julio Caballero**, Email: jcaballero@utalca.cl, Centro de Bioinformática y Simulación Molecular (CBSM), Facultad de Ingeniería, Universidad de Talca, Casilla 747, Talca 3460000, Chile.

12. Molecules (Call For Papers): Special Issue: **Structure and Function of Metalloenzymes.** Journal: Molecules (ISSN 1420-3049), JCR IF = 3.06. Last Date: 2019-Nov-

30. Topics: catalytic power of enzymes; computer-aided drug design; bio-desulfurization; computational methods in chemistry and biochemistry; metalloenzymes; biological membranes; docking and virtual screening; computational enzymatic catalysis. Workshop Associated: [EJIBCE](#), Encontro de Jovens Investigadores de Biologia Computacional e Estrutural, Portugal, 2018. Editor: [Dr. Sérgio Filipe Sousa](#), Email: sergiofsousa@med.up.pt, UCIBIO/REQUIMTE, BioSIM - Departamento de BioMedicina, Faculdade de Medicina da Universidade do Porto, Porto, Portugal.

13. Molecules (Published): Special Issue: [GPCR Mechanism and Drug Design](#). Journal: *Molecules* (ISSN 1420-3049), JCR IF = 3.06. Last Date: 2019-Nov-30. Topics: data science; drug design and discovery; computational chemistry; structural biology; molecular modeling; molecular docking; computational mutagenesis; G-protein-coupled receptors; protein-protein interactions; protein-ligand interactions. Workshop Associated: [EJIBCE](#), Encontro de Jovens Investigadores de Biologia Computacional e Estrutural, Portugal, 2018. Editor: [Dr. Irina Moreira](#), Email: irina.moreira@cnc.uc.pt, Center for Neuroscience and Cell Biology (CNC), University of Coimbra (UC), Portugal.

14. Molecules (Published): Special Issue: [From Computational Chemistry to Complex Networks](#). Journal: *Molecules* (ISSN 1420-3049), JCR IF = 3.06. Topics: Quantum Mechanics /Molecular Mechanics (QM/MM), Drug-target, protein-protein and other Docking methods, Monte Carlo (MC) methods, Quantitative Structure-Activity/Property Relationships (QSAR/QSPR) models, Graph theory and Complex Networks Topological Indices (TIs), Protein Structure Networks, Protein Interaction Networks (PINs) and Proteome. Editor: [Prof. Humbert González-Díaz](#), Email: mol2net.chair@gmail.com, Current Affiliation: IKERBASQUE Professor, Dept. of Organic Chemistry II, University of the Basque Country UPV/EHU, 48940, Leioa, Biscay, Basque Country, Spain.

15. Molecules (Call For Papers): Special Issue: [Natural Products for Neurodegenerative Diseases](#). Journal: *Molecules* (ISSN 1420-3049), JCR IF = 3.06. Last Date: 2019-Oct-31. Topics: Medicinal chemistry; Natural products; Photochemistry reactivity; Aporphines, oxoaporphines, and oxoisoaporphines; Coumarins. Editor: [Prof. Eduardo Sobarzo-Sanchez](#), Email: eduardo.sobarzo@ucentral.cl, Instituto de Investigación e Innovación en Salud, Facultad de Ciencias de la Salud, Universidad Central de Chile, Chile.



entropy

16. Entropy (Call for Papers): Special Issue: [Statistical Inference from High Dimensional Data](#). Journal Entropy (ISSN 1099-4300), JCR IF = 2.419. Editors: [Prof. Carlos Fernández-Lozano](#). Department of Computer Science, Faculty of Computer Science, University of A Coruña, CITIC, A Coruña 15071, Spain.

17. Entropy (Call for Papers): Special Issue: **Biological Statistical Mechanics**. Journal Entropy (ISSN 1099-4300), **JCR IF = 2.419**. Last Date: **2019-Nov-15**. Topics: cell differentiation, biocomplexity, order and organization, ecology, epidemics, correlation dynamics, complex networks, systems biology. Editors: **Prof. Alessandro Giuliani**, Email: alessandro.giuliani@iss.it, Environment and Health Department, Istituto Superiore di Sanità, Roma 00161, Italy. Prof. **Mariano Bizzarri**, Department of Experimental Medicine, Systems Biology Group Lab, Sapienza University of Rome, Rome, **Italy**.

18. Entropy (Published): Special Issue: **Graph and Network Entropies**. Journal Entropy (ISSN 1099-4300), **JCR IF = 2.419**. Topics: network sciences; walk entropies; algebraic graph theory; spectral methods; matrix functions. Editor: **Prof. Ernesto Estrada**, Email: ernesto.estrada@strath.ac.uk, Department of Mathematics & Statistics, University of Strathclyde, Glasgow G11XQ, **United Kingdom**. Current Affiliation: ARAID Professor, Institute of Applied Mathematics (IUMA), University of Zaragoza, **Spain**.



applied sciences

19. Applied Sciences (Published): Special issue entitled: **Applied Artificial Neural Networks**. Journal Applied Sciences (ISSN 2076-3417), **JCR IF = 2.217**. Topics: Evolutionary Computation; Artificial Neural Networks; Artificial Intelligence; Feature Selection; Machine Learning. Editor: **Prof. Marcos Gestal**. Email: marcos.gestal@udc.es, Computation Sciences and Information Technologies Department, Faculty of Computer Science, University of A Coruña, 15071, A Coruña, **Spain**.

20. Applied Sciences (Published): Special issue entitled: **Complex Networks and Machine Learning: From Molecular to Social Sciences**. Journal Applied Sciences (ISSN 2076-3417), **JCR IF = 2.217**. Topics: machine learning, complex networks, systems biology, protein networks, metabolic networks, ecosystems, artificial neural networks, social, financial, and legal networks. Editors: **Prof. Maykel Cruz-Monteagudo**, Email: mCruz@westcoastuniversity.edu, West Coast University, Miami Campus, FL, **USA**, **Prof. David Quesada**, Director of Dept. of Mathematics, Miami Dade College (MDC), Miami, FL, **USA**. Email: dquesada@mdc.edu, **Prof. Humbert González-Díaz**, Email: mol2net.chair@gmail.com, IKERBASQUE Professor, Dept. of Organic Chemistry II, University of the Basque Country UPV/EHU, 48940, Leioa, Biscay, **Basque Country, Spain**.

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USEDAT Integrating Labs Photo Galley



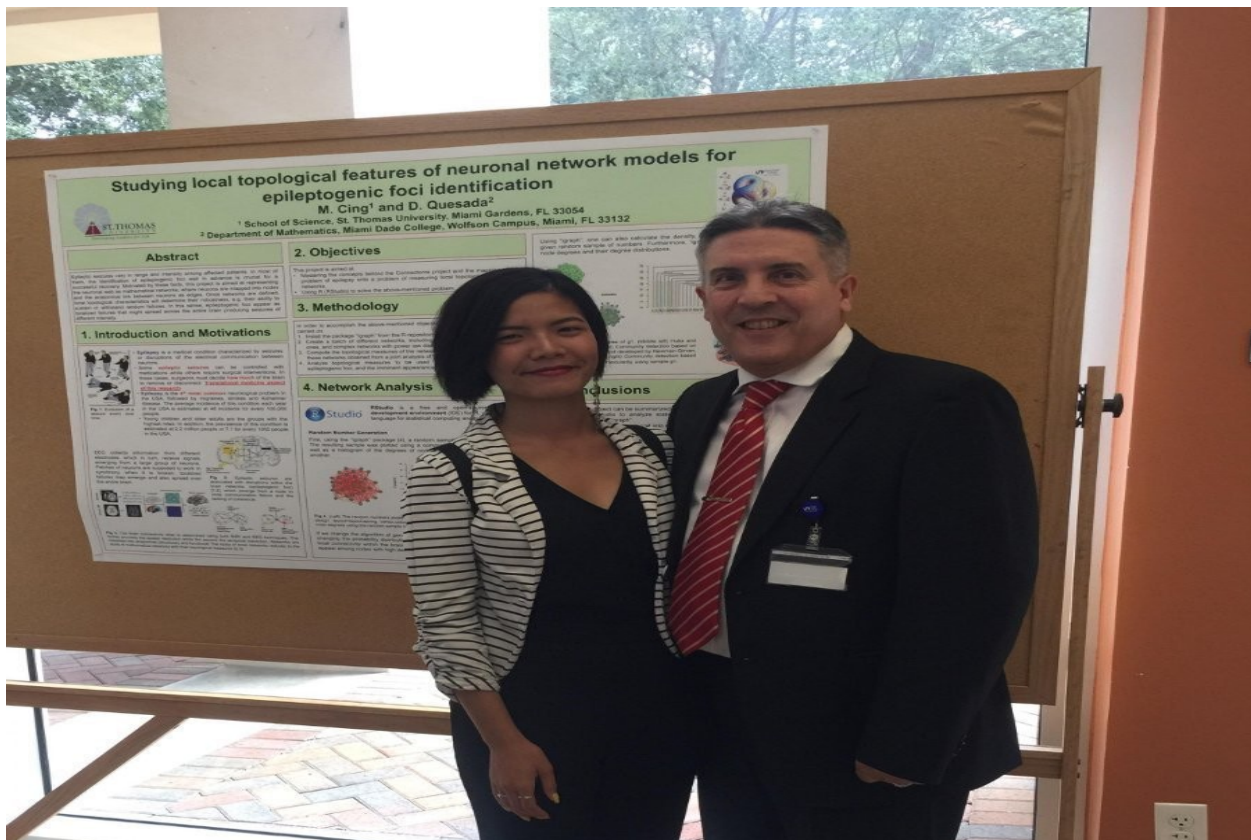
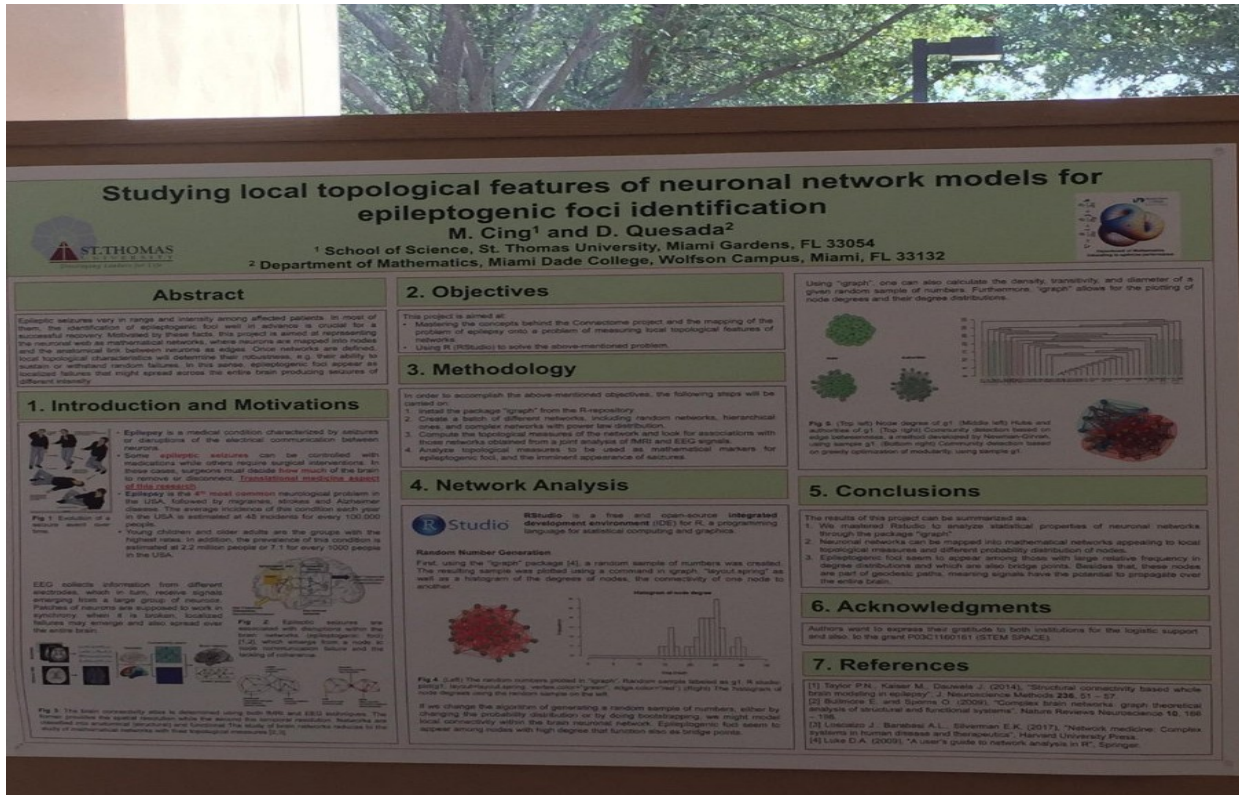
USEDAT ICN NSF-CREST Comput Nanotox: [Prof. Jerzy Leszczynski](#), Dir. Interdisciplinary Center for Nanotoxicity (ICN), Dept. of Chemistry and Biochemistry, Jackson State University (JSU), USA, with collaborators and students.



USEDAT UFPB-UNC Chapel Hill: Assoc Prof. [Prof. Eugene Muratov](#) University of North Carolina (UNC), Chapel Hill , NC, USA with Prof. [Marcus Tullius Scotti](#) Universidade Federal da Paraíba (UFPB) and UFPB USEDAT Students and Researchers, Joao Pessoa, Brazil, 2019.



USEDAT SRI MDC: Prof. [David Quesada](#) with students at SRI Summer School, Miami Dade College (MDC), FL, USA.



USEDAT SRI MDC: Prof. [David Quesada](#) with student and poster details at SRI Summer School, Miami Dade College (MDC), FL, USA.



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USEDAT GTPB - The Gulbenkian Training Programme in Bioinformatics: Prof. [Pedro L. Fernandes](#), with students of Bioinformatics Training, Instituto Gulbenkian de Ciencia (IGC), Lisbon.



USEDAT GTPB - The Gulbenkian Training Programme in Bioinformatics (@mygtpb): Train-the-Trainer event, attached to the BPBR16 course. First day, how learning works, training techniques. Prof. [Pedro L. Fernandes](#), with Ragnhild Reehorst Lereim, Vincenza Colonna, Domenica D'Elia, Allegra Via, Kim Gurwitz, David Philip Judge, Inês Fragata, Herminia Gnu, Marta Pingarilho, Jure Dimec and KeLin at Instituto Gulbenkian de Ciência, Lisbon, Portugal.



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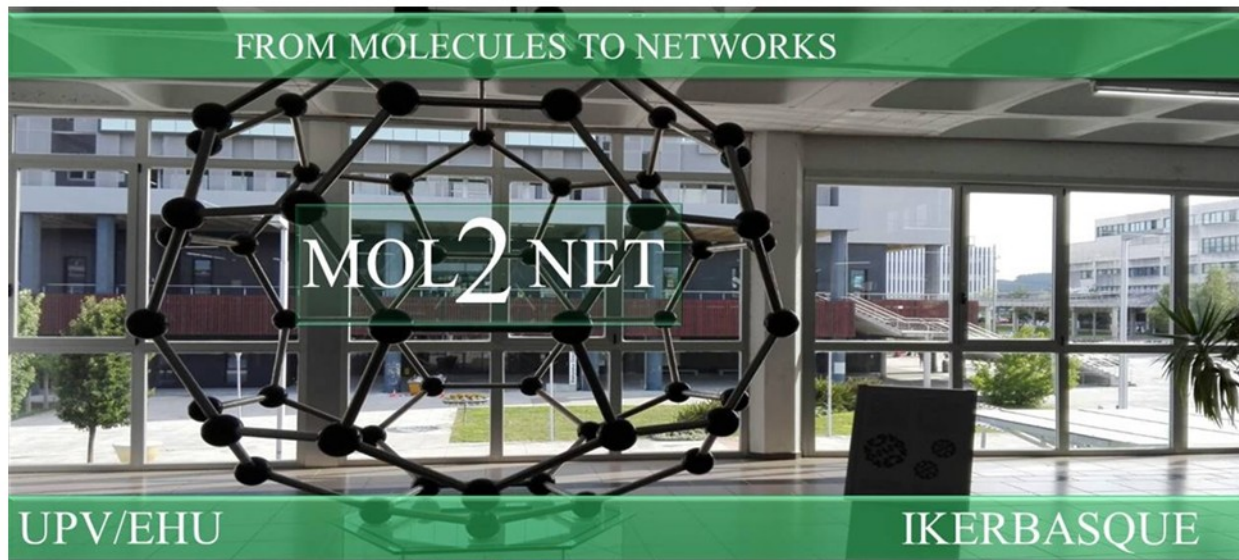
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DETAILS

[List of accepted submissions \(135\)](#)

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