MOL2NET: FROM MOLECULES TO NETWORKS (PROCEEDINGS BOOK), Vol. 4.

FROM MOLECULES TO NETWORKS

MOL2NET

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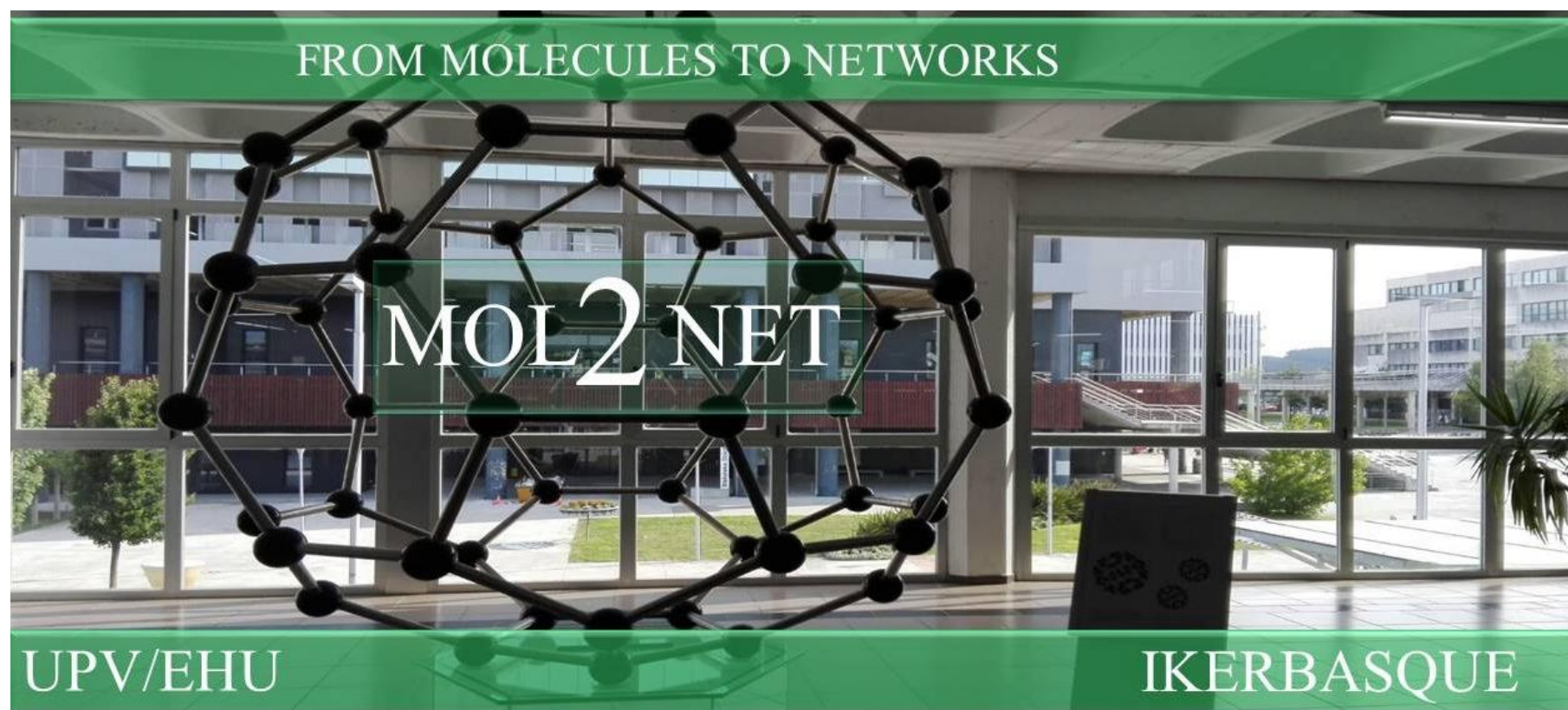
MOL2NET 2017, International Conference on Multidisciplinary Sciences (4th edition)

MOL2NET: FROM MOLECULES TO NETWORKS (PROCEEDINGS BOOK) Vol. 4.

YEAR-ROUND CONFERENCE
15 January–15 December 2018

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01. Welcome Message & Proceedings

Welcome from the Chair
[MOL2NET 2015] [MOL2NET 2016] [MOL2NET 2017] [FACEBOOK (>10K followers)]
[Welcome Videos] [官话] [हिन्दी] [Euskera] [Castellano] [Português] [Français]

[CLICK HERE TO SUBMIT NEW ABSTRACT]
LAST DAY FOR SUBMITTING COMMUNICATIONS 2018-Dec-22
ONLINE DISCUSSION FORUM OPEN FROM 2018-Dec-23 TO 2019-Jan-05
Dear colleagues worldwide, we are glad to invite you to MOL2NET-04, International Conference on Multidisciplinary Sciences, **ISSN**: 2624-5078, **ISBN**: 978-3-03842-820-6, MDPI SciForum, Basel, Switzerland, 2018. 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 Biolog**y, and **Complex Networks Sciences**. We suggest you to **download** the [Template File] to write your communication and to **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).

Sessions & Workshops

01. Welcome Message & Proceedings

02. SRI-10: Summer Research Inst. Symp. (Chemistry, Phys., Med., Nano., Bioinf., etc.), MDC, Miami, FL, USA, 2018

03. USINEWS-02: US-IN-EU World. Science Workshop Series (Chem., Phys., Omics., Nano., etc.), UMN, Duluth, USA, 2018

04. BIOCHEMPHYS-01: International Workshop (Med. Chem., Biotech., Phys. Chem.), CNAM, Paris, France, 2018

05. WCUCW-02: West Coast Univ. Capstone Workshop (Chem., Bioinf., Med., etc.), WCU, Miami, USA, 2018

06. WRSAMC-03: Workshop in Med. Chem. (Org. Chem., Nat. Prod., etc.), UFPB, Paraiba, Brasil, 2018

07. EJIBCE-02: Meeting in Struct. Comput. Biol. (Bioinf., Med. Chem., etc.), UPORTO, Portugal, 2018

08. OTISAD-01: Workshop on Intell. Decis. & Opt. (Systems, Data Analysis, etc.), UANL, Mexico, 2018

09. ICBSM-02: International Conf. (Bioinf., Simul., Data Analysis, & Mod.), UTALCA, Talca, Chile, 2017

10. IWMEDIC-06: Int. Workshop in Med. Info. (Image Proc., Data Sci., etc.), UDC, Coruña, Spain, 2018

11. IWIMSM-02: Iberoamerican Workshop on Model. & Simul. Meth., Valencia, Spain, 2018

12. LAWSCI-02: Challenges in Law, Tech., Life, and Soc. Sci., UPV/EHU, Bilbao, Spain, 2018

13. AWP-04: Academic Week of Physics, UNIFAL-MG, Alfenas, Brazil, 2018

14. MODEC-03: Workshop on Nat. Prod. & Agro. Proce. in Amazon, UEA, Ecuador, 2018

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 Template], or use the for other workshops: [BioChemPhys Template], [WRSAMC template] , [MODEC Template], [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 author (publication) or attendance (posting) certificate for conference and/or workshops (All the year)

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 Online participation: 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 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.

Notes 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.

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.

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, **is responsibility of authors**, to perform a **checking similarity**, 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.** 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.
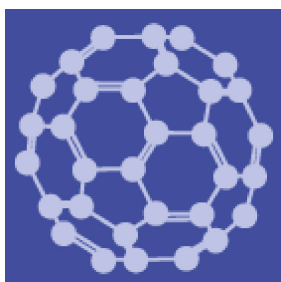
Call for Collaborators, Editors, Chairpersons, Sponsors

[EN] We sincerely invite you to join MOL2NET Conference Series or one of the worldwide associated workshops; please, sent a direct email to the chairperson: Prof. González-Díaz H., IKERBASQUE Professor, Email: mol2net.chair@gmail.com. You are encouraged to nominating and/or personally applying for a position or active role in some of the following modalities, or other modalities of collaboration suggested by you:

(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).

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. Please, check the following list of past and present special issues associated to our conference:
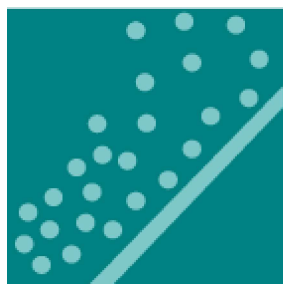
Nanomaterials (Published): Special issue entitled: Experimental Nanosciences, Computational Chemistry, and Data Analysis. Journal Nanomaterials (ISSN 2079-4991), **JCR IF = 3.55**. Editors: Prof. González-Díaz H, UPV/EHU, Spain, Prof. B. Rasulev , NDSU, USA,Dr. Shameer Khader, Philips, Cambridge, MA, USA, Prof. H. Kušić, UZ, Croatia.
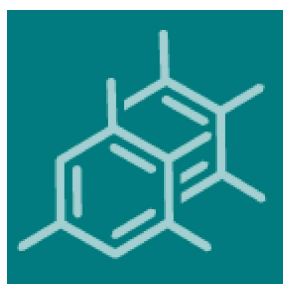

IJMS (Published): Special issue entitled: Data Analysis in Molecular Sciences. Journal: International Journal of Molecular SciencesIJMS (ISSN 1422-0067), **JCR IF = 3.257**. Topics: Cheminformatics, Computational Chemistry, Bioinformatics, Data Analysis, Proteomics, Biological Networks, Editors: Prof.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

Entropy (Call for Papers): Special issue entitled: **Biological Statistical Mechanics**. Journal Entropy (ISSN 1099-4300), **JCR IF = 1.821**. Topics: cell differentiation, biocomplexity, order and organization, ecology, epidemics, correlation dynamics, complex networks, systems biology. Editors: Prof. Alessandro Giuliani. 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.

Entropy (Call for Papers): Special issue entitled Graph and Network Entropies. Journal Entropy (ISSN 1099-4300), **JCR IF = 1.821**. Topics: network sciences; walk entropies; algegraic graph theory; spectral methods; matrix functions. Editor: Prof. Dr. Ernesto Estrada, Department of Mathematics & Statistics, University of Strathclyde, Glasgow G11XQ, UK.
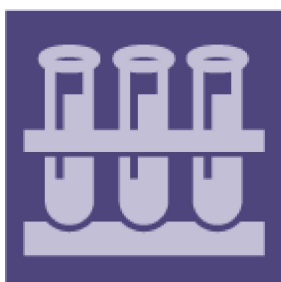

Molecules (Call For Papers): Special Issue: **GPCR Mechanism and Drug Design**. Journal: *Molecules* (ISSN 1420-3049), **JCR IF = 3.098.** Topics: data science; drug design and discovery; computational chemistry; structural biology; molecular modeling; molecular docking; computational mutagenesis; G-protein-coupled receptors; protein–protein interactions; protein–ligand interactions. Editor: Dr. Irina Moreira, Email: irina.moreira@cnc.uc.pt, Center for

Neuroscience and Cell Biology (CNC), University of Coimbra (UC), Portugal. Workshop Associated: EJIBCE, Encontro de Jovens Investigadores de Biologia Computacional e Estrutural, Portugal, 2018.

Molecules (Call For Papers): Special Issue: **Structure and Function of Metalloenzymes**. Journal: *Molecules* (ISSN 1420-3049), **JCR IF = 3.098.** 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. 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. Workshop Associated: EJIBCE, Encontro de Jovens Investigadores de Biologia Computacional e Estrutural, Portugal, 2018.

Applied Sciences (Call for Papers): Special issue entitled: **Complex Networks and Machine Learning: From Molecular to Social Sciences**. Journal Applied Sciences (ISSN 2076-3417), **JCR IF = 1.679**. 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. Dr. David Quesada, Director of Dept. of Mathematics, Miami Dade Colege (MDC), Miami, FL, USA. Email: dquesada@mdc.edu, Prof. González-Díaz H., IKERBASQUE Professor, Dept. of Organic Chemistry II, University of the Basque Country UPV/EHU , 48940, Leioa, Biscay, Spain. Email: mol2net.chair@gmail.com

Associated Workshops

In addition, you can participate both online or in person (face-to-face) in some of the workshops we organize in different universities worldwide (see workshops section). Publication of all communications of the workshops will be also 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. Some of the workshops planned to be held in 2018 edition are: SRI-10, St. Thomas University (STU) and Miami Dade College (MDC), Miami, FL, USA (Multidisciplinary Sciences); WCUCW-02, West Coast University (WCU), Miami, FL, USA (Multidisciplinary Sciences); WMCUP-01, University of Padova (UP), Padova, Italy (Medicinal Chemistry); LAWSCI-01, University of the Basque Country UPV/EHU, Bilbao, Spain (TICs, Bioethics, Social, and Legal Sciences), etc.; see other workshops in the list of sections at left panel.

Past Editions

MOL2NET-03, the 3rd edition of this conference series, was held in **2017**. This conference received >250 communications, submitted by >450 authors registered, and included >10 workshops in: USA, Spain, Portugal, Brazil, etc.. Some of the world top universities and centers represented in the lists of committee members and/or authors were: **Harvard** Medical School, Boston, USA; **Stanford** School of Medicine, USA; **Virginia** Commonwealth University (VCU), USA; University of**Minnesota Duluth**, MN, USA; Conservatoire National des Arts et Métiers, **CNAM París**, France; University of **Pennsylvania**, USA; **Miami** Dade Collegue (MDC), USA;**EMBL-EBI** European Bioinformatics Institute, Cambridge, UK; **CAS** Chinese Academy of Science, China; **ZJU** Zhejiang University, China.

MOL2NET-02, the 2nd edition of this conference series, was held in 2016. This 2nd conference published 150 communications of 400+ authors 30+ universities of 20+ countries. Some of the world top universities and centers represented in the lists of committee members and/or authors were: Harvard Medical School, Boston, USA; Stanford School of Medicine, USA; Virginia Commonwealth University (VCU), USA; University of Minnesota Duluth, MN, USA; Conservatoire National des Arts et Métiers, CNAM París, France; University of Pennsylvania, USA; Miami Dade Collegue (MDC), USA; EMBL-EBI European Bioinformatics Institute, Cambridge, UK; CAS Chinese Academy of Science, China; ZJU Zhejiang University, China.

MOL2NET-01, the first edition of this conference series, was held in 2015. This first conference attracted more than 100 papers and 300+ authors and/or committee members representing 30+ universities of 20+ countries. Some of the world top universities and centers represented in the lists of committee members and/or authors were: Harvard Medical School, Boston, USA; Stanford School of Medicine, USA; Virginia Commonwealth University (VCU), USA; University of Minnesota Duluth, MN, USA; Conservatoire National des Arts et Métiers, CNAM París, France; University of Pennsylvania, USA; Miller School of Medicine,University of Miami, USA; EMBL-EBI European Bioinformatics Institute, Cambridge, UK; CAS Chinese Academy of Science, China; ZJU Zhejiang University, China.

People, Media Channels, and Social Networks

We are uploading flyers and promotional videos (in different languages) to the MOL2NET accounts in different social networks such as: FACEBOOK group with**>10000 followers**; RESEARCHGATE project, LINKEDIN, and TWITTER account @mol2net. In addition, we have uploaded topic-specific pages with lists of contacts of people related to the conference. In this page you can find people with research interests focused on one specific area such as Organic Chemistry, Computational Chemistry, Materials or Nanoscience, etc.

Influences & Sister Conferences

MOL2NET conference series is inspired on various Sciforum conference series, specially on the ECSOC Electronic Conference Series in Organic Chemistry organized during more than 20 years (22nd edition in 2018) by Prof. Julio Seijas at Department of Organic Chemistry, Faculty of Sciences, Campus Lugo, University of Santiago de Compostela (USC), Spain. In consonance, we are glad to list Prof. Siejas in the scientific committee of MOL2NET and we invite all colleagues to participate also in ECSOC conference. In addition, MOL2NET committee members would like to recommend other conferences with some topics in common such as: IWBBIO, International Work-Conference on Bioinformatics and Biomedical Engineering, Chairperson: Prof. Ignacio Rojas, et al., Univerity of Granada, 2018 edition. NetSci: International School and Conference on Network Science.

THANK YOU FOR YOUR SUPPORT!!!

Sincerely yours

MOL2NET Chairman

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*Note: This committee is for MOL2NET Conference Series, to see the committees of each specific workshops associated to the conference visit the page of this workshop.

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*Translating biomedical research into commercial opportunities*

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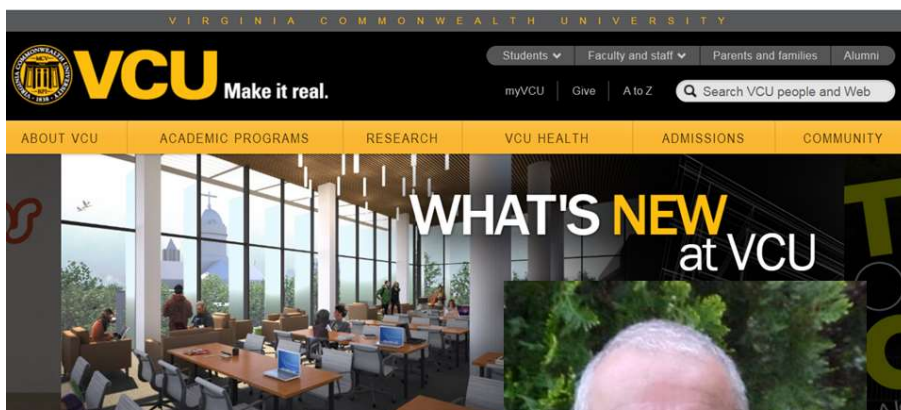
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Prof. Geza Toth, Ikerbasque Professor, Department of Physics, University of the Basque Country (UPV/EHU), Campus Buscay, Spain.

THANK YOU FOR YOUR SUPPORT!!!

Founder Chairman

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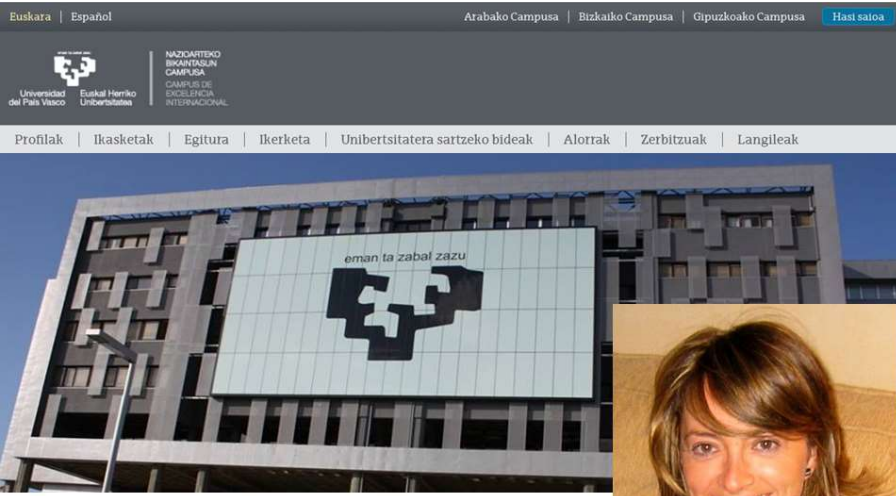UPV/EHU , 48940, Leioa, Biscay, Spain.
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MOL2NET Assoc. Journals Issues

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 atwww.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. Please, check the following list of past and present special issues associated to our conference:

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

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

Entropy (Call for Papers): Special issue entitled: **Biological Statistical Mechanics**. Journal Entropy (ISSN 1099-4300), **JCR IF = 1.821**. Topics: cell differentiation, biocomplexity, order and organization, ecology, epidemics, correlation dynamics, complex networks, systems biology. Editors: Prof. Alessandro Giuliani. 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.

Entropy (Call for Papers): Special issue entitled **Graph and Network Entropies**. Journal Entropy (ISSN 1099-4300), **JCR IF = 1.821**. Topics: network sciences; walk entropies; algebraic graph theory; spectral methods; matrix functions. Editor: Prof. Dr. Ernesto Estrada, Department

of Mathematics & Statistics, University of Strathclyde, Glasgow G11XQ, UK.

Molecules (Call For Papers): Special Issue: **GPCR Mechanism and Drug Design**. Journal: *Molecules* (ISSN 1420-3049), **JCR IF = 3.098**. 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. Editor: Dr. Irina Moreira, Email:irina.moreira@cnc.uc.pt, Center for Neuroscience and Cell Biology (CNC), University of Coimbra (UC), Portugal. Workshop Associated: EJIBCE, Encontro de Jovens Investigadores de Biologia Computacional e Estrutural, Portugal, 2018.

Molecules (Call For Papers): Special Issue: **Structure and Function of Metalloenzymes**. Journal: *Molecules* (ISSN 1420-3049), **JCR IF = 3.098**. 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. 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. Workshop Associated: EJIBCE, Encontro de Jovens Investigadores de Biologia Computacional e Estrutural, Portugal, 2018.

Applied Sciences (Call for Papers): Special issue entitled: **Complex Networks and Machine Learning: From Molecular to Social Sciences**. Journal Applied Sciences (ISSN 2076-3417), **JCR IF = 1.679**. 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. Dr. David Quesada, Director of Dept. of Mathematics, Miami Dade Colege (MDC), Miami, FL, USA.
Email: dquesada@mdc.edu, Prof. González-Díaz H., IKERBASQUE Professor, Dept. of Organic Chemistry II, University of the Basque Country UPV/EHU , 48940, Leioa, Biscay, Spain. Email: mol2net.chair@gmail.com

02. SRI-10: Summer Research Institute Symposium, MDC, Miami, FL, USA, 2018

NOTES: Before to submit your communication we strongly recommend to read to read carefully the **notes to participants** at the end of the welcome message and/or the notes in the following page [Notes to authors] about publication model, copyright, authors responsibilities, *etc*.

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LAST SUBMITTING DAY FOR COMMUNICATIONS 15/12/2018
ONLINE DISCUSSIONS OPEN 15/12/2018 - 25/12/2018

Welcome Message

Dear colleagues worldwide welcome to the Summer Research Institute (SRI) Symposium of the School of Science, Technology, and Engineering Management of Saint Thomas University (STU) and Miami Dade College (MDC). SRI series have research and education objectives providing undergraduate students, master, and phd students as well as research associated and professor hands-on experiences and computational projects. The workshop is dual including both in person participation (mostly for STU-MDC students and professors) and online participation (including students and professors from abroad). It covers multidisciplinary topics in science ranging from modern techniques of molecular biology, statistical analysis, mathematical modeling, computational physics, bioinformatics, nano sciences and a large variety of characterization techniques to the social, legal, and educational implications of these techniques.

For the third time, this year, the memories of the SRI series will be hosted online by the MOL2NET conference series. It means, that all communications will be published online at Sciforum platform. All presentations will be peer reviewed and a DOI number will be assigned. MOL2NET conference of Sciforum is one of the platforms with international recognition for scientific exchange. The variety of topics included within this new edition acknowledges the inter-disciplinary, teamwork, and networking of modern science. Feel free to contact researchers and participants to foster more collaboration efforts.

Last Edition

The last edition SRI-09 received a total of 27 submissions. Special thanks to our partner Miami Dade College (MDC) and the grant **STEM-SPACE P03C1160161**. The received contributions provided funding for equipment, logistics, and minor activities associated with the SRI. Ten speakers from and local Technological companies came to St. Thomas to share their wisdom as an in kind contribution. During this last edition, students exchanged experiences with researchers from University of Miami, Florida International University (FIU) and also from NASA. To see another previous edition you can follow the link SRI-08 and witness the quality of 38 submissions with a total of 21 publications.

MDPI Associated Journals Issue (Organized by SRI 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. Please, check the following special issue associated to our conference:

Applied Sciences (Call for Papers): Special issue entitled: Complex Networks and Machine Learning: From Molecular to Social Sciences. Journal Applied Sciences (ISSN 2076-3417), **JCR IF = 1.679**. Topics: machine learning, complex networks, systems biology, protein networks, metabolic networks, ecosystems, artificial neural networks, social, financial, and legal networks. Editors: Prof. D. Quesada, Director of Dept. of Mathematics, Miami Dade Colege (MDC), Miami, FL, USA. Prof. M. Cruz-Monteagudo, West Coast University, Miami Campus, FL, USA, FCT Fellow University of Porto Portugal, Consultant, Center for Computer Science (CCS), University of Miami, FL, USA. Prof. González-Díaz H., IKERBASQUE Professor, Dept. of Organic Chemistry II, University of the Basque Country UPV/EHU , Leioa (Great Bilbao), Biscay, Spain.
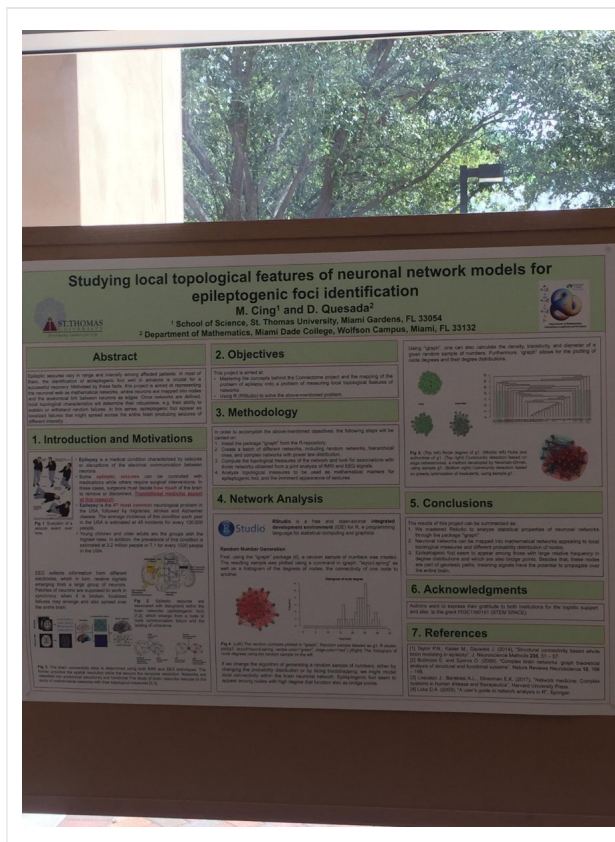
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Hide published submissions (24) and accepted abstracts (5)

Submissions

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Title	Poster	Authors	
Precision Medicine: Carbon Nanotubes as Potential Treatment for Human Brain Disorders-Based Mitochondrial Dysfunctions with a First Principles DFT-Study		Patrícia de Oliveira, Michael Gonzàlez-Durruhty, José María Monserrat, Solange Binotto Fagan	Show Abstract
New tool useful for drug discovery validated through benchmark datasets		Juan Castillo-Garit, Yoan Martínez-López, Yaile Caballero, Stephen Barigye, Yovani Marrero-Ponce, Reisel Millán Cabrera, Julio Madera, Efrain Chaluisa Quishpe, Francisco Torrens	Show Abstract
Predicting Compound-Protein Interactions in GPCR Network		Víctor Yáñez, Amanda Sánchez-Recillas	Show Abstract
A novel QSAR model to predict epidermial growth factor inhibitors		Riccardo Concu, Maria Natalia Dias Soeiro Cordeiro	Show Abstract
Prediction of pH-dependent aqueous solubility of druglike molecules of different chemical behavior		Laura Machin, Luis Alberto Torres-Gomez	Show Abstract
Multivariate classification of a series of organic compounds of pharmaceutical interest using MODESLAB methodology		Luis Alberto Torres-Gomez, Juan Carlos Polo, Yaima Garcia Guevara, Tapiwa Brine Mutsauri	Show Abstract

Title	Poster	Authors	
Modeling and prediction of anti-inflammatory activity in compounds of natural and synthetic origin		Luis Alberto Torres-Gomez, Yaima Garcia Guevara, Enoel Hernández Barreto	Show Abstract
PTML Model Prediction of Preclinical Activity		Harbil Bediaga, Sonia Arrasate Gil	Show Abstract
Gaussian basis set of triple zeta quality for atoms Fr through Lr: Application in DFT calculations of molecular properties		Amanda Ziviani de Oliveira, Cesar Turczyn Campos, Igor Badke Ferreira, Francisco Jorge, Lucas Sousa Carvalho Martins, Paulo Fantin	Show Abstract
Surveying Alignment-free Features for Ortholog Detection in Related Yeast Proteomes by using Supervised Big Data Classifiers		Deborah Galpert Cañizares, Alberto Fernández, Francisco Herrera, Agostinho Antunes, Reinaldo Molina Ruiz, Guillermin Agüero-Chapin	Show Abstract
Plasma-Based Water Purifier: Design And Testing Of Prototype with Different samples of water		Suraj M	Show Abstract
Chemical constituents isolated from *Mandevilla dardonoi* (Apocynaceae)		Francisca Lins, Josean Tavares, Marcelo da Silva, José de Melo, George Santos, Joanda Silva, Laiane Pereira, Lucas Abreu	Show Abstract
Predicting Proteasome Inhibition using Atomic Weighted Vector and Machine Learning		Juan Castillo-Garit, Yoan Martínez-López, Efrain Chaluisa Quishpe, Yaile Caballero, Stephen Barigye, Francisco Torrens	Show Abstract
Ligand-Based and Structure-Based virtual screening for the discovery of natural inhibitor the Hepatitis C Virus		Renata Priscila Costa Barros, Marcus Scotti	Show Abstract
PROPOSITION *IN SILICO* OF BENZOIC ANALOGS AGAINST *Staphylococcus aureus*	N/A	Alex Monteiro, Jessika Viana, Renata Barros, Marcus Scotti, Luciana Scotti	Show Abstract
A proposal for distributed processing for large scale virtual screening using Python		Alex Camargo, Vinicius Seus	Show Abstract
Ternary Phase Diagrams of Viral Proteins: The Example of H1N1 Influenza	N/A	Yunjoo Bae, Daniel Graham	Show Abstract
Fatiguing Data to Protect against Cyber Security Extortions: A counter-intelligence methodology	N/A	Dr. Anthony Vincent	Show Abstract
Generating optimal features to find out potent molecules against dengue virus: pharmacophore and QSAR approaches		Kazi Amirul Hossain	Show Abstract

Title	Poster	Authors	
MOLECULAR MODELING OF NUCLEOTIDE DERIVATIVES OF 2.5-DIHYDROFURAN-2,5-DIOL FOR EVALUATION OF POTENTIAL ANTITUBERCULAR ACTIVITY		Alex Monteiro, Marcus Scotti, Luciana Scotti	Show Abstract
Triterpenoids identified by GC-MS in chloroform/methanol extract from leaves of *Cissus incisa*	N/A	Deyani Nocedo-Mena, Mauricio González-Ferrara, María del Rayo Camacho-Corona	Show Abstract
Antihyperalgesic activity of quillaic acid obtained from *Quillaja saponaria* Mol.	N/A	Maité Rodríguez-Díaz, Carla Delporte, Sylvia Arrau, Bruce Cassels, Hugo Miranda, Gabriela Valenzuela, Andrés Barriga	Show Abstract
Challenges for implementing Next Generation Sequencing (NGS) of benthic macrofauna challenges, in the evaluation of marine environmental quality		Gerardo* Martí-Chillón, Ana* de Luis, Mónica* Díez-Díaz, Javier Torres Gavilá, José Rafael García-March, José Tena Medialdea, Francisco Codoñer	Show Abstract
Hyperheuristics for indirect elicitation of outranking model's parameters in Project Portfolio Optimization		Nelson Rangel-Valdez, Eduardo Fernandez, Laura Cruz-Reyes, Claudia Gomez-Santillan, Lucila Morales-Rodriguez	Show Abstract

List of Accepted Abstracts (5) Toggle list

Effect of localized mechanical vibration assisted self-assembly of particles on inherent defects.

Sayantan Das

Submitted: 26 Oct 2018

Abstract: Show Abstract

Carvacrol Encapsulated in Gellan Gum Hydrogel Enhancing The Antibacterial Activity

Adila Jaafar, Norafida Hasnu, Mas Jaffri Masarudin, Zulkarnain Zainal, Nur Aisyah Nasuha Mohd Azam, Norhayati Hashim

Submitted: 12 Jun 2018

Abstract: Show Abstract

Magnetic and transparent glasses: A structural approach by different spectroscopic techniques

Roger Fernandes, Douglas Franco, Valmor Mastelaro, Marcelo Nalin

Submitted: 11 Oct 2018

Abstract: Show Abstract

Non-parametric bootstrap confidence interval for inflection temperatures during the thermogravimetry of carbon nanotubes

Eric Ferreira, Raphael Borges, Cristiana Magalhães

Submitted: 10 Oct 2018

Abstract: Show Abstract

Use of Simulation For Engineering Enhancement

Karim Ennouri

Submitted: 23 Oct 2018

Abstract: Show Abstract

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03. USINEWS-02: US-IN-EU Worldwide Science Workshop Series, UMN, Duluth, USA, 2018

USINEWS-02
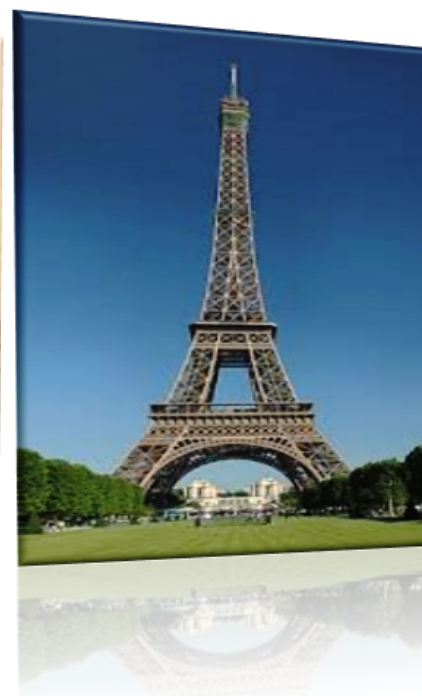
[MOL2NET 2015] [MOL2NET 2016] [MOL2NET 2017] [FACEBOOK (>10K followers)]
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(YEAR-ROUND PUBLICATION, OPEN ACCESS, AND FREE OF CHARGE)

USINEWS-02; US-IN-EU Worldwide Science Workshop Series is aimed to become a reference international science workshop series. This workshop is associated to MOL2NET-04 International Conference Series on Multidisciplinary. In fact, the publication of communications is at the online platform SciForum maintained by the editorial MDPI, Basel, Switzerland. After publication of papers is closed we shall open the online platform and the author 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). To see a detailed schedule of this workshop/section and all the conference follow this link[MOL2NET workshops schedule]. The University of Minnesota, MN, USA, the NSIT Netaji Subhas Institute of Technology, New Delhi, India, the University of Basque Country (UPV/EHU) and IKERBASQUE, Basque Foundation for Sciences, Biscay, Spain, are the main host institutions (see chairpersons below).

USINEWS focused on the interchanges of ideas among researchers working in U.S., Europe, India, etc. with colleagues from other countries across the world. The foundations of this workshop are in the multiple collaborations of Professors / Researchers of Indian like Dr. Suhbash C. Basak, University of Minnesota, USA, Prof.Ashok. K. Dubey, NSIT Netaji Subhas Institute of Technology, New Delhi, India, Prof. Kunal Roy, Jadavpur University, Dr. Shameer Khader, Philips Healthcare, Cambridge, MA, USA, with their international colleagues at Virginia Commonwealth University (VCU), University of Basque Country (UPV/EHU), IKERBASQUE, Basque Foundation for Sciences, and many other institutions in US-EU, India, and other countries.

The workshop is inspired on the Indo-U.S. Workshops series organized by Dr. Suhbash C. Basak during many years, as example of multicultural melting pot devoted to promote interdisciplinary collaborations in science. The works on this initiative started in 1990; the first event was organized in 1998 at Visva Bharati University, West Bengal, India. The Lecture Series was mainly to train young scholars. The third line of events was geared to benefit the South American scientists and young scholars. Two events have been held in Colombia. Some reports of these workshops are: *[J. Chem. Inf. Comput. Sci.*, 1999, 39 (2), pp 179–179], [*J. Chem. Inf. Comput. Sci.*, 2001, 41 (3), pp 479–479], [*J. Chem. Inf. Model.*, 2006, 46 (1), pp 1-1], These workshops included:

(1) Indo-US Workshop on Mathematical Chemistry Series, beginning in 1998 in India and having six more events both in USA and India

(2) Indo-US Lecture Series on Discrete Mathematical Chemistry, four events mainly focusing on the training of young scholars.

(3) Mathematical Chemistry Workshops of the Americas (involving countries of North and South Americas)

This INDOWSCI workshop is associated to MOL2NET-04 International Conference on Multidisciplinary Sciences, MDPI Sciforum, Switzerland, HQ UPV/EHU, Bilbao, Spain. Consequently, it aims to promote results on Multidisciplinary Science (All Areas), including but not limited to, the following **topics of interest:** 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. See the following note to authors on **topics outside the scope** of the conference and associated workshops [Note on topics].

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Preliminary communications 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.

Comments on previous works 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).

In any case, **it is the authors responsibility,** to ensure the veracity of the contents, checking similarity to other works, and carry out a proper citation of previous works. The committee is not responsible of this previous aspects in this publishing modality. In this sense, we strongly recommend the authors to use online text-similarity checking services 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.

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Show all published submissions (37) and accepted abstracts (5)

Submissions

List of Papers (37) Toggle list

Title	Poster	Authors	
Molecular docking approach to identify potential anticancer compounds targeting ALOX5 for the treatment of Pancreatic Cancer		Ravina Khandelwal, Anuraj Nayarisseri	Show Abstract
Structure Based docking studies for the identification of small molecule targeting mTOR for the treatment of Breast cancer		Khushboo Patidar, Anuraj Nayarisseri	Show Abstract
"Prediction Reliability Indicator": A new tool to judge the quality of predictions from QSAR models for new query compounds		Kunal Roy, Pravin Ambure, Supratik Kar	Show Abstract
Chemometric modeling of toxicity of contaminants of emerging concern to *Dugesia japonica* and its interspecies correlation with daphnia and fish: QSTR and i-QSTTR approaches		Kazi Hossain, Kunal Roy	Show Abstract
Chemometric modeling of refractive index of polymers using 2D descriptors: A QSPR approach		Pathan Mohsin Khan, Bakhtiyor Rasulev, Kunal Roy	Show Abstract
Ecotoxicological risk assessment and prioritization of pharmaceuticals using QSTR approaches		Kabir Khan, Emilio Benfenati, Kunal Roy	Show Abstract
Multimodal Perspectives of Nanotechnology and Nanoparticles in Drug Delivery		Baishakhi De, Anubhav Nagal, Rajeev K Singla	Show Abstract
Phytochemical Profiling and Antioxidant Activity of Aqueous Extract of *Aegle marmelos* Fruit Shell		Ankita Chaubey, Ashok Dubey	Show Abstract
Isolation of Novel Hyaluronidase Inhibitor from the Hard Shell of Coconut		Rajeev Singla, Mohammed Ali, Ashok Dubey	Show Abstract
Inhibition of *Staphylococcus aureus* and its biofilm by the metabolites of endophytic *Streptomyces* sp. ADR1		Radha Singh, Ashok Dubey	Show Abstract
PTML: Perturbation-Theory Machine Learning notes		Humbert Gonzalez-Diaz	Show Abstract
Interactions of complex neural networks with different proteins from six brain regions, in Alzheimer's disease.		Christhian Villanueva Medina, Scarlett Pérez olea, Sonia Arrasate Gil	Show Abstract
Drug protein interaction and its biological activity in the treatment of Alzheimer's disease		Scarlett Pérez Olea, Christhian Villanueva Medina, Sonia Arrasate Gil	Show Abstract
Prediction of Activity for Antimalarial Nanoparticle Delivery Systems		Diana Urista Márquez	Show Abstract

Title	Poster	Authors	
Clients profile evaluation attended in Barra do Garças municipality aesthetic clinics, Mato Grosso, Brazil		Thaís Alves, Bruna Rhaynaha Godoy, Ana Vitória Menezes, Lívia Maria de Almeida, Daniela Silva Delmondes, Pablo Delmondes, Jaqueline Santos Lopes	Show Abstract
PTML Knowledge-Based System for Multi-Output Prediction of Anti-Melanoma Compounds		Jose Cordero Cortes	Show Abstract
PTML Model for Alignment-free Prediction of Protein Targets of Anti-Melanoma Drugs		Mayra Valdez, Sonia Arrasate	Show Abstract
ISOLATION AND CHARACTERIZATION OF BACTERIAL CONSORTIA WITH CAPACITY TO DEGRADE HYDROCARBONS		Everardo Briseño Silva, Valentin Toro Castillo, Rafael Jimenez Mejía	Show Abstract
SUSTAINABILITY TRANSFORMATION IN TEACHING ORGANIC CHEMISTRY LABORATORY AT UNIVERSITY OF THE BASQUE COUNTRY		Iker Montes Bageneta, Sonia Arrasate Gil, Eneritz Anakabe Iturriaga, Urtzi Akesolo, Maria Merino Maestre, Sara López	Show Abstract
PREDICTIVE LIGNIN DEGRADATION STATISTICAL MODEL		Abigail Copca Granados	Show Abstract
Adolescent behavioral profile with acne vulgaris: case reports		Rosiellen Carvalho, Daniela Silva Delmondes, Shirley Prado, Pablo Delmondes	Show Abstract
Synthesis and application of Schiff based metal complexes of thiosemicarbazide in electrochemical sensors		CHANDRA MOHAN, Sulekh Chandra	Show Abstract
Studies on statistically optimized binary ethosomal gel encapsulated with Carvedilol: Ex-vivo permeation and Pharmacodynamic assessment in male Wistar albino rats		ANANDA KUMAR CHETTUPALLI, Sunil Kumar Thota	Show Abstract
Method development and validations of Apixaban in bulk and its formulations by UV-spectroscopy (area under curve)		NARENDER BOGGULA	Show Abstract
Development and validation of RP-HPLC method for the estimation of Tigecycline in bulk and its parenteral dosage form		Akiful M, Sandeep Reddy, Gowri Mulagada, Vasudha Bakshi	Show Abstract
PHYTOCHEMICAL SCREENING AND ANTHELMINTIC ACTIVITY OF ROOT EXTRACT OF *HUGONIA MYSTAX LINN* AGAINST *PHERETIMA POSTHUMA* – AN *IN VITRO* STUDY	N/A	NARENDER BOGGULA	Show Abstract
A preliminary assessment of the differences between the Malaysian and Bangladesh strains of the highly lethal Nipah virus		Proyasha Roy, Sumanta Dey, Tathagata Dutta, Ashesh Nandy, Subhas Basak	Show Abstract
H1N1 – First 100 Years: Regions of Least Variability in Neuraminidase Gene Sequence		Proyasha Roy, Tathagata Dutta, Ashesh Nandy	Show Abstract

Title	Poster	Authors	
Cissus incisa: a potential source of therapeutic agents		Deyani Nocedo-Mena, María del Rayo Camacho-Corona, Mauricio González-Ferrara	Show Abstract
The Diagnosis and Treatment of Niekmann Pick Disease (NPD)		Madhu Babu, Kiran Gangarapu, Hemanthkumar boyina, Krishnaprasad devarakonda	Show Abstract
SCREEING OF HYDRO-ALCOHOLIC EXTRACT OF FRUITS OF *LUFFA CYLINDRICA LINN.* ON ASPIRIN PLUS PYLORUS LIGATED RAT MODEL: FOR ITS ANTI-ULCER ACTIVITY	N/A	Krishna Prasd Devarakonda, PRASHANTHI GANDHAMALLA, sreelakshmi GK, VASUDHA BAKSHI	Show Abstract
LIVER CANCER IN CHILDREN		NALLAGIRI CHARANRAJ	Show Abstract
MVVM design pattern for asynchronous events in information system		Bernabe Ortega-Tenezaca, Viviana Quevedo-Tumailli, Lenin Ochoa Carrión, Ronny Rodríguez Cabrera, Luis Uvidia Armijo	Show Abstract
Development and characterization of isradipine compression coated controlled release mini-tablets		Sateesh Kumar Vemula, Rajendra Kumar Jadi, Sridhar Babu Gummadi, Raja Sridhar Rao Ponugoti	Show Abstract
PHYTOCHEMICAL AND PHARMACOLOGICAL EVALUATION OF ANTI- AMNESIC EFFECT OF *MORUS ALBA LINN* IN WISTAR RATS	N/A	Prathibha R, Manohari R, Aswini S, Sai priya R, Sandhya R, Vasudha B, HemanthKumar B	Show Abstract
The regulation of emerging technologies: is it possible to stem the tide?	N/A	Aliuska Duardo-Sanchez	Show Abstract
ISOLATION AND CHARACTERIZATION OF BACTERIAL CONSORTIA WITH CAPACITY TO DEGRADE HYDROCARBONS	N/A	Valentin Toro Castillo, Everardo Briseño Silva, Rafael Jimenez Mejía	Show Abstract

List of Accepted Abstracts (5) Toggle list

"Evaluation of *Galphimia glauca* stem methanol extract fractions for Central Nervous System Depressant and Muscle relaxant activities"

BABA SHANKAR RAO GARIGE, Srisailam Kesheti, Uma Vattikuti, Vasudha Bakshi

Submitted: 26 Oct 2018

Abstract: Show Abstract

EVALUATION OF ANTI-EPILEPTIC ACTIVITY OF LEAF EXTRACT OF *DILLENIA INDICA* LINN ON EXPERIMENTAL MODELS OF EPILEPSY IN MICE

nerella mounika

Submitted: 02 Nov 2018

Abstract: Show Abstract

Neuroprotective effect of Aripiprazole on cerebral ischemia/reperfusion in wistar rats

Vasudha Bakshi, G Hima Bindu G

Submitted: 02 Nov 2018

Abstract: Show Abstract

PSYCHOPHARMACOLOGICAL STUDIES OF the WHOLE PLANT OF *MARSILEA MINUTA*

ram mohan, BABA SHANKAR RAO, Ganapathy Seru, vasudha B

Submitted: 30 Oct 2018

Abstract: Show Abstract

Mt-QSAR, ChemBL vs MRN antibacterials entrophy.

Carlos Cornelio Reynoso

Submitted: 03 Aug 2018

Abstract: Show Abstract

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04. BIOCHEMPHYS-01: International Workshop on Med. Chem., Biotech., and Phys. Chem., CNAM, Paris, France, 2018

[CLICK HERE TO SUBMIT NEW ABSTRACT]

BIOCHEMPHYS-01: International Franco-Tunisian workshop on
Med. Chem., Biotech., and Phys. Chem., Cnam, Paris, France, 2018

***Submission Date Extended**: We are pleased to announce that the both abstract submission and article submission dates has been extended up to **December 15, 2018**, in response to numerous requests and due to the increased interest in Biochemphys 2018. You can still register at the Sciforum website to submit your abstracts and/or login to upload your communications.

Dear colleagues worldwide,

Greetings from BIOCHEMPHYS-01!

You are cordially invited to participate to the first International Franco Tunisian Workshop on Medicinal Chemistry, Biotechnology, and Physical Chemistry at Cnam, Paris, France, 2018. This scientific workshop is organized by Professors and Researchers of the Laboratory of Molecular Chemistry (CMGPCE) and the Laboratory of Systems & Applications of Information & Energy Technologies (SATIE) (at Cnam, Paris, France) with their Tunisian colleagues who participate to the UTIQUE Hubert Curien Program (PHC UTIQUE managed by Campus France and CMCU). The Tunisians partners are Professors and Researchers at the Laboratory of interfacing and advanced materials (LIMA, Monastir University), Biotechnology Center of Sfax (CBS), the Higher Institute of Biotechnology of Sfax (ISBS) and Unité de Recherche "Physique des Matériaux Isolants et Semi-isolants" (PMISI, Faculty of Sciences of Sfax).

The host institution, Conservatoire national des arts et métiers, Cnam, is a higher education and research institution dedicated to adult continuing education. It holds a unique, original position in the French educational landscape with nearly 150 educational centers in France and a large presence worldwide. Since its foundation in 1794, Cnam has closely combined academic knowledge and professional skills with a strong relationship with the industry. In a context marked by new economic and societal expectations, the Research in Cnam is very dynamic, and guaranty a high-level scientific positioning. It covers a large variety of domains varying from chemistry, biology, bio-informatic to physics, mathematics and material science.

This workshop series is planned to be held each academic term an. It is devoted to fostering both education and research in multidisciplinary sciences with emphasis in Molecular Sciences (Organic and Medicinal Chemistry), Physical-chemistry, Biochemistry, Nanotechnology, Materials Sciences, Cheminformatics, Physics, …. Researchers and students from other institutions around the world are welcomed. All accepted papers receive a DOI number and are published online before being published at the end of year on the conference proceedings book with ISSN and ISBN numbers.

Both participation and publication are totally free of cost!!! No charges will be paid neither by the authors, nor by their institutions.

The BIOCHEMPHYS-01 is in large measure targeted for graduate and PhD students, chemists and bioinformaticians researchers and scientists involved in areas related to Medicinal Chemistry, Cheminformatics and /or Bioinformatics, Biophysics, Physics, Protein Engineering, Biosensors and Chemical Sensors, Biomarker detection, Modelling and Simulation. Research work related with the use of new materials for photocatalytic applications and energy storage are also welcome.

Steps for Participation to BIOCHEMPHYS workshop

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(6) Log in to post comments, questions, or answers in a section or one of the workshops

(7) Contact chairpersons if you need author (publication) or attendance (posting) certificate for conference and/or workshops (all year)

Publications are expected to be short papers consisting of 2-3 pages summarizing the results of the research project, PhD thesis, MSc work, or Degree dissertation, etc. The deadline for the abstract submission is November 15, 2018 (extended up to **December 15, 2018**). The comments on previous works as short notes to comment about the more interesting points, highlights, etc. of works previously published by the authors or other groups are also accepted. In this case, committee and/or external reviewers also only check the scope and apparent scientific soundness.

Review and Publication

This type of communications 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 as for an online Preprint service. Therefore, all works receive DOI numbers and are indexed in GoogleScholar. The works may also receive comments from registered participants (public post-publication review). The authors are encouraged to submit their works to peer-reviewed scientific journals of MDPI or other editorials during or after finalization of the conference, as per SciForum copyright rules. After publication of papers is closed, we shall open the online platform, and the authors (professors, researchers, and students) will be able to post online comments, questions, 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.)

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(2) IKERBASQUE, Basque Foundation for Science, 48011, Bilbao, Biscay, Spain.

Dr. Aliuska DUARDO-SANCHEZ (Law.Lic., Ph.D. TICs & Legal Sciences) Post-Doctoral Research Associate, Program Juan de La Cierva (JdC), Chair in Law and The Human Genome, Department of Public Law, Faculty of Law, University of Basque Country (UPV/EHU), Biscay, Leioa 48940, Spain.

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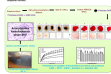
Hide published submissions (32) and accepted abstracts (10)

Submissions

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Title	Poster	Authors	
Polyanionic Molybdate Powders as Promising Electrode Materials Based on NASICON $Fe_2 (MoO_4)_3$ Networks		Thamer ALOUI, Najla FOURATI, Hajer GUERMAZI, Samir GUERMAZI, Chouki ZERROUKI	Show Abstract
Sb_2S_3 thin films: effect of PEI polymer substrate on physical properties		Sameh ben ameur, hajer Guermazi	Show Abstract
Dual-modality probe for MRI and photoacoustic imaging: synthesis, and relaxometric characterization		Marie Devreux, Fabienne Dioury, Céline Henoumont, Clotilde Ferroud, Sophie Laurent	Show Abstract
Transient currents and conduction mechanisms in unfilled and ZnO filled epoxy matrix		Salwa Moussa, Fatma Namouchi, Hajer GUERMAZI	Show Abstract
Modelling and simulation of SAW delay line sensors with COMSOL Multiphysics		Bilel Achour, Nadia Aloui, Najla Fourati, Chouki Zerrouki, Nourdin Yaakoubi	Show Abstract

Title	Poster	Authors	
Prime importance of the supporting electrolyte in the realization of molecularly imprinted polymers		Meriem Mokni, Zouhour Mazouz, Ghada Attia, Najla Fourati, Chouki Zerrouki, Ali Othmane, Asma Omezzine, Ali Bouslama	Show Abstract
Electrical study of new anthracene derivatives for electronics applications		Ghada Attia, Safa Teka, Mustapha Majdoub, Rafik Ben Chaabanne	Show Abstract
Electrocatalytic Oxidation of Flumequine by Electrogenerated PPy-Ag Modified Electrode: Electrochemical and sensing properties.		Houssem E. E. Sakhraoui, Naima Maouche, Nadia Ktari, Rafik Kalfat	Show Abstract
The biodeterioration and blackening of vinyl glues: A new microbial cause and triaryl butene derivatives as new biocide	N/A	Karim Jalleli, Fatma Abdmouleh, Mousser Hedrich, Fatma Trigui, Manel Ben Ali, Pascal Pigeon, Siden Top, Mamdouh Ben Ali, Maher Bougacha, Gérard Jaouen, Mehdi EL ARBI	Show Abstract
Comparison of total phenols content and *DPPH* radical-scavenging activity of four *Psidium* species.	N/A	Dailenys Marrero Morfa, Liliana Vicet Muro, Dany Siverio Mota, Julio García Lahera, Onel García Espinosa, Maria Jorge Rodriguez, Susana Castro Torres	Show Abstract
Development of an electrochemical biosensor for Δ9-tetrahydrocannabinol detection based on gold surfaces functionalized with self-assembled monolayers	N/A	tlili amal, Mina souiri, Wahiba Douki, Ali Othmane, Hechem saadaoui	Show Abstract
From *In Vitro* to *In Cellulo*: Evaluation of Anti-TNFα Activity of a New Series of Small Molecules		Aïda MASCRET, Hadley MOUHSINE, Damien CABRERA, Christophe RICCO, Maité SYLLA-IYARRETA VEITIA, Marc PORT, Jean-François ZAGURY	Show Abstract
Study of acute toxicity of an aqueous abstract obtained from the flowers of *Kigelia africana* in Balb/c mice	N/A	Liset Alvaré Morfa, Jorge Pérez Donato, Enoel Hernández Barreto, Sergio Sifontes Rodríguez	Show Abstract
Chemometric Characterization of Chemlali Extra-Virgin Olive Oil Adulteration Mixed with Soybean Oil, Corn Oil and Sunflower Oil	N/A	malika drira, hazem jabeur, Mohamed BOUAZIZ	Show Abstract
Qualitative phenolic profile of Rumex tunetanus flowers and stems using ultra-high-performance liquid chromatography coupled to quadrupole-time-of-flight mass spectrometry and their antioxidant activity	N/A	Jouda Abidi, Sonda Ammmar, Mohamed BOUAZIZ	Show Abstract

Title	Poster	Authors	
Evaluation of bacteria of aquatic origin as fish probiotic in vitro		MOUNA jlidi, Asmahen Akremi, Adel HAJ BRAHIM, Houda HMANI, Lobna DAOUD, Manel BEN ALI, Nabil SOUISSI, Samir BEJAR, Mamdouh BEN ALI	Show Abstract
Imbalance Glutathione Biosynthesis in ASD: A kinetic patterns "in vivo"	N/A	Carmen Jiménez-Espinoza, Francisco Marcano Serrano, José González- Mora	Show Abstract
Utilisation of click chemistry in medicinal chemistry. Applications to the synthesis of new bioactive triarylmethanes.	N/A	Ameni Hadj Mohamed, Mehdi El Arbi, Moncef Msaddek, Maité Sylla-Iyarreta Veitia	Show Abstract
Characterization of a novel protease from *Anoxybacillus kamchatkensis*strain M1V with biotechnological interest		Sondes MECHRI, Khelifa Bouacem, Nadia Zaraî Jaouadi, Hatem Rekik, Mouna Ben Elhoul, Maroua Omrane Benmrad, Hocine Hacene, Samir Bejar, Amel Bouanane-Darenfed, Bassem Jaouadi	Show Abstract
A novel detergent-stable protease from *Penicillium chrysogenium* X5 and its utility in textile fibres processing	N/A	Maroua OMRANE, Emna MOUJEHED, Mouna Ben Elhoul, Sondes Mechri, Samir Bejar, Riadh Zouari, Ayda Baffoun, Bassem Jaouadi	Show Abstract
Production, partial purification, characterization, and application as laundry detergent additive of an alkalophilic protease from *Bacillus velezensis* strain F35		Wacim BEJAR, Hatem REKIK, Sondes Mechri, Nadia JAOUADI, Samir BEJAR, Najah JMAL, Bassem JAOUADI	Show Abstract
***Salicola* sp. strain SBJ9: a novel extremely halophilic bacterium with an interesting protease activity**		Lobna DAOUD, Adel HADJ BRAHIM, Houda HMANI, Asmahen AKREMI, Mouna JLIDI, Manel BEN ALI, Samir BEJAR, Naser ALIYE FETO, Mamdouh BEN ALI	Show Abstract
Purification and biochemical characterization of a novel detergent-stable serine alkaline protease from *Bacillus safensis* strain RH12	N/A	Hatem Rekik, Nadia Zaraî Jaouadi, Fares Gargouri, Wacim Bejar, Fakher Frikha, Najah Jmal, Samir Bejar, Bassem Jaouadi	Show Abstract
First draft genome sequencing of the *Salicola* genus	N/A	Lobna DAOUD, Adel HADJ BRAHIM, Houda HMANI, Mouna JLIDI, Manel BEN ALI, Samir BEJAR, Naser ALIYE FETO, Mamdouh BEN ALI	Show Abstract

Title	Poster	Authors	
Bacillus sp.BCLRB2: An efficient diazotrophic Halotolerant PGPB strain		Adel HADJ BRAHIM, Daoued Lobna, Jlidi Mouna, Akremi Asmahen, Hmani Houda, Ben Ali Manel, Naser FETO, Samir BEJR, Mamdouh BEN ALI	Show Abstract
Halotolerant PGPB Seed biopriming Induces wheat salinity tolerance		Adel HADJ BRAHIM, Jlidi Mouna, Hmani Houda, Daoued Lobna, Ben Ali Manel, Akremi Asmahen, Naser FETO, Samir BEJR, Mamdouh BEN ALI	Show Abstract
Antimicrobial and anticancer activities of bisacodyl and it's deacetylated metabolite DDPM		Abdmlouleh Fatma, Ricco Christophe, El Arbi Mehdi, Sylla-Iyarreta Veitía Maité, Ben Ali Mamdouh, Ferroud Clotilde	Show Abstract
Identification of new analgesic candidates through virtual *in silico* screening and *in vivo* experimental test.		Arelys López-Sacerio, Yudith Cañizarez-Carmenate, Juan Castillo-Garit	Show Abstract
Structure-antimicrobial activity relationship of a series of functionalized arylbenzothiazoles		Abdmlouleh Fatma, Mehdi El Arbi, Maité Sylla-Iyarreta Veitía, Mamdouh Ben Ali, Clotilde Ferroud	Show Abstract
Synthesis of some new diarylmethanes by McMurry coupling reaction: characterization and antibacterial activity	N/A	Ameni Hadj Mohamed, Meral Görmen, Mehdi El Arbi, Moncef Msaddek, Maité Sylla-Iyarreta Veitia	Show Abstract
ANTIVIRAL ACTIVITY OF THE ESSENTIAL OIL OF CONYZA CANADENSIS	N/A	Manel Ben Ali, Lobna DAOUD, Adel HAJ BRAHIM, Houda HMANI, Mouna jlidi, Samir BEJAR, Mamdouh BEN ALI	Show Abstract
Assessment of antioxidant and antibacterial properties of some Tunisian plants	N/A	Manel Ben Ali, Houda HMANI, Lobna DAOUD, Mouna jlidi, Adel HAJ BRAHIM, Samir BEJAR, Mamdouh BEN ALI	Show Abstract

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Natural and Economic biodegradation of feather using a new keratinase from *Actinomadura viridilutea* strain DZ50

Mouna Ben Elhoul, Nadia Zaraî Jaouadi, Hatem Rekik, Maroua Omrane Benmrad, Sondes MECHRI, Samir Bejar, Bassem Jaouadi

Submitted: 01 Dec 2018

Abstract: Show Abstract

A highly convenient synthesis process for the recovery of powerful antioxidants hydroxytyrosol via catalytic oxidation method

NOURZED FRIKHA, Soumaya Bouguerra, Mohamed BOUAZIZ

Submitted: 23 Nov 2018

Abstract: Show Abstract

CANCER SIGNAL INHIBITION THROUGH HSP PERTURBATION IN BREAST CANCER CELL LINE-MCF-7

Yusuf Tutar

Submitted: 11 Dec 2018

Abstract: Show Abstract

Characterization and overexpression of a glucanase from a newly isolated *B. subtilis* strain

Houda HMANI, Lobna DAOUD, Manel BEN ALI, Adel HAJ BRAHIM, Mouna JLIDI, Samir BEJAR, Mamdouh BEN ALI

Submitted: 01 Dec 2018

Abstract: Show Abstract

Conversion process for tyrosol to hydroxytyrosol via montmorillonite KSF as catalyst

Soumaya Bouguerra, Mohamed Bouaziz

Submitted: 28 Nov 2018

Abstract: Show Abstract

Expression of a Thermo-stable Xylanase from the Thermophilic anaerobic bacterium *Caldicoprobacter algeriensis* sp. TH7C1[T]

sonia mhiri, Amel Bouanane, Sawssan Neifar, Monia Mezghani, Rihab Ameri, Sahar Trabelsi, Samir Bejar

Submitted: 29 Nov 2018

Abstract: Show Abstract

Investigation of *GSTM1* and *GSTT1* gene polymorphisms on mitochondrial disease in a Tunisian population.

Raouia Ghorbel, Ghada Ben Salah, Rania Ghorbel, Imen Chamkha, Leila Ammar-Keskes, Faiza Fakhfakh

Submitted: 01 Dec 2018

Abstract: Show Abstract

Isolation of *Erwinia amylovora* Bacteriophage from Soil and Pear Trees Plant Tissues

Asmahen Akremi, Mouna Jlidi, Adel Haj Brahim, Manel Ben Ali, Lobna Daoud, Houda Hmani, Samir Bejar, Naser Aliye Feto, Mamdouh Ben Ali

Submitted: 29 Nov 2018

Abstract: Show Abstract

Optimisation of Monoglyceride production with esterification of glycerol by oleic acid via KSF as catalyst

Asma Chaari, Soumaya Bouguerra, Mohamed Frikha

Submitted: 02 Dec 2018

Abstract: Show Abstract

Synthesis of tyrosol derivatives through 2-phenylethanol conversion by catalytic process

Rania Ben hamida, NOURZED FRIKHA, Soumaya Bouguerra, Mohamed BOUAZIZ

Submitted: 23 Nov 2018

Abstract: Show Abstract

05. WCUCW-02: West Coast University Capstone Workshop, WCU, Miami, USA, 2018

WCUCW-02

NOTES: We suggest you to **download and use** the [Template File] to write your communication. We also strongly recommend you to **read carefully** the[Instructions to authors] about publication model, copyright, authors responsibilities, *etc*.

[CLICK HERE TO SUBMIT NEW ABSTRACT]

Dear colleagues worldwide, we invite you to join us at WCUCW-02 West Coast University Capstone Workshop, 2018, Miami, FL, USA. This is the Capstone workshop for West Coast University (WCU), Miami, FL, USA. This workshop series held each academic term is devoted to fostering both education and research in multidisciplinary sciences. Professors, researchers, post-docs, Ph.D., M.Sc. and degree students worldwide are invited to submit their contributions to be published online in Sciforum platform, Basel, Switzerland, **open access and totally free of cos**t. We specially welcome students completing their General Education courses at WCU. These capstone courses students form groups of three and take on the roles of scientist, medical researcher, or public health professional, all of them approaching an assigned topic from their field of expertise. They are each required to devise a study on their topic, pretend to conduct it, generate logical data to support a hypothesis, write an academic paper sharing their findings, and defend their data in a presentation. The workshop education goals focus on professors and students in the WCU Miami campus Capstone course. However, we also welcome researchers and students from other nationwide WCU campuses and researchers from other institutions around the world. The Capstone workshop is associated with MOL2NET-04 International Conference on Multidisciplinary Sciences, MDPI Sciforum, Switzerland, HQ UPV/EHU, Bilbao, Spain. It will therefore **run both online and in person.** The workshop runs online at the platform SciForum maintained by the editorial MDPI, Basel, Switzerland. It runs in person at WCU, Miami campus, during the Capstone course. The **topics of interest** include, but are not limited to, the following: Multidisciplinary Science (all areas), Health Science (all areas), Chemistry (all areas), Biology and Life Sciences (all areas), Environmental Science (all areas), Social Sciences (all areas), Biomedical Engineering, Mathematics (Applied), Data Analysis, Education. See the following note to authors on **topics outside the scope** of the conference and associated workshops [Note on topics].

Steps for Participation
(0) Register, Sign in/Login, to Sciforum platform (all year)
(1) Submit the title and abstract, select a section or workshop (do not upload paper here)
(2) Wait for Sciforum abstract acceptance email, follow the link, and/or login to upload paper(doc and pdf format)
(3) Download template doc and prepare your communication [Template File]
(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 year)

(6) Log in to post comments, questions, or answers in a section or one of the workshops
(7) Contact chairpersons if you need author (publication) or attendance (posting) certificate for conference and/or workshops (all year)
Notes to Participants
To see a detailed schedule of this workshop/section and of the entire conference follow this link: [MOL2NET workshops schedule]
Preliminary communications 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 as for an online Preprint service. Therefore, all works receive DOI numbers and indexed in GoogleScholar. The works may also receive comments from registered participants (public post-publication review). The authors are encouraged to submit their works to peer-reviewed scientific journals of MDPI or other editorials during or after finalization of the conference, as per SciForum copyright rules.
Comments on previous works 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 also only check the scope and apparent scientific soundness. The works may also receive comments from registered participants (public post-publication review). After publication of papers is closed, we shall open the online platform, and the authors (professors, researchers, and students) will be able to post online comments, questions, 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.)
We strongly recommend that you carefully read the following **notes to participants** about publication model, copyright, authors' responsibilities, *etc*. Be aware,**it is the author's responsibility** to ensure the veracity of the contents(checking similarity to other works) and to carry out a proper citation of

previous works. The committee is not responsible of these aspects in this publishing modality. We therefore strongly recommend the authors to use online text-similarity checking services 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 Journal Special Issue

In parallel, members of committees and/or authors of different workshops are encouraged to edit special issues for different journals of the editorial MDPI (http://www.mdpi.com/). This year WCUCW-02 shall be associate to the one special issue. The authors of papers submitted to the workshop are encouraged to complete their works in full version papers and submit to the journal as well. Please, check details about topic of the issue. Take also into consideration that publication in the workshop is free of charge but article processing charges may be levied to authors of the journal. 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. The details of the issue are:

Applied Sciences (Call for Papers): Special issue entitled: Complex Networks and Machine Learning: From Molecular to Social Sciences. Journal Applied Sciences (ISSN 2076-3417), **JCR IF = 1.679**. Topics: machine learning, complex networks, systems biology, protein networks, metabolic networks, ecosystems, artificial neural networks, social, financial, and legal networks.

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Professor Melissa Cueto, MAInstructor II, West Coast University, Miami, FL, USA, Adjunct Prof., University of Miami, Coral Gables, FL, USA.
Prof. Dr. Maykel Cruz-Monteagudo, West Coast University, Miami Campus, FL, USA.

Show all published submissions (12) and accepted abstracts (3)

Submissions

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Title	Poster	Authors

Title	Poster	Authors	
National Strategy to CombatWildland Fires: A Public Policy		Daphne Gaston, Kathryn Ayres	Show Abstract
Global Warming and Climate Change		Elba Soza, Kathryn Ayres	Show Abstract
The Business of Disaster		Daniel Fouladi, Kathryn Ayres	Show Abstract
A Case Study of the Dietitian's Role in Rehabilitation of Stroke Patients through Medical Nutrition Therapy		Delia Alviarez, Kathryn Ayres	Show Abstract
Idealized correlations: prediction of solubility of fullerene in organic solvents	N/A	Alla Toropova, Andrey Toropov, Emilio Benfenati	Show Abstract
Web Application for Real Time Data Visualization of Heat Sensor	N/A	Bernabe Ortega-Tenezaca, Viviana Quevedo-Tumailli, Víctor Cerda Mejía, Octavio Guijarro Rubí, Estela Guardado Yordi, Amaury Pérez Martínez	Show Abstract
Isolation of *Erwinia amylovora* Bacteriophage from Soil and Pear Trees Plant Tissues	N/A	Asmahen Akremi, Mouna Jlidi, Adel Haj Brahim, Manel Ben Ali, Lobna Daoud, Houda Hmani, Samir Bejar, Naser Aliye Feto, Mamdouh Ben Ali	Show Abstract
Use of integrated software, applied to the elaboration of didactic material for students with hearing disability at the basic intercultural education center of deaf	N/A	Viviana Quevedo, Bernabé Ortega-Tenezaca	Show Abstract
Incidence of the use of didactic material for students with hearing disability at the basic intercultural education center of deaf		Viviana Quevedo, Bernabé Ortega-Tenezaca	Show Abstract
Antibacterial activities of triterpenes from leaves of *Cissus incisa*		Deyani Nocedo-Mena, Elvira Garza, Mauricio González-Ferrara, María del Rayo Camacho-Corona	Show Abstract
***Cryptosporidium spp.* prevalence in sheep from commercial sites in the State of Mexico, Mexico during Summer.**	N/A	María Uxúa Alonso-Fresán, Maria de Lourdes Ordoñez-Sánchez, Alberto Barbabosa-Pliego, Benjamín Valladares-Carranza, Valente Velázquez-Ordoñez	Show Abstract
Machine learning techniques and the identification of new potentially active compounds against *Leishmania infantum*.	N/A	Naivi Flores Balmaseda, Susana Rojas Socarrás, Juan Alberto Castillo Garit	Show Abstract

List of Accepted Abstracts (3) Toggle list

A Nanoquimioinformatic model to predict anticancer activity in glioblastoma tumor

María Blanco, Sonia Arrasate

Submitted: 28 Aug 2018

Abstract: Show Abstract

The Benefits of Physical Therapy for Stroke Patients

Mario Gutierrez, Kathryn Ayres

Submitted: 29 Oct 2018

Abstract: Show Abstract

The Role of Special Victim Units in Health Care and Justice

Gabriel Fontela, Kathryn Ayres

Submitted: 29 Oct 2018

Abstract: Show Abstract

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06. WRSAMC-03: Workshop in Medicinal Chemistry, UFPB, Paraiba, Brasil, 2018

WRSAMC2018, 3rd Edition

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Welcome Message from Chairs

Dear all we are glad to welcome you to a new edition of the series of Workshops on Research in Sciences Applied to Medicinal Chemistry (WRSAMC) 2018. This workshop series is organized by researches from Department of Chemistry, Programa de Pós-Graduação em Produtos Naturais e Sintéticos Bioativos (PgPNSB - Postgraduate Program in Natural Products and Synthetic Bioactive) and Hospital Universitário of Universidade Federal da Paraíba (UFPB). This year, as well as last year, WRSAMC *is dedicate to the* PgPNSB 40th Anniversary. More specifically, this year WRSAMC hosts the first symposium in Paraiba for chemical studies of natural products.

1st Paraiban Symposium on Chemicals for Natural Products (I SIMPEQPN)

The 1st Paraiban Symposium on Chemicals for Natural Products (I SIMPEQPN) will take place from 9 to 11 October 2018 in the Auditorium of the Rectory of the Federal University of Paraíba, in João Pessoa. To celebrate the 40th anniversary of PPgPNSB, the scientific committees and organizers of I SIMPEQPN are developing a versatile scientific program around the current and exciting topic: Chemicals for Natural Products. The symposium will have as main theme the chemical studies of natural products, among them: spectroscopic techniques, chromatographic, synthesis, quality control, among others. Guests from the institution and outside will present / discuss aspects related to natural history, cultivation, breeding, quality control, ethnobotany, ethnopharmacology, phytochemistry, pharmacology, among other research areas, conferences and lectures that will take place during the three days of the event. There will also be poster sessions as well as oral presentations. Participants will receive certificates and abstracts of papers will be published in online proceedings. -150 participants; -Presentations in posters and oral; -Speeches; -Conferences. Please, check official SIMPEQPN event page in Facebook as well.

I Simpósio Paraibano de Estudos Químicos de Produtos Naturais (I SIMPEQPN)

O I Simpósio Paraibano de Estudos Químicos de Produtos Naturais (I SIMPEQPN) acontecerá de 9 a 11 de outubro de 2018 no auditório da Reitoria da Universidade Federal da Paraíba, em João Pessoa. Para celebrar o 40º aniversário da PPgPNSB, os comitês científicos e organizadores do I SIMPEQPN estão desenvolvendo um programa científico versátil em torno do atual e excitante tema: Estudos Químicos de Produtos Naturais. O simpósio terá como tema principal os estudos químicos de produtos naturais, entre eles: técnicas espectroscópicas, cromatográficas, síntese, controle de qualidade, entre outros. Convidados da instituição e externos apresentarão/debaterão aspectos relacionados à história natural, cultivo, melhoramento, controle de qualidade, etnobotânica, etnofarmacologia, fitoquímica, farmacologia, entre outras áreas de investigação, em conferências e palestras que ocorrerão ao longo dos três dias de evento. Haverá também apresentação sessões de pôsteres, além das apresentações orais. Os participantes receberão certificados e os resumos dos trabalhos serão publicados em anais online. -150 participantes; -Apresentações em pôsteres e oral; -Palestras; -Conferências.

I SIMPEQPN Coordenação Geral
Prof. Marcus Tullius Scotti (Coordenador Docente), Departamento de Química, Centro de Ciências Exatas e da Natureza, Universidade Federal da Paraíba - Campus I, Cidade Universitária, CEP: 58.051-900 João Pessoa - Paraíba - Brasil, Emails: mtscotti@gmail.com, mscotti@ccae.ufpb.br ,

Prof. Vicente Carlos de Oliveira Costa (Vice-coordenador Docente), Instituto de Pesquisa em Farmacos e Medicamentos, Universidade Federal da Paraíba - Campus I, Cidade Universitária, CEP: 58.051-900, João Pessoa - Paraíba – Brasil.

Msc. Ana Rita Rodrigues de Almeida Silva (Coordenadora Discente)

Msc. Laisla Rangel Peixoto (Vice-coordenadora Discente)
WRSAMC - SIMPEQPN - Mol2Net Association

Both WRSAMC workshop series and SIMPEQPN simposium are associated to MOL2NET-04 International Conference on Multidisciplinary Sciences, **ISSN**: 2624-5078, **ISBN**: 978-3-03842-820-6, MDPI SciForum, Basel, Switzerland, 2018. Consequently, the present page of the conference will serve as both: (1) publication media for communications, posters, or plenary conferences (videos) and also (2) online discussion media to post comments, questions, and answers about the workshops, respectively. Participants on both events, **online discussions** at the end of the year and workshop along the year, are entitled to receive attendance certificates from both the WRSAMC workshop and the MOL2NET conference. The WRSAMC will be held in person however, the workshop will remain **open all the year for submission and publication of communications** online via the platform SciForum.

Notes to Participants

Submission process has the following steps: 1-Registration, 2-Submission of abstract, 3-Wait for abstract acceptation email, 4-Upoload of full communication, 5-Wait for communication approval/publication emails. After you successfully register, you can submit your paper online. Communications are expected to be short papers 1-3 pages. Please, donwload and use the following template WRSAMC template to submit your communication.

Be aware:

on step 1, you should select MOL2NET 2017, International Conference on Multidisciplinary Sciences, 3rd edition (Conference).

on step 2, you should select WSRAMC2017 workshop in research sciences applied in medicinal chemistry.

Before to submit your work be aware that the editorial publication model of this workshop is similar to a PREPRINT service. It means that works presented here have to be considered only as preliminary communications and not as final post-print versions of journal papers. In this sense, even when all the works published are revised by at least one member of the committee and/or external reviewer this level of revision checks only apparent scientific soundness and general scientific interest.

In a second level, collective post-publication review, the works published may receive comments (published in the form of posts) from all the participants registered in the conference. The authors are prompted to use all these opinions to write the full versions of their works and submit them to publication in a peer-reviewed scientific journals according to SciForum copyright rules. Some workshops will use specialized services to checked for possible similarity. In any case, **the authors are the only one responsible for** the veracity of the contents, checking similarity to other works, and proper citing or under-citing of previous works, etc.

WRSAMC Workshop Series Chairs

Prof. Marcus Tullius Scotti, Departamento de Química, Centro de Ciências Exatas e da Natureza, Universidade Federal da Paraíba - Campus I, Cidade Universitária, CEP: 58.051-900 João Pessoa - Paraíba - Brasil, Emails: mtscotti@gmail.com, mscotti@ccae.ufpb.br

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Session Chairs:
Prof. Dr. Luciana Scotti, Hospital Universitário, Universidade Federal da Paraíba - Campus I, Cidade Universitária, João Pessoa - Paraíba - Brasil
Prof. Dr. Marcus T. Scotti, Departamento de Química, Centro de Ciências Exatas e da Natureza, Universidade Federal da Paraíba - Campus I, Cidade Universitária, João Pessoa - Paraíba - Brasil

Hide published submissions (48) and accepted abstracts (3)

Submissions

List of Papers (48) Toggle list

Title	Poster	Authors	
TERPENES: NATURAL COMPOUNDS WITH POTENTIAL USES IN LUNG CANCER CHEMOTHERAPY		Rafaela Silva, Luciana Felinto, Maria Ferreira	Show Abstract
Phytochemical characterization of the Protein Fraction Dioscorine, obtained from Tubers of *Dioscorea cayennensis*		Aleson de Sousa, Francielly de Araújo, Giulian da Silva Sá, Nathália Galvão Silva, Kamila Bezerra, Carlos Gadelha	Show Abstract
An alternative for healing through the use of lectins: an overview		Lucas Coêlho Bernardo, Nathalia Regina Galvão Silva	Show Abstract
IN SILICO STUDIES TO EVALUATE INTERACTIONS BETWEEN KAURANE-TYPE DITERPENES AND THE DIHYDROFOLATE REDUCTASE – THYMILIDINE SYNTHASE OF THREE *LEISHMANIA* SPECIES.		Chonny Herrera-Acevedo, Daissy Monroy-Velandia, Areli Flores-Gaspar, Ericsson Coy-Barrera	Show Abstract
Contribution to the phytochemical study of *Ocotea gardneri* (MEISN) MEZ (Lauraceae).		Glayanne Gomes de Melo, Laisla Peixoto, Maria Madalena Silva Teles, Natanael Ramos de Lima, Gabriela de Sousa, Fiama Figueiredo, José Maria Filho	Show Abstract
Chemical constituents isolated from *Mandevilla dardonoi* (Apocynaceae)		Francisca Lins, Josean Tavares, Marcelo da Silva, José de Melo, George Santos, Joanda Silva, Laiane Pereira, Lucas Abreu	Show Abstract
Preparation of Hemissíntéticos molecular hybrids of the Diterpeno ent-7-Acetotraquiloban-18-OIC acid and its hydroxyl derivative		THAIS ALMEIDA SANTOS MARCELO SOBRAL DA SILVA	Show Abstract

Title	Poster	Authors	
Phytochemical research of _Cordia rufescens_ A.DC		Nikole Durand Trigueiro, Ana Rita Silva, Jociano Lins, Carlos Arthur Veloso, Emille Wannick Silva, Pedro Figueiredo, Diego Igor Araújo, Vicente Carlos Costa	Show Abstract
Chemometrics and Molecular Modeling applied to coumarin derivatives as potential multitarget inhibitors in _Mycobacterium tuberculosis_		Jéssika de Oliveira Viana, Mayara Santos Maia, Gabriela Cristina Soares Rodrigues, Marcus Tullius Scotti, Luciana Scotti	Show Abstract
CHEMISTRY OF ARBORININE AND PHARMACOLOGICAL ACTIVITIES		Ernestine epse Zondegoumba, Whistler Tankoua, Rodrigo Santos, Olivier Ndogo, Barthélémy Nyassé, Francisco Mendonça Junior, Luciana Scotti, Maria de Lima, Marcus Scotti	Show Abstract
Antimalarial acridine N-acylidrazonic derivatives: ADME in silico studies and molecular		Ana Ligia da Pereira, Ricardo Moura, Francisco Mendonça Júnior, Luciana Scotti, Marcus Scotti	Show Abstract
Chemical characterization and antimicrobial activity of the essential oil from _Leptohyptis macrostachys_ (Benth.)Harley & J.F.B. Pastore		Emille Wannick Reinaldo da Silva, Andreza Barbosa Silva Cavalvanti, Ana Rita Rodrigues de Almeida Silva, Pedro Thiago Ramalho Figueiredo, Laísa Vilar Cordeiro, Carlos Arthur Gouveia Veloso, Edeltrudes de Oliveira Lima, Vicente Carlos de Oliveira Costa	Show Abstract
Efeito adjuvante de Zingiber Officinale L. em pacientes com câncer		Andressa Viegas	Show Abstract
Phytochemistry and anticancer potential of graviola (Annona muricata)		Andressa Viegas, Thyago dos Santos, Liliane Costa	Show Abstract
Virtual Screening of 1,2-Diazoles Compounds for Chagas Disease: A Prediction Model		NATÁLIA DE SOUSA, RENATA PRISCILA BARROS, JOSÉ ALIXANDRE LUÍS, LUCIANA SCOTTI, MARCUS TULLIUS SCOTTI	Show Abstract
Effect of Canabidiol in the Treatment of Epilepsy		Wandemberg Neto, Gabriela Lourenço, Carla Costa, Raiza Góis, Stella Moreira, Sávio Araújo, Claudia Silva, Vanessa Dantas	Show Abstract

Title	Poster	Authors	
PHYTOCHEMICAL CHARACTERIZATION, EVALUATION OF PROTEIN CONTENT AND BIOPROSPECTION OF LECTINS AND TRYSTIN INHIBITORS IN EXTRACT OF *Sesbania virgata* **(Cav.) Poir SEEDS**		Giulian César Sá, Nathália Regina Silva, Kamila Bezerra, Francielly de Araújo, Aleson de Sousa, Carlos Alberto Gadelha	Show Abstract
The application of Delta-9-tetrahydrocannabinol (THC) against cannabis use disorder.		Gabriela Lourenço, Carla Liandra da Costa, Rony Costa, Stella Alice Moreira, Sávio Lucas de Araújo, Claudia Silva, Wandemberg Neto, Raiza de Góis	Show Abstract
PHENOLIC COMPOUNDS AND ANTIOXIDANT ACTIVITY *Pavonia glazioviana***GÜRKE**		Camila Silva, Maysa Dayane Félix, Ana Karoline Aquino, Micaelly Oliveira, Yanna Carolina Teles, Maria de Fatima Souza	Show Abstract
MORINGA OLEIFERA: **A NEW PERSPECTIVE FOR THE SYNTHESIS OF NATURAL PRODUCTS**		Kamila Bezerra, Nathália Galvão Silva, Aleson de Sousa, Giulian Sá, Francielly de Araújo	Show Abstract
Application of Self-Organizing Maps generated from Molecular Descriptors of diterpenoids in Chemotaxonomy Studies of Lamiaceae Family		Andreza Cavalcanti, Marcelo Silva, Vicente Costa, Renata Barros, Luciana Scotti, Josean Tavares, Marcus Scotti	Show Abstract
Efeito adjuvante de *Zingiber Officinale* **L. em pacientes com câncer**		Andressa Viegas	Show Abstract
Contribution to the knowledge of the species *Hancornia speciosa* **Gomes: A bibliographical review**		RAMON DE LIMA, LEÔNIA BATISTA, JOSEAN TAVARES	Show Abstract
Antimicrobial evaluation of sutures containing *Lippia sidoides* **Cham essential oil.**		Lília Linden, Isabela Farias, Alessandra Estevam dos Santos, Karoline Da Silveira, Fábio Sampaio	Show Abstract
Phytochemical investigation and tocolytic activity of the methanolic extract of *Evolvulus linarioides* **Meisn. (Convolvulaceae)**		Laiane Pereira, Rayane Pessoa, Gleice da Silva, Indyra Figueiredo, Josean Tavares, Vicente Costa, Fabiana Cavalcante, Marcelo da Silva	Show Abstract
In silico analysis of cytotoxicity, rate of absorption and molecular docking of natural products against protease, integrase and HIV-1 reverse transcriptase		Alex Monteiro, Isadora Luna, Marcus Scotti, Luciana Scotti	Show Abstract

Title	Poster	Authors	
CARQUEJA: CHEMICAL COMPOSITION AND FRAMACOLOGICAL EFFECTS		Laiane Gonçalves, Brenda Tavares, Fernanda Galdino, José de Andrade, Letícia Abrantes, Maria Rita de Sousa, Paula Gabriela Lira, Lázaro Robson Pereira	Show Abstract
Synthesis of Lophirone C using coconut peroxidase		Tamyrys Bento, Luis Rodrigues, Luiz Silva, José Barbosa-filho, Flávio Borges, Bruno Oliveira, Maria Eduarda Maia, Gabrielly Duarte	Show Abstract
The use of the Ginkgo Biloba plant and its interaction with other drugs		Raiza Góis, Wandemberg Neto, Cláudia Silva, Lucas Amaral, Vanessa Dantas, Daniela Barros, Lúcio Castellano, Paulo Bonan	Show Abstract
Anxiolytic effects of oral administration of L-Theanine: a revision		Stella Moreira, Wandemberg Neto, Gabriela Lourenço, Carla Costa, Sávio Araújo, Daniela Barros	Show Abstract
A review on the hypoglycemic effect of the leaf tea of A*verrhoa carambola*		João Cavalcanti, Iago Duarte, João Ventura, Maria Almeida	Show Abstract
Use of *Hypericum perforatum* (HP) for the treatment of psychiatric disorders: moderate to severe unipolar depression		Claudia Kowalesky, Daniela Barros, Vanessa Dantas, Lucas Amaral, Raiza Góis, Gabriela Palitot, Paulo Bonan, Lúcio Castellano	Show Abstract
The Anti-Inflammatory Effects of the Zingiber officinale Roscoe		Lucas Amaral, Raiza Góis, Cláudia Kowalesky, Natália Pazos, Paulo Bonan, Lucio Castellano, Daniela Barros, Vanessa Dantas	Show Abstract
Physicochemical analysis of honey samples produced in Paraíba (Brazil)		Maysa Dayane Felix, Paulo Pereira Junior, Camila Silva, Edilene Teles Moreira, Elizabeth Lafayette, Yanna Carolina Teles	Show Abstract
Phytochemical study of *Psidium araça* Raddi		Ana Karoline Aquino, Wallison Dias, Ewerton Lima, Camila da Silva, Maysa Félix, Paulo Pereira Júnior, Maria de Fátima de Souza, Yanna Teles	Show Abstract

Title	Poster	Authors	
Phytochemical analysis of the hydroethanolic extract of peels from *Passiflora edulis* fo. *flavicarpa* Degener and potential vasorelaxant effect *ex vivo*.		Bárbara Cabral, Jovelina Samara Alves, Tays Amanda Gonçalves, Priscilla Maria Maciel, Isac Medeiros, Silvana Zucolotto	Show Abstract
Antioxidant effects of chemical compounds in black tea		Fernanda Silva Galdino, Brenda de Oliveira Tavares, José Isaac Alves de Andrade, Kamylla Kellen Alves de Andrade, Laiane Batista Gonçalves, Lázaro Robson de Araújo Brito Pereira, Maria Rita Araruna de Sousa, Victória Myllena de Souza Leonardo	Show Abstract
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Quality control and quantitation of catechin and epicatechin from leaves of Maytenus rigida Mart		Diego de Araújo, Anny Fernandes, Rodrigo de Andrade, Josean Tavares, Marcelo da Silva	Show Abstract
Evaluation of the antioxidant and photoprotective activity of *Xylopia langsdorffiana* St-hill & Tul.		Rodrigo de Andrade, Diego de Araújo, Yuri do Nascimento, Josean Tavares, Marcelo da Silva	Show Abstract
PHENOLIC COMPOUNDS ISOLATED FROM *EUPHORBIA PHOSPHOREA*		André de Albuquerque, Roseana de Araújo Ramos, Lucas Abreu, Yuri do Nascimento, Josean Tavares, Vicente Carlos Costa	Show Abstract
Phytochemical prospection of *Azadirachta indica* stem bark ethanolic extract and evaluation of its toxicity against *Drosophila melanogaster*		Paula Patricia Marques Cordeiro, Dárcio Luiz de Sousa Júnior, Joycy Francely Sampaio dos Santos, Larissa da Silva, Luiz Jardelino de Lacerda Neto, Maria Apoliana Costa dos Santos, Francisco Assis Bezerra da Cunha, Henrique Douglas Melo Coutinho	Show Abstract
TERPENES: NATURAL COMPOUNDS WITH POTENTIAL USES IN LUNG CANCER CHEMOTHERAPY		Rafaela Silva, Luciana Felinto, Maria Ferreira	Show Abstract

Title	Poster	Authors	
Phytochemical profile of leaves extract of *Azadirachta indica* A. Juss and toxicity against *Drosophila melanogaster*		Dárcio Sousa Júnior, Paula Cordeiro, Zildene Silveira, Nair Macêdo, Aline Boligon, Joycy dos Santos, José da Costa, Francisco da Cunha	Show Abstract
Phytochemical investigation of *Erythroxylum rimosum* O. E. Schulz		jociano lins, Ana Rita Silva, Nikole Trigueiro, Pedro Figueiredo, Emille Silva, Carlos Veloso, Anderson Pinheiro, Vicente Costa	Show Abstract
Phytochemicals of Punica granatum L. in inflammatory bowel diseases: a overview		Joilsa Cândidos dos Santos, Andreyna Pereira Nascimento, Gabriela da Silva Nascimento, Caroline Duarte Siqueira Araruna	Show Abstract
Sterols identified by GC-MS in fraction of hexane extract of *Cissus incisa*	N/A	Deyani Nocedo-Mena, María del Rayo Camacho-Corona, Mauricio González-Ferrara	Show Abstract
Analysis of chemical composition of *Cissus incisa* leaves by GC/MS	N/A	Deyani Nocedo-Mena, Mauricio González-Ferrara, María del Rayo Camacho-Corona	Show Abstract

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ANTIBACTERIAL ACTIVITY OF BROMELIACEAE NATIVE CAATINGA SPECIES: A COMPARATIVE STUDY

Mayara Gomes

Submitted: 13 Sep 2018

Abstract: Show Abstract

Use of *Damnacanthal* for the treatment of breast cancer

Sávio Lucas de Araújo, Gabriela Lourenço, Carla Liandra da Costa, Wandemberg de Albuquerque Neto, Stella Alice Moreira, Vanessa Dantas, Daniela de Barros

Submitted: 07 Sep 2018

Abstract: Show Abstract

Contribution to the knowledge of the species Hancornia speciosa Gomes: A bibliographical review

RAMON LIMA, LEONIA BATISTA, JOSEAN TAVARES

Submitted: 18 Sep 2018

Abstract: Show Abstract

07. EJIBCE-02: Meeting of Young Researchers in Structural Computational Biology, Porto, Portugal, 2018

EJIBCE-02

Welcome Message
EJIBCE-02, UP, PORTO, PORTUGAL, 2018

About The Meeting of Young Researchers in Structural Computational Biology (EJIBCE 2018), see last edition (EJIBCE 2017), aims at bringing together the Portuguese scientific community working in the field in a free-of-charge meeting, to provide a forum for discussion and sharing with no strings attached. This Sixth edition builds on the success of previous editions in Porto, Lisbon, Coimbra, Oeiras and Coimbra, which gathered ca. 60 participants and had over 10 oral communications in each edition.

Mission & Objectives

Given the current economic situation in Europe, and particularly in Portugal, it is increasingly harder to obtain funding and to have an optimistic approach to science and collaborations. Besides, the recent austerity measures put in place by the Portuguese government led many researchers to join groups and institutes abroad, and eventually lose touch with the Portuguese scientific community and developments. After obtaining a doctoral degree or finishing a postdoctoral appointment, many Portuguese scientists abroad look back to their country looking for an opportunity to continue their careers and contribute to the development of Portuguese science. Others wish to remain abroad, but at the same time reach out to the Portuguese community and cultivate stronger ties to its researchers. However, what groups are there on Computational Structural Biology? What do they actually focus on? Are they open to collaborations?

This meeting was created in order to answer these and other similar questions. Its main goal is to provide a simple no-frills environment where Portuguese researchers in Computational Structural Biology, active both in Portugal and abroad, can meet and get to know each other's research and ambitions. Ultimately, we hope that in doing so, we will be able to stimulate new collaborations and broaden the horizons of the Portuguese community of Computational Structural Biologists.

EJIBCE 2018 builds up on the format of previous editions, focusing on a small number of oral communications interspersed with several breaks to encourage discussion and exchange of ideas. Throughout the day, 12 researchers will present their results. Seven will be selected from the submitted abstracts by the Scientific Committee, based on the quality and originality of the work, and will be given 15 minutes to speak, followed by a short discussion. The remaining 5 oral communications will be delivered by invited keynotes, who will be given 25 minutes to speak plus 10 for discussion.

Invited Keynotes

- Diogo Santos-Martins (Scripps Research Institute, California, USA)
- Ana Newton (Yale University, USA)
- João Henriques (University of Copenhagen, Denmark)
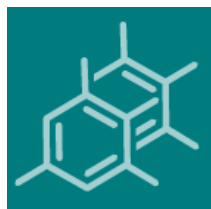- Marta Carneiro (ZoBio B.V., The Netherlands)

- Joana Pereira (Max Planck Institute, Tübingen, Germany)

Website: http://ejibce.github.io

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MDPI Associated Journal Special Issue

Molecules (Call For Papers): Special Issue: **GPCR Mechanism and Drug Design**. Journal: *Molecules* (ISSN 1420-3049), **JCR IF = 3.098**. 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. Editor: Dr. Irina Moreira, Email: irina.moreira@cnc.uc.pt, Center for Neuroscience and Cell Biology (CNC), University of Coimbra (UC), Portugal. Workshop Associated: EJIBCE, Encontro de Jovens Investigadores de Biologia Computacional e Estrutural, Portugal, 2018.

Molecules (Call For Papers): Special Issue: **Structure and Function of Metalloenzymes**. Journal: *Molecules* (ISSN 1420-3049), **JCR IF = 3.098**. 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. 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. Workshop Associated: EJIBCE, Encontro de Jovens Investigadores de Biologia Computacional e Estrutural, Portugal, 2018.

Chairpersons

Dr. Irina Moreira, E-mail: irina.moreira@cnc.uc.pt
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Dr. Nuno S Cerqueira, Email: nscerque@fc.up.pt,
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Advisory Chairperson

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Session Chairs:
Dr. Irina Moreira, Center for Neuroscience and Cell Biology (CNC), Universidade de Coimbra, Coimbra, Portugal, Bijvoet Center for Biomolecular Research, Faculty of Science-Chemistry, Utrecht University, Utrecht, The Netherlands.

Hide published submissions (24) and accepted abstracts (7)

Submissions

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Title	Poster	Authors	
Generating optimal features to find out potent molecules against dengue virus: pharmacophore and QSAR approaches	N/A	Kazi Amirul Hossain	Show Abstract

Title	Poster	Authors	
Mini-review on the applications and perspectives of a new simplex machine learning approach in chemistry and biology	N/A	Muhammad Farman, Asma Hammami, Abir Sarraj-Laabidi, Nabil Semmar	Show Abstract
pH effects on PG/PC and PS/PC lipid binary mixtures	N/A	Pedro Rafael Magalhães, Diogo Vila-Viçosa, Tomás Silva, Miguel Machuqueiro	Show Abstract
Is the 5,10-methylenetetrahydrofolate cofactor synthesized through a non-enzymatic or enzymatic mechanism?		Henrique Fernandes, Sérgio Sousa, Nuno Cerqueira	Show Abstract
Application of QM/MM Methods in the Study of PNPOx	N/A	André Pina, Sérgio Sousa, Nuno Cerqueira	Show Abstract
From All Atom to Coarse Grain: Molecular Dynamic Simulation of Imprinting Process on a Silica Xerogel	N/A	Riccardo Concu, Maria Natalia Dias Soeiro Cordeiro	Show Abstract
Influence of codon 35 amino acid insertion in HIV-1 protease: insights from molecular dynamics		João Luís, Ana Mata, Nuno Alves, Carlos Simões, João Pereira-Vaz, Daniela Vaz, Vítor Duque, Rui Brito	Show Abstract
Experimental and Computational Studies Addressed to 1,3-Dipolar Cycloadditions of D-Erythrose 1,3-Dioxane 1,5-Lactone with *Regio- and Stereo-selectivity*	N/A	Cristina de Sousa, António Ribeiro, António Fortes, Nuno Cerqueira, Maria Alves	Show Abstract
pH-dependent permeability of outer membrane protein G: an in silicostudy		Inês Pires, Miguel Machuqueiro	Show Abstract
Evaluation of Different Scoring Functions for Docking and Virtual Screening against GPCR Drug Targets		Tatiana Vieira, Rita Magalhães, Nuno Cerqueira, Sérgio Sousa	Show Abstract
Creation of a Structural Database for Inhibition of Biofilm Formation	N/A	Rita Magalhães, Tatiana Vieira, Henrique Fernandes, Nuno Cerqueira, André Melo, Manuel Simões, Sérgio Sousa	Show Abstract
New phosphorylated amino acid parametrization to correctly reproduce their acid/base equilibria, including in protein binding events		Nuno Oliveira, Inês Pires, Miguel Machuqueiro	Show Abstract
The importance of unstructured termini in the aggregation cascade of beta-2-microglobulin: insights from molecular simulations of D76N mutant	N/A	Rui João Loureiro, Diogo Vila-Viçosa, Miguel Machuqueiro, Eugene Shakhnovich, Patrícia Faísca	Show Abstract
Exploring the Catalytic Mechanism of the Malonyl-Acetyl Transferase Domain of Human Fatty Acid Synthase		Pedro Paiva, Sérgio Sousa, Maria Ramos, Pedro Fernandes	Show Abstract
Accelerating the DszD enzyme for the Biodesulfurization of Crude Oil and Derivatives		Pedro Ferreira, Sérgio Sousa, Pedro Fernandes, Maria Ramos	Show Abstract

Title	Poster	Authors	
Unraveling the catalytic mechanism of Tryptophan synthase, a drug target against Mycobacterium tuberculosis	N/A	Carla S. Silva Teixeira, Sérgio F. Sousa, Nuno M. F. S. A. Cerqueira	Show Abstract
Combined experimental and computational studies devoted to the synthesis of 1,4-lactones		Juliana F. Rocha, David S. Freitas, Jennifer Noro, Carla S. Silva Teixeira, Cristina E. A. Sousa, Sérgio F. Sousa, Maria J. Alves, Nuno Cerqueira	Show Abstract
Single vs Multi Conformational QM/MM approach for enzymatic catalysis: The case of study of the HBP Sdesulfinase from the 4S pathway	N/A	João Sousa, Sérgio Sousa, Pedro Fernandes, Maria Ramos	Show Abstract
The pH-dependent membrane stability and insertion mechanism of GALA peptide	N/A	J Ricardo Dias, Tomás Silva, Miguel Machuqueiro	Show Abstract
Computational campaign to discover novel human 20S proteasome inhibitors		Pedro Fernandes, Romina Guedes, Bruno Victor, Rita Guedes	Show Abstract
PypKa: a python module for flexible Poisson-Boltzmann based pKa calculations with proton tautomerism	N/A	Pedro Reis, Diogo Vila-Viçosa, Walter Rocchia, Miguel Machuqueiro	Show Abstract
Estimating pKa shifts of encapsulated drugs through a CpHMD approach.		Diogo Reis, Miguel Machuqueiro, Diogo Vila-Viçosa	Show Abstract
Screening of the Binding Trajectories of Inhibitors via Tunnels using Novel Software CaverDock	N/A	Gaspar Pinto, Ondrej Vavra, Piia Kokkonen, Jiri Filipovic, Adam Jurcik, David Bednar, Barbora Kozlikova, Jiri Damborsky	Show Abstract
In silico **design of halogenated carbohydrate mimetics as potential halogen-bonding ligands**		Rafael Nunes, Nuno M. Xavier, Paulo J. Costa	Show Abstract

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The influence of conformational diversity on enzyme catalysis

Ana Rita Calixto, Maria Ramos, Pedro Fernandes

Submitted: 20 Dec 2018

Abstract: Show Abstract

COARSE GRAIN-MOLECULAR DYNAMICS SIMULATIONS OF CYCLIC PEPTIDE NANOTUBES ON BIOLOGICAL MEMBRANES FOR DIFFERENT NEGATIVE CHARGE CONTENT

Martin Calvelo, Barbara Claro, Margarida Bastos, Rebeca Garcia-Fandiño

Submitted: 11 Dec 2018

Abstract: Show Abstract

Comparing Molecular Dynamics Force Fields in Bacteria Membrane Models

Antonio Peón, Bárbara Claro, Margarida Bastos, Ángel Piñeiro, Rebeca Garcia-Fandino

Submitted: 11 Dec 2018

Abstract: Show Abstract

Drug-Target Interaction Prediction: End-to-End Deep Learning Approach

Nelson Monteiro, Bernardete Ribeiro, Joel Arrais

Submitted: 12 Dec 2018

Abstract: Show Abstract

Folding of cyclic peptides stabilized by halogen bonds

Diogo Vila-Viçosa, Rafael Nunes, Paulo Costa

Submitted: 13 Dec 2018

Abstract: Show Abstract

Implementation of a biocomputing platform to settle a new drug discovery pipeline towards post-synaptic receptors.

Rui Ribeiro

Submitted: 17 Dec 2018

Abstract: Show Abstract

The impact of using single atomistic long range cutoff schemes with the GROMOS 54A7 force field

Tomás Silva, Diogo Vila-Viçosa, Pedro Reis, Bruno Victor, Matthias Diem, Chris Oostenbrink, Miguel Machuqueiro

Submitted: 04 Jan 2019

Abstract: Show Abstract

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08. OTISAD-01: Workshop on Intelligent Decision and Optimization of Complex Systems, UANL, Nuevo Leon, Mexico, 2018

OPTISAD-18

[CLICK HERE TO SUBMIT NEW ABSTRACT]

Welcome Message

Dear colleagues, we are pleasant to invite you to the international workshop OPTISAD'18, Workshop of the Thematic Network to Support The Intelligent Decision and Optimization of Complex and Large Scale Systems, Conacyt, Mexico. The topics of interest include Intelligent Optimization, Multi-criteria Decision Making, and Fuzzy Sets and Systems and Applications. The topics also include the application in the previous areas other methods like Machine Learning, Statistics, Artificial Intelligence, Artificial Neural Networks, Deep Learning, Big Data analysis, etc. In addition, the workshop focus on the applications of all kind of computational techniques to Decision-making in the Optimization of large systems in Omics, Biotechnology, Systems Biology, Chemical Biology, Chemical Engineering, Medicine, Social Sciences, Education, Economics, Industry, Transport, Ecology and Environmental Sciences, etc. We suggest you to **download** the [Template File] to write your communication and to **read carefully** the [Instructions to authors] about publication model, copyright, authors responsibilities, *etc*.

Chairperson:

Dr. Fernando López Irarragorri, Professor at the Autonomous University of Nuevo Leon (UANL), México.

Committee:

Dr. Igor Litvinchev, Professor at the Universidad Autónoma de Nuevo Leon (UANL), México.

Dr. Viacheslav Kalashnikov, Professor at the Instituto Tecnológico de Monterrey (ITESM), México.

Dr. Eduardo R. Fernández González, Professor at the Universidad Autónoma de Sinaloa (UAS) , México.

Dr. Jorge A. Navarro Castillo, Professor at the Universidad Autónoma de Sinaloa (UAS), México.

Dr. Juan C. Leyva López, Professor at the Universidad de Occidente (UdO) , México.

Dra. Laura Cruz Reyes Professor at the Instituto Tecnológico de Ciudad Madero (ITCM), México.

Dr. Rafael A. Espin Andrade, Professor at the Universidad Autónoma de Coahuila (UAC), México.

Dr. Maxim Todorov, Professor at the Universidad de las Americas de Puebla(UDLAP), México

Dr. Rafael Caballero Fernández, Universidad de Malaga (UM), España.

Dra. Rosario C. Garza Rios, Universidad Técnica de la Habana (CUJAE), Cuba.

Advisory Chairman

Prof. Humbert González-Díaz, IKERBASQUE Professor, Email: mol2net.chair@gmail.com
(1) Department of Organic Chemistry II, University of the Basque Country UPV/EHU , 48940, Leioa, Biscay, Spain.
(2) IKERBASQUE, Basque Foundation for Science , 48011, Bilbao, Biscay, Spain.

Session Chairs:
Dr. Fernando López, UANL, Nuevo Leon, Mexico

Show all published submissions (8) and accepted abstracts (6)

Submissions

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Title	Poster	Authors	
Primal-dual and general primal-dual partitions in linear semi-infinite programming with bounded coefficients		Abraham Barragán, Lidia Hernández, Maxim Todorov	Show Abstract
A brief review of multi-objective optimization proposals that interactively incorporate preferences.		Mercedes Perez-Villafuerte, Laura Cruz-Reyes, Nelson Rangel-Valdez, Claudia Gomez-Santillan, Hector Fraire-Huacuja, Maria Morales-Rodriguez	Show Abstract
Optimal Scheduling for Precedence-Constrained Applications on Heterogeneous Machines		Carlos Soto, Alejandro Santiago, Héctor Fraire, Bernabé Dorronsoro	Show Abstract
Portfolio optimization with incorporation of preferences and many criteria		Efrain Solares, Eduardo Fernandez, Jorge Navarro	Show Abstract
Project Portfolio Optimization under Temporal Constraints with uncertainty		Fausto Balderas-Jaramillo, Eduardo Fernandez, Claudia Gomez-Santillan, Nelson Rangel-Valdez, Laura Cruz-Reyes	Show Abstract
Modeling Personality Influence over Preference Model's Parameter Values		Jorge Castro-Rivera, Maria Lucila Morales Rodriguez, Nelson Rangel-Valdez, Claudia Gómez-Santillán, Laura Cruz-Reyes, Hector Joaquín Fraire-Huacuja	Show Abstract
PROJECT PORTFOLIO SELECTION FROM A PRIORITY RANKING WITH SYNERGIC EFFECTS		Claudia Gómez-Santillán, Eduardo Fernandez, Nelson Rangel-Valdez, Hector Fraire-Huacuja, Laura Cruz-Reyes	Show Abstract
A review of some methods that incorporate decision-maker preferences in multi-objective evolutionary optimization using a multi-criteria classification method	N/A	Julia Patricia Sanchez-Solis, Eduardo Fernández, Laura Cruz-Reyes, Gilberto Rivera-Zarate, Luis Cisneros	Show Abstract

List of Accepted Abstracts (6) Toggle list

A new outranking-based approach to the constrained sorting problem.

Omar Gaxiola, Eduardo Fernandez, Jorge Navarro

Submitted: 09 Nov 2018

Abstract: Show Abstract

Solving a multicriteria waste collection problem using a non trade-off interactive method

Laura Delgado Antequera, Francisco Ruiz, Fátima Pérez, Rafael Caballero

Submitted: 17 Oct 2018

Abstract: Show Abstract

Comparison of three metaheuristic models to solve portfolio optimization problems considering decision-maker preferences through an outranking-based approach

Gilberto Rivera, Laura Cruz-Reyes, Eduardo Fernandez, Gibran Porras, Nelson Rangel

Submitted: 10 Nov 2018

Abstract: Show Abstract

Incorporating the principles of outranking theory into mathematical programming to solve many-objective project portfolio problems in an interactive way

Gilberto Rivera, Eduardo Fernandez, Claudia Gomez, Ramses Guerrero, Patricia Sanchez

Submitted: 10 Nov 2018

Abstract: Show Abstract

THE INTERVAL OUTRANKING APPROACH AND ITS FURTHER DEVELOPMENTS

Eduardo Fernández, Jorge Navarro

Submitted: 30 Oct 2018

Abstract: Show Abstract

Vehicle and Crew bus scheduling with multi attributes

Francisco Meza Fierro, Fernando Lopez Irarragorri, Yasmin Rios Solis

Submitted: 10 Oct 2018

Abstract: Show Abstract

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09. ICBSM-02: International Conference in Bioinformatics, Simulations and Modeling, UTALCA, Talca, Chile, 2017

iCBSM-02

[REGISTER/LOG IN TO SUBMIT]

Dear colleagues iCBSM-02: Second International Conference in Bioinformatics, Simulations and Modeling, Talca, Chile, 2017. This second version of iCBSM will be held at the Centro de Bioinformática y Simulación Molecular (CBSM) which is associated to the School of Bioinformatics Engineering, Faculty of Engineering, Universidad de Talca, Chile. The conference aim is to maintain and strengthen the research collaborations already initiated with the research groups participating in the previous version of the congress (2015). In addition, it seeks to extend international cooperation networks with research groups located in North America and Europe, mostly in lines of research that are still weak in our group.

Target Audience

This conference is in large measure targeted at graduate and PhD students, bioinformatics engineers, researchers and scientists involved in areas related to Medicinal chemistry, Biophysics, Computational Materials chemistry and Biochemistry, Protein Engineering and Biotechnology and Bioinformatics/Genomics. Available spaces: **80-100 attendants**.

Abstract preparation and submission

The program will be built around talks from accepted abstracts and international/national invited speakers. Abstracts will fall into two categories: oral and poster presentation. We kindly invite all interested graduate and PhD students, as well as postdocs and researchers, to submit your abstracts. The deadline for the abstract submission, either for oral presentation or poster format, is **October 15, 2017**. The Word template for the preparation of abstracts (in **english**) can be downloaded from the link: Abstract_iCBSM-2017.doc, and these must be submitted via the link [Submit New Abstract].

MOL2NET DOI Indexing and MDPI Journals Issues Publication

This year iCBSM is associated to MOL2NET International Conference Series on Multidisciplinary Sciences, MDPI Sciforum, Basel,Switzerland, UPV/EHU, Bilbao, Spain. In this sense, all the abstracts and video conferences of the iCBSM conference will be published on the Sciforum site in open access modality totally free of charge and indexed with a doi number.

In parallel, the authors are welcome to send full written versions of their papers or talks to some of the special issues edited by members of the MOL2NET committee for different journals of the editorial MDPI (http://www.mdpi.com/). Some of these special issues are now in call for papers, submissions are welcome *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. Once you are registered, click here to go to the submission form. In order to send a proposal of special issue contact the chairperson of the conference Prof. González-Díaz H.

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- Dr. Jans Alzate Morales, CBSM, University of Talca
- Dr. Julio Caballero, CBSM, University of Talca
- Dr. Ingo Dreyer, CBSM, University of Talca
- Dra. Wendy Gonzalez, Director CBSM, University of Talca
- Dr. Gonzalo Riadi, CBSM, University of Talca
- Dr. Horacio Poblete Vilches, DI and CBSM, University of Talca
- Dra. Ariela Vergara-Jaque, DI and CBSM, University of Talca
- Dra. Janin Riedelsberger, CBSM, Universidad de Talca

Advisory Committee

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(2) IKERBASQUE, Basque Foundation for Science , 48011, Bilbao, Biscay, Spain.
ORCID: https://orcid.org/0000-0002-9392-2797

Session Chairs:
Professor Jans Alzate Morales, Centre for Bioinformatics and Molecular Simulations (CBSM), Faculty of Engineering, University of Talca

Show all published submissions (18) and accepted abstracts (13)

Submissions

List of Papers (18) Toggle list

Title	Poster	Authors	
Modeling and Analysis of AG:IGE Interface of House Dust Mite Allergens of Group 1		Tania Churasacari, Daniela Zapata, Janny Maza, Alicia Arica, Roberto Pineda, Santiago Justo	Show Abstract
Molecular Dynamics and In Silico Analysis of Oligomerization Surfaces of CYND Enzymes		Aldhair Médico, Cristian Bustamante, Roberto Pineda, Santiago Justo	Show Abstract
IDENTIFICATION OF GENES ASSOCIATED TO COLD ACCLIMATION IN *Eucalyptus nitens* BY ANALYSIS OF GENE EXPRESSION *in silico*.		Sebastián Silva, Marta Fernández	Show Abstract
COMPUTATIONAL STUDY OF HYBRID PLA-PEG NANOPARTICLES AS ANTIPLATELET DRUG CARRIERS		Maria Francisca Matus, Iván Palomo, Cristian Vilos	Show Abstract
3D-PP: a tool for discovering conserved 3D protein patterns		Alejandro Valdés-Jiménez, Josep Larriba-Pey, Miguel Reyes-Parada, Gabriel Nuñez-Vivanco	Show Abstract
Understanding the covalent inhibition of Clavulanate against β-lactamases (TEM-1 and KPC-2) with QM/MM screening methods.	N/A	Rubén Fritz, Jans Alzate Morales, Marc Van Der Kamp, Jim Spencer, Adrian Mulholland	Show Abstract
A proposed new measure to verify the general version of Chargaff 2nd rule.	N/A	Camilo Fuentes Beals, Gonzalo Riadi Mahias, Karen Oróstica, Ignacio Vidal	Show Abstract
RIP-MD: A tool to study residue interaction networks in protein molecular dynamics	N/A	Sebastian Contreras-Riquelme, Jose-Antonio Garate, Tomas Perez-Acle, Alberto Martin	Show Abstract
EVOLUTIONARY VARIATIONS IN HLH DOMAIN MODULATES THE FAST INACTIVATION PHASE IN CALCIUM SELECTIVE TRP CHANNELS.	N/A	Lisandra Flores, Kattina Zavala, Juan C Opazo, Daniel Bustos, Wendy Gonzalez, Seabastian Brauchi	Show Abstract
Structural insight on the Hsp90-binding modes of Naphthoquinone derivatives. Molecular Modeling study for antitumoral drug design		Claudio Godoy-Castillo, Jorge Gonzalez, Jorge Soto-Delgado	Show Abstract
Can Fusion Transcripts between a transposable element and an exon generate piRNAs in mouse (Mus musculus)?	N/A	Bairon Hernández, Gonzalo Riadi	Show Abstract
Elucidating the role of the intracellular pH sensing mechanism of TASK-2 K_2P channel		Daniel Bustos, Francisco Sepúlveda, Guierdy Concha, Leandro Zúñiga, Wendy González	Show Abstract

Title	Poster	Authors	
Stochastic Modeling of Gene Regulatory Networks in *Escherichia coli*	N/A	Rodrigo Santibáñez, Daniel Garrido, Alberto Martin	Show Abstract
Xenopus snc-RNA genes are predominantly located within TEs and are differentially expressed in regenerative and non-regenerative stages after spinal cord injury.		Daniela Araya, Braulio Valdebenito, Johany Peñailillo, Juan Larrain, Gonzalo Riadi	Show Abstract
Structural characterization of the FcDFR1-Dihydroflavonols interactions using Molecular dynamic symulation		Carolina Parra-Palma, María Moya-León, Patricio Ramos	Show Abstract
Study of the translocation mechanism of octopamine in the dopamine transporter. New insights from molecular simulation studies.	N/A	sandra arancibia, Angélica Fierro	Show Abstract
Assessing the halophilic character of ADP-dependent sugar kinases from the archeon order *Methanosarcinales*		Pablo Cea, Felipe González-Ordenes, Victor Castro-Fernández, Victoria Guixé	Show Abstract
Assessing the effect of calcium and magnesium ions in the structural stability of the protein kinase A through molecular dynamics simulations	N/A	Jocelyn Solorza, Rodrigo Recabarren, Jans Alzate Morales	Show Abstract

List of Accepted Abstracts (13) Toggle list

In silico characterization of a rhamnogalacturonan endolyase gene from the Chilean strawberry

Angela Méndez-Yáñez, María Alejandra Moya-León

Submitted: 03 Jan 2019

Abstract: Show Abstract

ANALYSIS IN SILICO OF TRANSCRIPTIONAL AND FUNCTIONAL REGULATION IN *ARABIDOPSIS THALIANA* OVER-EXPRESSING A *PINUS RADIATA* D. DON *MADS10*

Tamara Mendez, Raúl Herrera, Andrea Vega, Rodrigo Gutierrez

Submitted: 17 Dec 2018

Abstract: Show Abstract

Drug repositioning in receptors of monoaminergic proteins and nicotinic acetylcholine receptors with possible polypharmacological effect

Fabián Ramírez, Gabriel Nuñez-Vivanco, Miguel Reyes-Parada

Submitted: 27 Dec 2018

Abstract: Show Abstract

Characterization of ligand protein interactions in mesophilic and thermophilic organisms using data mining techniques

alejandra Bravo

Submitted: 19 Dec 2018

Abstract: Show Abstract

Computational study of the structure and binding site features of FaEXPA2 an α-expansin protein involved in ripening of Strawberry fruit

Felipe Valenzuela-Riffo, Luis Morales-Quintana

Submitted: 19 Dec 2018

Abstract: Show Abstract

Improving Transposable Element annotation using RNA-seq data

Braulio Valdebenito Maturana, Gonzalo Riadi Mahias

Submitted: 13 Dec 2018

Abstract: Show Abstract

Mechanistic insight of the cationic cycloaddition reaction between iminium cation and *N*-vinylpyrrolidone

Yeray Rodriguez, Margarita Gutiérrez, Arnold Romero-Bohórquez, Jans Alzate Morales, Jorge Soto-Delgado

Submitted: 12 Dec 2018

Abstract: Show Abstract

Modelling and structural characterization of PrXTH from *Radiata pine*: *in-silico* interaction with putative substrates

Cristian Carrasco, Yazmina Stappung, Raúl Herrera

Submitted: 14 Dec 2018

Abstract: Show Abstract

Modelling starting enzyme-substrate complexes from human arginase I by the satisfaction of spatial restraints.

José L. Velázquez-Libera, Erix W. Hernández-Rodríguez, Carlos Navarro-Retamal, Julio Caballero

Submitted: 14 Jan 2019

Abstract: Show Abstract

Molecular dynamics simulations show secondary structure content dependence in the adsorption of the cold regulate protein COR15A of *Arabidopsis thaliana*

Carlos Navarro-Retamal, Helgi Ingólfsson, Anja Thalhammer, Dirk Hincha, Jans Alzate-Morales, Wendy González-Diaz

Submitted: 17 Dec 2018

Abstract: Show Abstract

New piperidine derivatives. Studies *in silico* on α7 nicotinic acetylcholine receptors

Jhon López, Angélica Fierro, Edwin Pérez, Jesús García-Colunga

Submitted: 14 Dec 2018

Abstract: Show Abstract

Rational design and biological activity of synthetic compounds as blockers of potassium channels TASK

Bárbara Arevalo, Niels Decher, Teresa Ramirez, Margarita Gutierrez, Wendy Gonzalez

Submitted: 03 Jan 2019

Abstract: Show Abstract

Structural pattern identification for human arginase-I inhibitors by 3D-QSAR modeling.

José L. Velázquez-Libera, Carlos Navarro-Retamal, Erix W. Hernández-Rodríguez, Julio Caballero

Submitted: 14 Jan 2019

Abstract: Show Abstract

10. IWMEDIC-06: International Workshop in Medical Informatics, UDC, Coruña, Spain, 2018

IWMEDIC-06, UDC, CORUÑA, SPAIN, 2018

IWMEDIC-06: International Workshop in Medical Informatics, UDC, Coruña, Spain, 2018

[MOL2NET 2015] [MOL2NET 2016] [MOL2NET 2017] [FACEBOOK (>10K followers)]
[Welcome Videos] [官话] [हिन्दी] [Euskera] [Castellano] [Português] [Français]

[CLICK HERE TO SUBMIT NEW ABSTRACT]

IWMEDIC-06 is the VI International Workshop on Medical Imaging, Medical Coding, and Clinical Data Analysis of University of Coruña (UDC). The IWMEDIC-06 workshop will be held in person and/or online (video conferences) at the University Hospital Complex of A Coruña , Hospital Médico Quirúrgico San Rafael, and Faculty of Computer Sciences, UDC in the summer of 2018. The chairman of this workshop is Prof. Alejandro Pazos; Ph.D., M.D., Chair and Director of Department of Computer Sciences, UDC, Coruña, Spain and head of the RNASA-IMEDIR group. The topics include, but are not limited to, Medical Imaging Processing, Medical Informatics, Medical Coding, Bioinformatics, Computer Aided Drug Desing, Data Analysis, etc. English will be the official language for online publication and presentations, as per MDPI rules, in person or online lectures may be in English, Spanish, or Galician.

Workshop Chairman

Prof. Alejandro Pazos

Ph.D., M.D., Chair Professor of Department of Information and Communication Technologies, Faculty of Computer Sciences, University of Coruña (UDC), Coruña, Spain

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Prof. González-Díaz H., IKERBASQUE Professor, Email: mol2net.chair@gmail.com
(1) Department of Organic Chemistry II, University of the Basque Country UPV/EHU , 48940, Leioa, Biscay, Spain.
(2) IKERBASQUE, Basque Foundation for Science , 48011, Bilbao, Biscay, Spain.
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(Online Publication)

Conference Proceedings

Video Conferences Playlists

Please, visit the channel of the RANASA-IMEDIR group and/or follow the present link to visualize all the video conferences presented o this workshop [IWMEDIC playlist]. You can see these conference also on the IWMEDIC - MOL2NET shared playlist as alternative landing page [IWMEDIC mirror]

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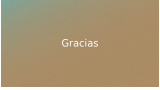Prof. Dr. med. Alejandro Pazos, RNASA-IMEDIR, Computer Sciences Faculty, University of Coruña, 15071 Coruña, Spain., INIBIC Institute of Biomedical Research, CHUAC, UDC, 15006 Coruña, Spain.
Ms. Cadela Rodriguez-Suarez, RNASA-IMEDIR, University of Coruña (UDC), Coruña, Spain

Show all published submissions (8) and accepted abstracts (4)

Submissions

List of Papers (8) Toggle list

Title	Poster	Authors	
Blockchain: posibilidades y aplicaciones al dominio de la medicina y los datos clínicos		David Lizcano	Show Abstract
Redesign and performance of an automatic segmentation method		Adrian Carballal, Carlos Fernandez-Lozano, Francisco Novoa, Nereida Rodriguez-Fernandez, Iria Santos, Marcos Garcia-Guimaraes, Guillermo Aldama-Lopez, Ramon Calviño-Santos, Jose Manuel Vazquez-Rodriguez, Alejandro Pazos	Show Abstract
Metodología para el análisis de expresión génica diferencial usando Machine Learning		Jose Liñares-Blanco	Show Abstract
How to define the quality of images		Adrian Carballal, Nereida Rodriguez, Iria Santos, Luz Castro, Juan Romero	Show Abstract
Infraestructure to support biomedical applications		Francisco Cedron, Adrian Carballal, Carlos Fernandez-Lozano, Cristian Munteanu, Alejandro Pazos	Show Abstract
AI in Civil Engineering: practical cases		Alberto González, Juan Dopico	Show Abstract
The role of Biomedical Infromatics in Exposome research		Guillermo Lopez-Campos, Enrique Calderin	Show Abstract
Deep Learning Applications	N/A	Cristian Robert Munteanu	Show Abstract

List of Accepted Abstracts (4) Toggle list

Application of Mass Spectrometry Imaging in Rheumatic Diseases

Beatriz Rocha, Berta Cillero Pastor, Cristina Ruiz Romero, Andrea Cuervo, Ron M. A. Heeren, Juan D. Cañete, Francisco J Blanco

Submitted: 05 Sep 2018

Abstract: Show Abstract

Predicción de enfermedad cardiovascular en pacientes de diálisis peritoneal con técnicas de machine learning

Carlos Fernandez-Lozano, Rafael Alonso Valente

Submitted: 05 Sep 2018

Abstract: Show Abstract

**Quantification in medical imaging: Application in the study of neurological diseases**

Virginia Mato Abad

Submitted: 04 Sep 2018

Abstract: Show Abstract

Sistema inteligente para uso de drones en asistencia sanitaria

Jose Maria Barreiro, Juan Alfonso Lara

Submitted: 03 Sep 2018

Abstract: Show Abstract

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11. IWIMSM-02: Iberoamerican Workshop on Modelization and Simulation Methods, Valencia, Spain, 2018

IWIMSM-02, UCV-ICMOL, VALENCIA, SPAIN, 2018
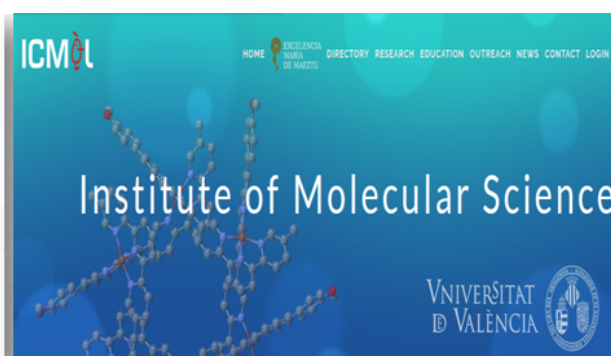
[CLICK HERE TO SUBMIT NEW ABSTRACT]

Welcome Message

We are glad to invite all colleagues worldwide to participate on the second edition of the workshop IWIMSM-02: Iberoamerican Workshop on Modelization and Simulation Methods, Valencia, Spain, 2018. This is a joint workshop promoted by professors of the Institute of Molecular Science (ICMol) and the Faculty of Pharmacy of the University of Valencia (UV), and the Catholic University of Valencia (UCV), Valencia, Spain. This workshop is associated to the MOL2NET International Conference Series on Multidisciplinary Sciences. MOL2NET (the conference running title) is the acronym of the lemma of the conference: From Molecules to Networks.

Scope and Target Audience

This conference is in large measure targeted at under-graduated, MSc, and PhD students, as well as Professors, Engineers, and Researchers focused on the application of Computational Modelling and Simulation techniques. The fields of application include, but are not limited to, Medicinal Chemistry, Computational Chemistry, Materials and Nanosciences, Bioinformatics, Biotechnology, Systems Biology, Biomedical Engineering, Environmental Sciences, Social Sciences, Scientometrics, etc. The algorithms used may also come from different areas including, but not limited to, Discrete Mathematics, Mathematical Analysis, Complex Networks Sciences, Statistics, Data Analysis, Artificial Intelligence, Machine Learning, Deep Learning, etc.

Abstract preparation and submission

Before to submit your communication we recommend to download and use the [Template File] to write your communication. We also strongly recommend you to read carefully the **notes to participants** at the following page [Instructions to authors] about publication model, copyright, authors responsibilities, *etc*. Submit your communications in two steps, first submit your title, authors, and abstract here: [Submit New Abstract]. Next, upload your communication after abstract approval.

Steps for Participation

(0) Register, Sign in/Login, to Sciforum platform [Sciforum login] (All the year)

(1) Submit the title and abstract, select a section or workshop (do not upload paper here) [Submit New Abstract] (until **Dec-15**)

(2) Wait for Sciforum abstract acceptance email, follow the link, and/or login to upload paper, doc and pdf format (until **Dec-15**)

(3) Download template doc and prepare your communication [Template File] (until **Dec-15**)

(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 (**Dec-15** to **Dec-20**)

(7) Contact chairpersons if you need author (publication) or attendance (posting) certificate for conference and/or workshops (All the year)

Steering Committee (Chairpersons)

Prof. Gloria Castellano, Email: gloria.castellano@ucv.esDirector of Department of Experimental Sciences and Mathematics, Catholic University of Valencia (UCV), Valencia, Spain.
Editor of NEREIS, ISSN: 1888-8550, Revista Iberoamericana Interdisciplinar de Métodos, Modelización y Simulación

Prof. Francisco Torrens, Email: Francisco.Torrens@uv.esInstitute of Molecular Science (ICMol), University of Valencia (UV), Valencia, Spain.

Scientific Committee (Local)

Prof. Jorge Gálvez, Full Prof., Department of Physical Chemistry, Faculty of Pharmacy, University of Valencia, Spain

Prof. Ramon García-Domenech, Full Prof., Department of Physical Chemistry, Faculty of Pharmacy, University of Valencia, Spain.

Prof. Facundo Pérez Giménez, Department of Physical Chemistry, Faculty of Pharmacy, University of Valencia, Spain.

Prof. Jesus V. De Julián Ortiz, Tenure-track 1, Department of Physical Chemistry, Faculty of Chemistry, University of Valencia, Spain.

Dr. Maria Galvez-Llompart, Department of Physical Chemistry, Faculty of Pharmacy, University of Valencia, Spain.

Dr. Riccardo Zanni, Department of Physical Chemistry, Faculty of Pharmacy, University of Valencia, Spain.

Scientific Committee (Abroad)

Prof. Alejandro Pazos, Ph.D., M.D., Director of Department of Computation, University of Coruña (UDC), Coruña, Spain.

Prof. Cristian R. Munteanu, Department of Computation, University of Coruña (UDC), A Coruña, Spain.

Prof. Juan M. Ruso, Department of Applied Physics, University of Santiago de Compostela (USC), Spain.

Prof. Natalia D.S. Cordeiro, Department of Chemistry and Biochemistry, University of Porto, Porto, Portugal.

Prof. Carolina Horta Andrade, Universidade Federal de Goias, Setor Leste Universitario, Goiania, Brazil.

Prof. Yovani Marrero-Ponce, University San Francisco de Quito, Cumbayá, Quito, Ecuador.

Advisory Chairman

Prof. González-Díaz H., IKERBASQUE Professor, Email: gonzalezdiazh@yahoo.es
(1) Department of Organic Chemistry II, University of the Basque Country UPV/EHU , 48940, Leioa, Biscay, Spain.
(2) IKERBASQUE, Basque Foundation for Science , 48011, Bilbao, Biscay, Spain.
ORCID: https://orcid.org/0000-0002-9392-2797

Session Chairs:
Prof. Dr. Francisco Torrens, Institute of Molecular Science (ICMol), University of Valencia (UV), Valencia, Spain.
Prof. Dr. Gloria Castellano, Director of Department of Experimental Sciences and Mathematics, Catholic University of Valencia (UCV), Valencia, Spain.

Show all published submissions (13)

Submissions

List of Papers (13) Toggle list

Title	Poster	Authors	
Post-emergence herbicidal activity of *Eucalyptus globulus* Labill. essential oil		M. Dolores Ibáñez, M. Amparo Blázquez	Show Abstract
Fitting method for vacuum ultraviolet spectrometer calibration using line ratio technique		Juan Luis González-Santander	Show Abstract
Molecular Docking Study of Phenolic Compounds with Chitosan: Planning of Biodegradable Hydrogels with Antioxidant Action		Daniela Silva Delmondes, Pablo Delmondes	Show Abstract
Application of molecular topology to the research of analogues to the E-β-Farnesene for plant louse pest control		Ignacio Rosa-Pardo, Lorena Andrés-Olmos Andrés-Olmos, Alex Barreras-Peñalver, Jorge Gálvez, Ramón García-Domenech	Show Abstract
Effect of the Mediterranean diet on body weight and waist circumference in patients with Amyotrophic Lateral Sclerosis (ALS)		Sandra Carrera Juliá, Carlos Barrios Pitarque, José Enrique de la Rubia Ortí, María Luz Moreno Sancho, Eraci Drehmer Rieger	Show Abstract
Effect of olive oil intake and vitamin C in body and fat tissue development		Eraci Drehmer, Mari Ángeles Navarro, Sandra Carrera, Mari Luz Moreno Sancho	Show Abstract
Main pathologies causing confiscation of equine livestock intended for human consumption		CARLA IBÁÑEZ SANCHIS, MARTA PARRA ESCRIBANO, ANTONIO CALVO CAPILLA	Show Abstract
***Saccharomyces boulardii*: probiotic yeast for craft beer production, growth analysis and biovolume estimation**		Joaquín Mulero-Cerezo, Álvaro Briz-Redón, Ángel Serrano-Aroca	Show Abstract
Sanitary portrayal of the animal husbandry in the south of Lebanon		CARLA IBÁÑEZ SANCHIS, BORJA MARTÍ PEIRÓ, ANTONIO CALVO CAPILLA	Show Abstract
Análisis de las alteraciones de la cáscara del huevo de gallina		Ramiro Soler, Joel Bueso	Show Abstract
Quantitative Structure-Antileukemic Activity Models of stilbenoids: A Theoretical Study		Adela León, Francisco Torrens, Gloria Castellano	Show Abstract
A new procedure for the Antioxidant capacity dpph assessment in small samples.		Marie Gombert, Alvaro Carrasco Garcia, Joaquin Carrasco Luna, Pilar Codoñer Franch	Show Abstract
A new simplex machine learning approach for analysis of structural chemical diversification processes. Comparison with other molecular modeling methods.	N/A	Abir Sarraj-Laabidi, Asma Hammami-Semmar, Nabil Semmar	Show Abstract

12. LAWSCI-02: Challenges in Law, Technology, Life, and Social Sciences, UPV/EHU, Bilbao, Spain, 2018

LAWSCI-02, UPVEHU, BILBAO, SPAIN, 2018

[LAWSCI01] [SUBMIT HERE] (Select MOL2NET Conference, Section LAWSci)

Dear colleagues worldwide,

We are glad to invite you to participate in the workshop LAWSci, Challenges in Law, Technology, Life, and Social Sciences. This workshop will be held from 25-30 April, **2018**, online at Sciforum platform. This is a workshop associated to the MOL2NET International Conference Series on Multidisciplinary Sciences, MDPI Sciforum, Switzerland, HQ UPV/EHU, Bilbao, Biscay, Spain.

LAWSci workshop series promotes multidisciplinary collaborations and debate in the frontiers of Law, Technology, Life, and Social Sciences. The interaction between bio-science and ICTs has forged great developments in many fields. However, the appreciation of these discoveries is sadly, all too often, accompanied by a lack of understanding of the legal implications. This conference series aims to provide a reference to the various legal avenues that are available for the protection of scientific advances, but also the legal instruments to protect society from unwanted effects. It constitutes a study of some of the legal implications of bioscience and ICT advances, weighing their impact on society and the law's role in shaping that effect.

In this sense, the presentations will be focused on legal trends in different fields covering, but not limited to: patentability in plants and human genomics, clinical procedures' standards, patients' personal data protection, informed consent, regulatory issues in drug discovery, biomedical research legislation, toxicology, medico-legal problems such as healthcare malpractice, medical insurance or ethics in medical practice, software protection in chemo-informatics, bioinformatics, medical informatics, and social sciences, taxes in the biotechnology industry and causality/liability in environmental pollution, criminology, *etc*. The conference will run on-line and free, saving traveling and participation costs (subscriptions, open publication, participation in forum, certificates, etc., are **free of cost**).

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Hide published submissions (11)

Submissions

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Title	Poster	Authors	
MOTIVATOR PROGRAM IMPLEMENTATION FOR VOLUNTARY BLOOD DONORS: "RED JUNE - USE YOUR INNER BEAUTY"		Pablo Delmondes	Show Abstract
Ethical and legal aspects of medical gene editing: towards a new eugenics		Ekain Payan-Ellacuria	Show Abstract
EL FENÓMENO DEL STALKING		Sheila Rivera	Show Abstract
Desajuste Conceptual del Término "Intimidación" en el lenguaje popular y el jurídico. Especial observación al caso de "La Manada"		Magali Moso	Show Abstract
EL DELITO DE TRATA DE PERSONAS EN EL CÓDIGO PENAL ESPAÑOL		Micaela García Pedriz Buldain	Show Abstract
El Sexting		Andrea López Freiría	Show Abstract
El ciberacoso como modalidad delictiva		Ariane Huebra	Show Abstract
LA PERSEGUIBILIDAD DE LOS DELITOS SEMIPÚBLICOS Y SU INJERENCIA EN EL ÁMBITO DE LOS DELITOS DE ABUSO Y AGRESIÓN SEXUAL: UNA REFLEXIÓN		Oriana Elejalde	Show Abstract
LOS CONSUMIDORES EN EL CÓDIGO PENAL ESPAÑOL: Artículos 281 y 283		David Saceda Domínguez	Show Abstract
Media influence on body self-perception in academics of the health area		Viviane Silva, Pablo Delmondes, Suiani Roewer	Show Abstract
ANÁLISIS ÉTICO Y JURÍDICO SOBRE EL USO DE LA TÉCNICA CRISPR-CAS9 EN LA TERAPIA GÉNICA APLICADA EN HUMANOS	N/A	Claudia Ramos	Show Abstract

13. AWP-04: Academic Week of Physics, UNIFAL-MG, Alfenas, Brazil, 2018

AWP-04

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Seeking to foster inter-locutions among undergraduate students, masters, students in the Pibid, faculty, researchers in the area of Physics and academic community and extra-academic in a more general way, it is intended to develop the academic week of Physics. During the event, lectures, presentation of papers and round tables are planned. Official Link: [Homepage]. Place: Federal University of Alfenas (UNIFAL-MG), Alfenas, Minas Gerais, Brazil. Date: October 24-26, 2018. Please, use the following template [AWP-04 Template] to compose your communication.

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Buscando propiciar interlocuções entre discentes da graduação, mestrado, atuantes no Pibid, corpo docente, pesquisadores da área de Física e comunidade acadêmica e extra-acadêmica de forma mais geral, pretende-se desenvolver a semana acadêmica da Física. Durante o evento estão previstas palestras, apresentação de trabalhos e mesas redondas. Lugar: Universidade Federal de Alfenas. Alfenas. Minas Gerais. Brasil. Fecha: 24 a 26 de Outubro, 2018. Página web: [Homepage].

MOL2NET Association

This workshop is associated with MOL2NET-04 International Conference on Multidisciplinary Sciences, MDPI Sciforum, Switzerland, HQ UPV/EHU, Bilbao, Spain. It will therefore **run both online and in person.** The workshop runs online at the platform SciForum maintained by the editorial MDPI, Basel, Switzerland.

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Submissions

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Title	Poster	Authors	
Protoboard com elementos Resistivos Orgânicos		HUGO METZ	Show Abstract
Máquina de Wimshurst : um projeto aplicado ao Ensino de Física		Gabriel Baldasso, Cassio Henrique Marculino, Francielli de Fatima David, Raphael César Pimenta, Frederico Toti	Show Abstract
Fim do Mundo um projeto para aprender Ciência e pensar sobre o futuro.		Francielli de Fatima David, Cassio Henrique Marculino, Gabriel Baldasso, Raphael César Pimenta, Amanda Silva, Frederico Toti	Show Abstract
MOTOR DE STIRLING UM ALIADO NO PROCESSO DE APRENDIZAGEM DA TERMODINÂMICA		Leticia Carolaine Faria, Cassio Henrique Marculino, Francielli de Fatima David, Gabriel Baldasso, Raphael César Pimenta, Lucas Fagundes, Frederico Toti	Show Abstract
Uma proposta do uso de vídeo-análise para o Ensino de Física		Cassio Henrique Marculino, Francielli de Fatima David, Ygor Silva, João Almeida, Vinicius Pimenta, Gabriel Baldasso, Amanda Silva, Raphael César Pimenta, Lucas Fagundes, Samuel Soltau	Show Abstract
Estudo das propriedades óticas de células solares de banda intermediária utilizando o método Split Operator		Ygor Silva, João Almeida, Gabriel Macedo, Anibal Bezerra	Show Abstract
A Física investiga: Será o Homem-Aranha um assassino por falta de conhecimento físico?		André Carvalhaes, Samuel Soltau	Show Abstract
Fourier Grid Hamiltonian aplicado ao estudo das propriedades ópticas e de transporte de células solares de banda intermediária simuladas computacionalmente usando a linguagem Julia.		João de Almeida, Ygor Lacerda, Cassio Henrique, Gabriel Macedo, Gabriel Marinho	Show Abstract

Title	Poster	Authors	
Introdução ao Ensino de Física de Partículas através de um jogo de cartas	Obrigado pela atenção. E-mail de contato: andersonfisica2050@gmail.com	Anderson Santos, Samuel Soltau	Show Abstract
REALIDADE AUMENTADA E SMARTPHONE COMO FERRAMENTAS NO ENSINO DE FÍSICA		RENAN CINTRA, Samuel Soltau	Show Abstract
Estudos Teóricos da interação de nanotubos de carbono com aminoácidos		Andrilene Alves, Wanderson Knupp, Ihosvany Rodriguez	Show Abstract
Uma proposta de uso do Tracker para a análise espectroscópica		João Paulo Cruz, Samuel Soltau	Show Abstract
Simulação de órbitas estelares na Galáxia: Uma aplicação de modelos semi-empíricos à Gravitação Universal	Obrigado pela atenção! Listas Contato: rafaeljpassosdominigues@gmail.com	Rafael Domingues, Artur Justiniano	Show Abstract

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Detecção do Exoplaneta WASP-76 b no Miniobservatório Astronômico da Unifal-MG

José Carlos da Silva, Artur Justiniano Roberto Júnior

Submitted: 10 Oct 2018

Abstract: Show Abstract

SEQUÊNCIA DIDÁTICA UTILIZANDO ROBÓTICA EDUCACIONAL E GAMIFICAÇÃO ATRAVÉS DO KIT EV3 LEGO

Marcos Tavares, Cristiana Magalhães

Submitted: 10 Oct 2018

Abstract: Show Abstract

SEQUÊNCIA DIDÁTICA UTILIZANDO ROBÓTICA EDUCACIONAL E GAMIFICAÇÃO ATRAVÉS DO KIT EV3 LEGO

Marcos Tavares

Submitted: 10 Oct 2018

Abstract: Show Abstract

Aproximação de massa efetiva aplicada à perovskitas híbridas de baixa dimensionalidade

Gabriel Machado, Anibal Bezerra

Submitted: 10 Oct 2018

Abstract: Show Abstract

Estudo fotocatalítico do $CuWO_4$ com e sem agente sacrifício para a degradação do corante Rodamina-B

Naiara Lima

Submitted: 08 Oct 2018

Abstract: Show Abstract

O ENSINO DIVERSIFICADO DO TEMA ENERGIA: UMA PROPOSTA DE ENSINO BASEADA NA TRÍADE CIÊNCIA, TECNOLOGIA E SOCIEDADE.

Guilherme Pereira, Thirza Sorpreso

Submitted: 11 Oct 2018

Abstract: Show Abstract

Obtenção de Curvas de luz de Estrelas Variáveis Eclipsantes no Observatório Astronômico da Universidade Federal de Alfenas

Fabiana Pinto, Artur Justiniano

Submitted: 11 Oct 2018

Abstract: Show Abstract

Obtenção de curvas de luz de estrelas hospedeiras de exoplanetas no observatório astronômico da universidade federal de alfenas.

João Carlos Alves, Artur Justiniano, José Carlos Silva

Submitted: 10 Oct 2018

Abstract: Show Abstract

Preparação e caracterização de materiais óxidos multifuncionais nanoestruturados a base de ZnO dopado com Zr e Mn

Isabella Silva de Souza, Hugo de Carvalho

Submitted: 11 Oct 2018

Abstract: Show Abstract

Solução numérica para a equação de Schrödinger uma alternativa para o ensino de mecânica quântica

Gabriel Macedo, Ygor Silva, João Almeida, Gabriel Marinho, Cassio Marculino, Anibal Bezerra

Submitted: 08 Oct 2018

Abstract: Show Abstract

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14. MODEC-03: Workshop on Natural Products and Agro-Industrial Procesess in Amazon, UEA, Puyo, Ecuador, 2018

MODEC, 3rd Edition

[Workshop Editorial & Full Committee]

MODEC 2018 (Submissions Open)

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MODEC2018, International Workshop on the Natural Products and Agro-Industrial Processes in Ecuadorian Amazon region

Welcome to the MODEC2018 workshop. This is Amazon State University's (UEA) first workshop, devoted to the promotion and application of the Multidisciplinary Sciences to the development of natural products and agro-industrial processes in Ecuadorian Amazon regions. This workshop runs both online and on location at the university. The online portion of the workshop is powered by the SciForum platform of MDPI, hosted by the MOL2NET International Conference Series on Interdisciplinary Sciences.

Additionally, the physical component of the workshop is also scheduled to run through the Department of Earth Sciences (Facultad de Ciencias de la Tierra) at Universidad Estatal Amazónica (UEA), Puyo, Ecuador. Please, contact the workshop chairmen for further details. Paper submission is already open and the publication of papers for conference purposes in SciForum platform is free of cost.

Publications are expected to be short papers consisting of 1-3 pages. Be aware that the submission is a two step process. First you must register and submit a tentative title, authors list and abstract. Next, you need to submit your full publication upon acceptance of the abstract by the committee. Full publications will be published online, free of charge, with doi number as soon as possible after acceptance. If you are planning to submit a publication, please use the following template, MODEC Template.doc. Click on the following link to register and/or submit your communication Sumit to MODEC here.

All submitted papers should fall under one of the following categories:

- Computational chemistry, Cheminformatics, and Bioinformatics
- Mathematical modeling
- Organic and Functional Foods
- BioTrade: Natural Products of the Amazon
- Production systems with agro-business and forestry purposes or biomass for energy purposes
- Environmental impacts
- Agro-industrial development processes

Schedule:
- Abstracts submission until 2018-Oct-01, Envio de los abstract hasta el 01 de octubre de 2018.
- Abstract acceptance until 2018-Oct-03.
- Communications submission until 2018-Nov-01.
- Communications acceptance until 2018-Nov-15.
- Communications publication until 2018-Nov-30.

 Please, click the following link to read the editorial paper with welcome message and call for papers as well as the full description of the workshop with details of topic, short biographies of the members of the committee, contact details, personal pictures, etc., [Workshop Editorial & Full Committee]
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Prof. Amaury Pérez Martínez received his Bs. in Chemical Engineering in 2002, his MSc degree in Chemical Engineering Processes and Analysis in 2007, and his PhD degree in Chemical Engineering in 2013. He has worked in the development of new technology in the Chemical Industry. Currently, he is an Assistant Professor of Agro industrial Engineering at Amazon State University (UEA) in Puyo, Ecuador. His research interests include philosophy of process design, simulation, and sustainable development

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Session Chairs:
Dr. Amaury Pérez Martínez

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Title	Poster	Authors	
MODEC03-2018, International Workshop on the Natural Products and Agro-Industrial Processes in Ecuadorian Amazon region		Amaury Pérez Martínez, Karel Dieguez Santana, Oscar Rivera-Borroto, Gerardo Casañola-Martín	Show Abstract
Obtaining microorganisms with cellulolytic activity in different regions of Ecuador		Jonathan Villavicencio, Carmen Salvador, Layanis Mesa, Maira Rojas, Pablo Londoño	Show Abstract
Recycled of commercial enzymes in the production of ethanol of II generation		Carmen Salvador Pinos, Adalis Mesa Noval, Leyanis Mesa Garriga, Erenio González Suárez	Show Abstract
Preliminary study of caffeine extraction from *Ilex guayusa* L. leaves using supercritical carbon dioxide.		Pablo Londoño-Larrea, Santiago Zapata, Mishell Lara-López, Estefanía Villamarín-Barriga	Show Abstract
Assessment of the best operating conditions in the enzymatic hydrolysis of pretreated bagasse for bagasse ethanol.		Carmen Salvador Pinos, Adalis Mesa Noval, Ángel Batallas Merino, Jonathan Villavicencio, Layanis Mesa Garriga, Erenio González Suárez	Show Abstract
Substitution of commercial enzymes for native ones from Ecuador: a university innovation		Carmen Salvador Pinos, Erenio González Suárez, Diana Concepcion Toledo, Amaury Pérez-Martínez, Karel Dieguez Santana	Show Abstract
Analyses of enzymatic hydrolysis of bagasse cane of sugar for obtention of ethanol employing a cocktail of natives commercials enzymes.		Ángel Batallas, Carmen Salvador, Jonathan Villavicencio, Humberto González Gavilánez, Layanis Mesa, Erenio González	Show Abstract
Polyphenols of chuchuhuazo (*Maytenus macrocarpa* bark*)* as antioxidant and preservative in fresh sausage.		Manuel Pérez Quintana, Cristian Correa, Luis Bravo, Reinier Abreu, Darwin Viáfara	Show Abstract
Vapor-phase antifungal activity of *Ocimum micranthum* from Ecuadorian Amazon rainforest		Bélgica Yaguache Camacho, Matteo Radice, Laura Scalvenzi	Show Abstract
Strategic diagnosis of the local development environmental system in rural communities of the colonized Amazonian Kichwa territory		Ruth Arias Gutiérrez, Manuel Pérez Quintana, Roberto González Sousa, Angelina Herrera Sorzano, Neyfe Sablon-Cossio	Show Abstract
Content of phenolic compounds in powders of six Amazonian vegetables and its effect as a phytobiotic additive for pigs	N/A	Willan Caicedo, Alex Flores, Manuel Pérez	Show Abstract

Title	Poster	Authors	
Thermal efficiency analysis of a discontinuous distiller for _Ocotea quixos_ from Amazon Region of Ecuador		Galo Cerda Mejía, Víctor Cerda Mejía, Amaury Peréz Martínez, Javier Dominguez Brito, Erenio Gonzales Suarez	Show Abstract
The Pig Manure Anaerobic Digestion. A tubular biodigester characterization in the Ecuadorian Amazon		Edwin Collahuaso González, Amaury Pérez-Martínez, Miguel Herrera-Robledo, Karel Diéguez-Santana	Show Abstract
Evaluation of the noise pollution of the Cevallos avenue, Ambato city, Ecuador, for the determination of critical points of affectation in the place, and to provide information that allows the generation of preventive and corrective measures to the problem		Pedro Peñafiel, Karem Cazares, Daniela Marizande	Show Abstract
EVALUATION OF AGROINDUSTRIAL RESIDUES OF THE SIERRA AND AMAZONIA IN THE OBTAINING OF MUSHROOMS _Pleurotus ostreatus var. Florida._		Julia Escobar, Mario Álvarez	Show Abstract
Evaluation of the operation parameters and the process quality of the obtaining of granulated panela in the parish of Tarqui, in the panela industry "El Valle"	N/A	Julia Escobar, Victor Cerda, Andrea Tapuy	Show Abstract

List of Accepted Abstracts (1) Toggle list

Use of cellulolytic enzymes from a strain of bacteria of the genus _Bacillus sp_. in the enzymatic hydrolysis process for production of second generation ethanol.

Carmen Salvador Pinos, Adalis Mesa Noval, Jonathan Villavicencio, Ángel Batallas Merino, Amaury Pérez-Martínez, Leyanis Mesa Garriga, Erenio González Suárez

Submitted: 14 May 2018

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