# CHEMBIOINFO-07: EJIBCE & Chem-Bioinfoinformatics Congress Coimbra, Portugal-München, Germany-Chapell Hill, USA, 2021


## CHEMBIOINFO-07: EJIBCE & Chem-Bioinfoinformatics Congress Coimbra, Portugal-München, Germany-Chapell Hill, USA, 2021 (Editorial)

Prof. Alexander Tropsha,[1] Prof. Eugene Muratov,[1] Prof. Paola Gramatica,[2] Prof. Weifan Zheng,[3] Dr. Irina Moreira,[4] Dr. Igor Tetko,[5] Dr. Yasset Perez-Riverol,[6] Prof. Humbert González-Díaz,[7,8,9,*]

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**Welcome Message**

Dear colleagues worldwide welcome to a joint call of CHEMBIOINFO-07: Chem-Bioinformatics Congress, **München, Germany-Chapel Hill, USA, 2021** (see this section) and EJBCE VIII Meeting of Young Researchers in Structural Computational Biology, **Coimbra, Portugal, 2021** (see next section). CHEMBIONFO & EJIBCE form an inter-university trans-Atlantic Chem-Bioinformatics, Computational Chemistry, and Computational Biology congress series. From the America's side the event is organized by professors of University of North Carolina (**UNC Chape Hill**), Chape Hill, NC, **USA**, and professors of North Carolina Central University (**NCCU**), Durham, NC, **USA**. From Europe's side the event is organized by professors and researchers of Helmholtz Zentrum München - German Research Center for Environmental Health (**GmbH**), **Germany**, The European Bioinformatics Institute (**EMBL-EBI**), Cambridge, **United Kingdom**, Center for Neuroscience and Cell Biology (**CNC**), University of Coimbra (**UC**), Coimbra, Portugal, the University of The Basque Country (**UPV/EHU**) and **IKERBASQUE**, Basque Foundation for Science, Bilbao, **Basque Country, Spain**. This congress is associated to the **MOL2NET** International Conference Series on Multidisciplinary Sciences. MOL2NET (From Molecules to Networks), International Conference on Multidisciplinary Sciences, **ISSN**: 2624-5078, MDPI SciForum, Basel, Switzerland.

**Topics of Interest.** CHEMBIOINFO series aims to bring together leading academics, researchers and scholars to share their experiences on all aspects of computational programing, modeling, simulations, or scientific computing dedicated to Computational Chemistry, Chemoinformatics, Bioinformatics, Systems Biology, Biocomputing, etc. We focus on applications to Medicinal Chemistry, Drug Design & Discovery, Pharmaceutical Industry, Natural Products Research, Toxicology, Vaccine Design, Biotechnology, Personalized Medicine, Biomedical Engineering, etc. We welcome contributions involving the following topic:

**Computational Chemistry & Chemoinformatics:** Quantum Chemistry, Functional Density Theory (DFT), Ab Initio Methods, Semi-Empirical Methods, Machine Learning (ML) Quantum Chemistry Potentials, Molecular Mechanics/Molecular Dynamics (MM/MD), Molecular Docking, etc.

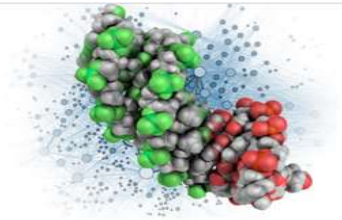
**Bioinformatics and Systems Biology:** Proteomics, Genomics, BLAST and sequence alignment, Meta-Genomics, Protein folding and Protein Structure prediction, RNA secondary structure prediction, Protein Interaction Networks (PINS), Gene Regulatory Networks (GRN), Metabolomics and Metabolic Networks, Synthetic Biology, Data Analysis, and related techniques.

**Computer Coding, Data Analysis, Artificial Intelligence, and Soft Computing.** The congress also deals with the development or application of computer languages, computational programs, and/or algorithms for the study of chemical and biological process and/or inspired on biological processes. This include programing in Python/Biopython, Perl/Bioperl, etc. Development or application of Machine Learning (ML), Artificial Neural Networks (ANN), Deep Learning Networks (DLN), Bayesian Networks, Random Forest, Classification Trees, Genetic Algorithms (GA), Swarm Intelligence (SI), Ant Colony Algorithms, Artificial Imune Systems, etc.

**Bioethics and Biolaw:** Last, not the least, the workshop deals with all the Legal, Regulatory, and Bioethics issues emerging from use of new experimental and ICTs in the previous areas such as Drug patenting, Genome patenting, Drug re-purposing patents, Chem-Bioinformatics Software and Models Copyrights, etc. GDPR and Personal data protection in Human Bioinformatics, etc.

**Modalities of Participation.** The congress series may run both in person and/or online depending on year. Participation in all modalities is not mandatory. In online/person presentations may include workshops, seminars, meetings with face-to-face discussion at both universities and/or online publication of papers, videos, etc.

**CHEMBIOINFO & EJIBCE Joint Call**



VIII EJIBCE

Coimbra, 20 de dezembro 2021

CENTER FOR NEUROSCIENCE AND CELL BIOLOGY

The present is a joint call of CHEMBIONINFO-07 with the VIII Meeting of Young Researchers in Structural Computational Biology (EJIBCE 2021). EJIBCE series 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 Eighth edition builds on the success of previous editions in Porto, Lisbon, Oeiras and Coimbra, which now counted with ca. 80 participants and had over 10 oral communications. The joint call also pursues increasing the contacts between CHEMBIOIFO and EJIBCE communities and with the participants of all other Mol2Net conference series congresses.

**EJIBCE 2021 Mission & Objectives.** Sharing and discussing ideas are the seeds for a robust scientific community. Given the current pandemic situation, promoting and encouraging an open spirit and collaboration between Computational Biology research groups in Portugal is increasingly necessary. Among other factors, this panorama showed the contribution but also a growing need for researchers capable of making the most of computational resources to generate quick, efficient, and rational responses to real, urgent, and unavoidable problems. This connection with Portugal becomes essential when returning to the country after a PhD, a post-doctorate, or any other prolonged period abroad. On the other hand, some researchers want to continue their work abroad but, at the same time, cultivate a close relationship with science in Portugal. But which groups are working on Structural Computational Biology in Portugal? And what research is carried out in these groups? Questions come naturally, and answers are not always easy to find. This meeting aims to answer some of these questions. It intends to make known the best that is done in this Structural Computational Biology area in Portugal and, on the other hand, to reveal what Portuguese researchers based abroad are studying. In this way, we want to provide a space where projects and results can be shared and discussed, with a stimulating collaboration view (at national and international level) and broadening the horizons of Structural Computational Biology in Portugal.

**CHEMBIOINFO & EJIBCE Papers Online publication.** This workshop 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 published in **open access totally free of cost** and a **DOI number will be assigned**. This include, conference papers, letters,, posters, etc. The platform also includes the possibility of online comments from researchers of both universities and colleagues worldwide as well. At the end of the year all contributions will be published in the Proceedings Book of the MOL2NET-05, International Conference on Multidisciplinary Sciences, **ISSN**: 2624-5078, MDPI SciForum, Basel, Switzerland.

**CHEMBIOINFO & EJIBCE Online Publication Steps:** As this joint pursuit to increasing the interactions between CHEMBIOIFO-EJIBCE community with all other Mol2Net conference participants and also with researchers worldwide we split the congress on two main stages. In 1st stage called Publication stage the participants will submit, upload, and publish their communications. In the 2nd stage, called Post-publication discussions, the participants will post comments or questions in the papers of other authors and/or answer to comments made by others about their own works. The steps are the following:

**CHEMBIOINFO & EJIBCE Publication stage**

(00) Register, Sign in/Login, to Sciforum platform **[Sciforum login]**
(01) Submit the title/abstract to workshop (do not upload paper here)
(02) Download template doc and prepare your communication
(03) Wait for Sciforum abstract acceptance email
(04) Follow the link in the email or login to upload paper (doc and pdf format)

**CHEMBIOINFO & EJIBCE Post-publication stage**

(05) Wait for paper acceptance and publication emails
(06) Follow link to proofread your paper
(07) Communicate with chairpersons if corrections are necessary
(08) Wait for advice of post-publication season starting
(09) Login to post comments, questions, or answer comments about your work
(10) Request author (publication) and/or reviewer (post) attendance certificate.

**MDPI JCR Journals Special Issues**

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 issues run 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 issues associated to the topic of the workshop.

International Journal of
*Molecular Sciences*

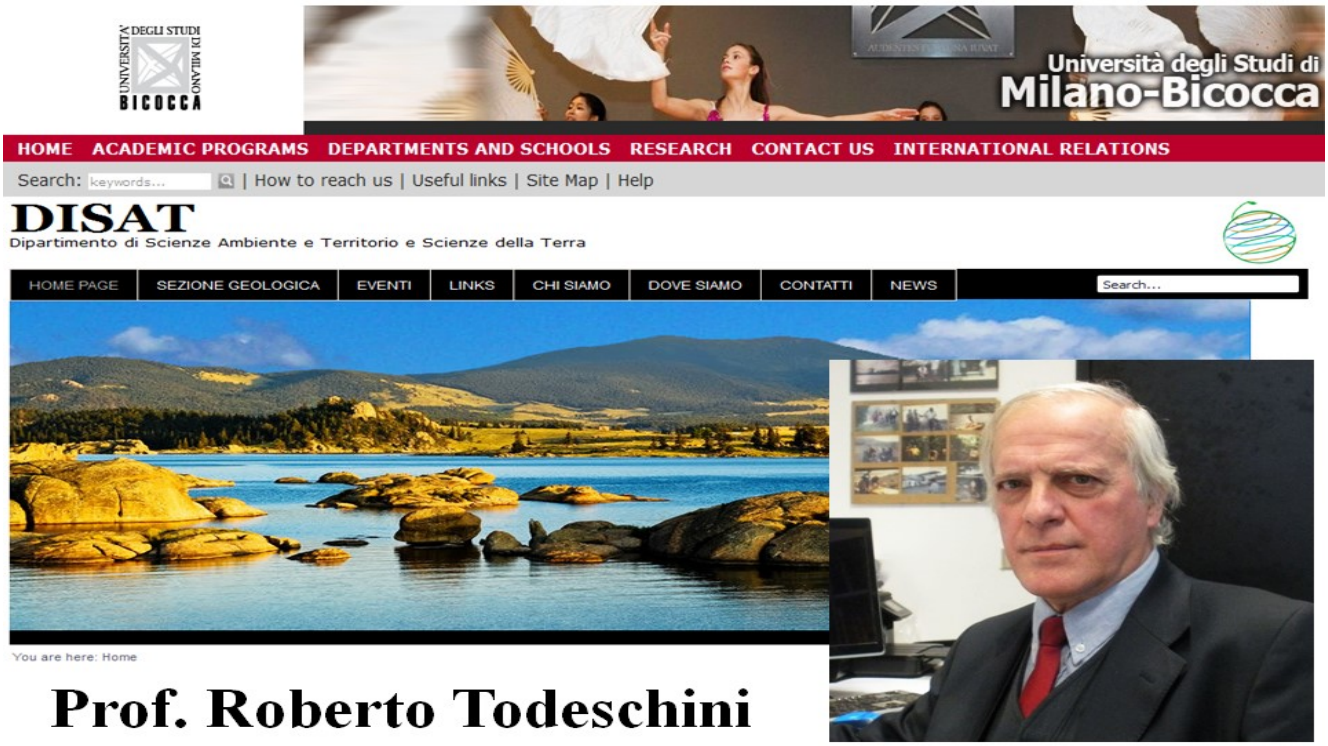
**IJMS (Call For Papers):** Special Issue: **Artificial Intelligence and Machine Learning in Drug Development**. Journal: International Journal of Molecular Sciences IJMS (ISSN 1422-0067), **JCR IF = 5.924**. Editor: Editor: Dr. **Irina Moreira**, Center for Neuroscience and Cell Biology (CNC), University of Coimbra, **Coimbra, Portugal**. Email: irina.moreira@cnc.uc.pt. Submissions until: **30 April 2022**.

**IJMS (Call For Papers):** Special Issue: **Complex Networks, Bio-Molecular Systems, and Machine Learning**. Journal: International Journal of Molecular Sciences IJMS (ISSN 1422-0067), **JCR IF = 5.924**. Editor: **Prof. Humberto González-Díaz**, Email: mol2net.chair@gmail.com, Department of Organic and Inorganic Chemistry, and Basque Center for Biophysics, University of the Basque Country (UPV/EHU) and Ikerbasque - Basque Foundation for Science, 48011 Bilbao, Biscay, **Spain**. Submissions until: **28 Feb 2022**.

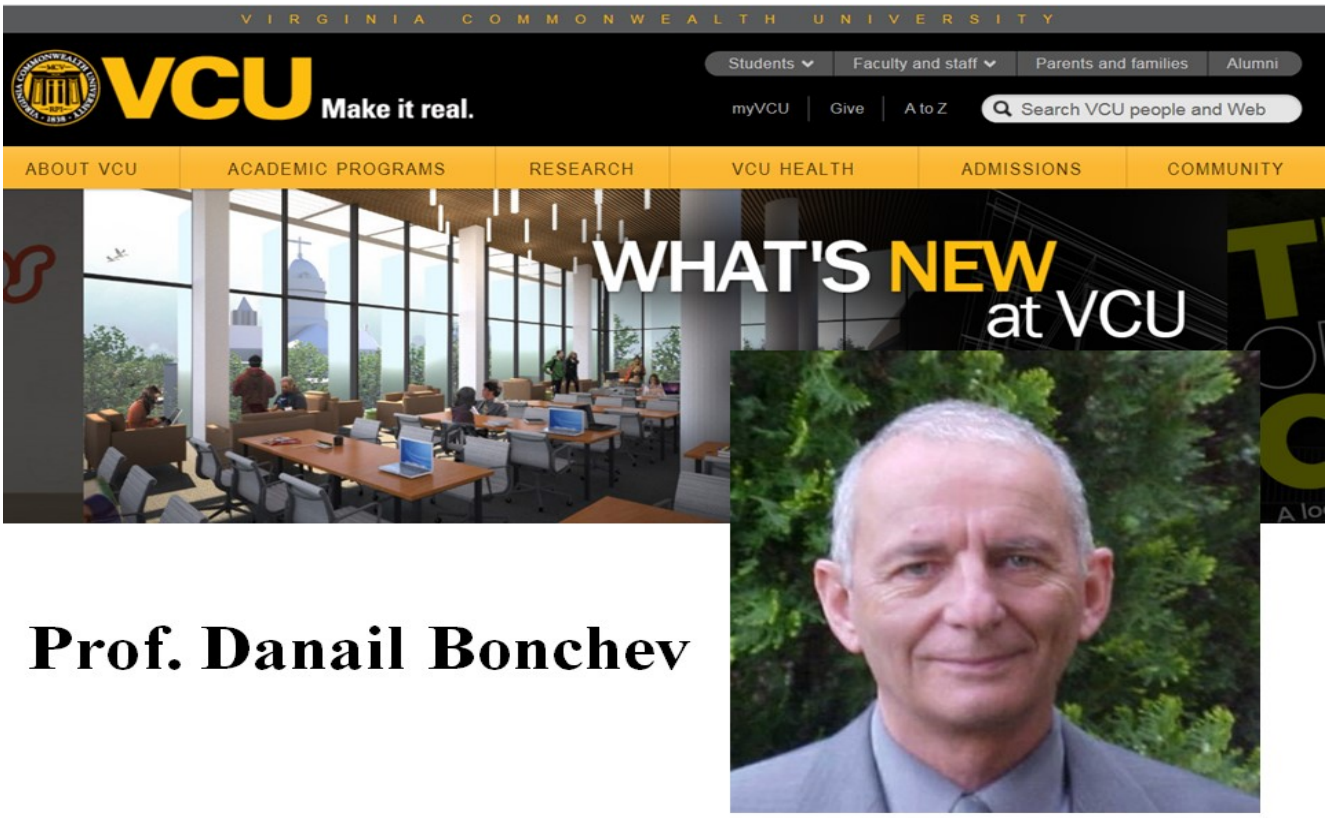
*BioChem*

**BIOCHEM (Call For Papers):** Special Issue: **Computational Analysis of Proteomes and Genomes**. Journal: *BioChem* (ISSN 2673-6411). Editor: Dr. **Irina Moreira**, Center for Neuroscience and Cell Biology (CNC), University of Coimbra, **Coimbra, Portugal**. Email: irina.moreira@cnc.uc.pt. Submissions until: **31 Dec 2022**.

**CHEMBIOINFO-07 Dedicated to Prof. R. Todeschini and Prof. Danail Bonchev**

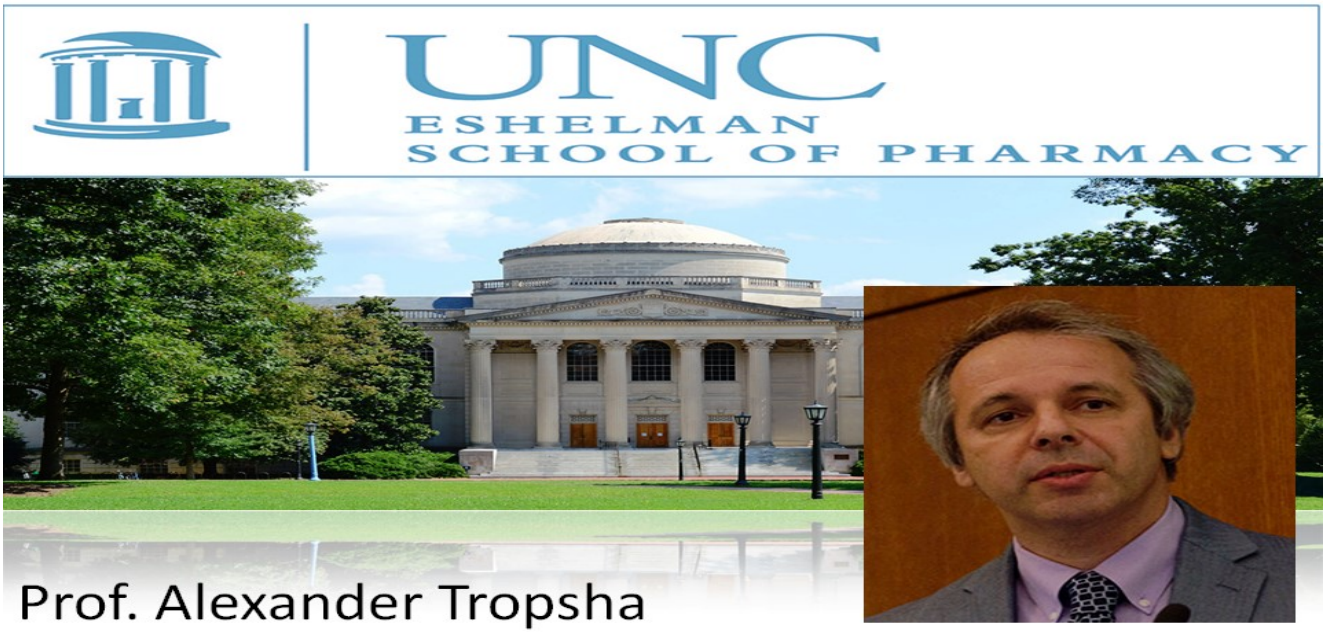



**Prof. Roberto Todeschini**, Department of Environmental Sciences, University of Milano-Bicocca, Milano,Italy.




**Prof. Danail Bonchev**, Center for the Study of Biological Complexity, Virginia Commonwealth University (VCU), Richmond, **USA**.

**CHEMBIOINFO-07 Co-Host Honor Chairpersons**

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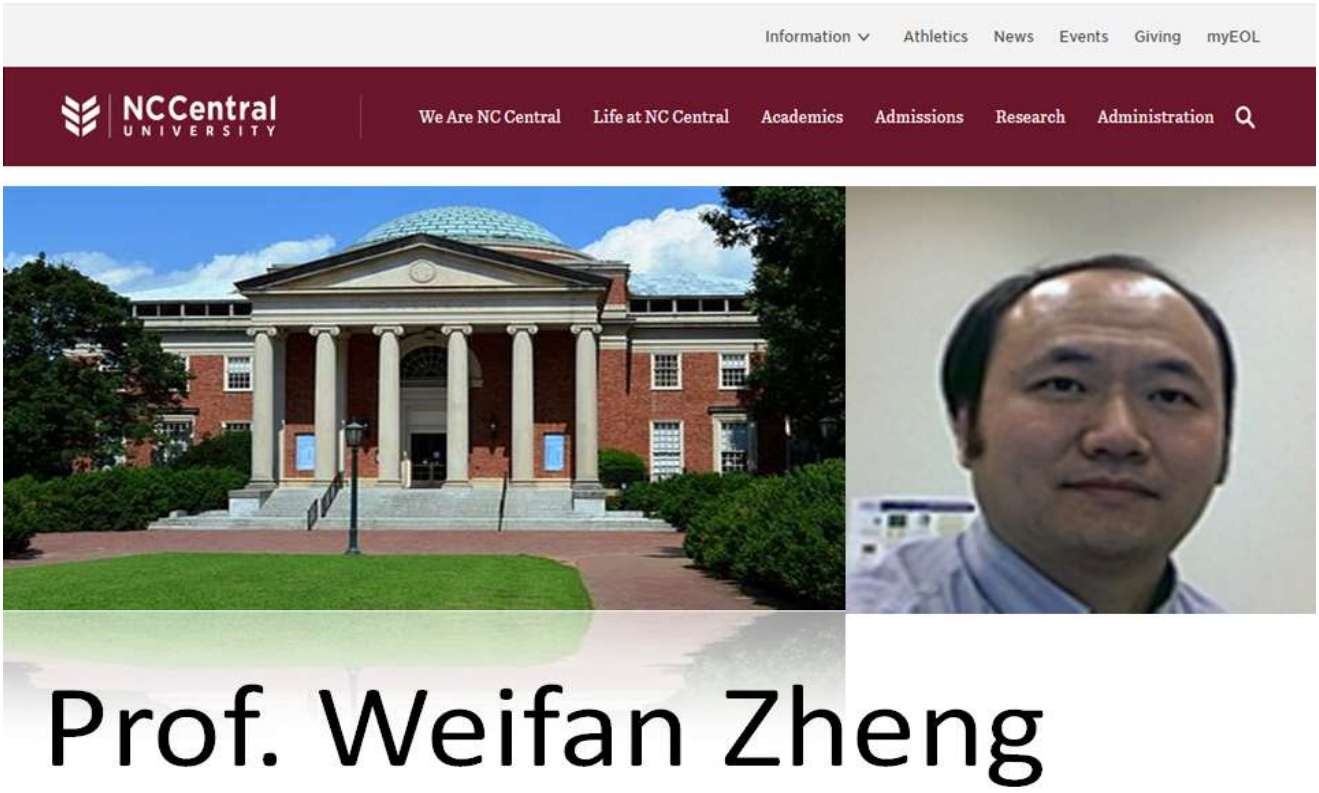
**Prof. Paola Gramatica**

Prof. **Paola Gramatica**, Full professor of Environmental Chemistry, Faculty of Sciences, Insubria University, **Italy**.

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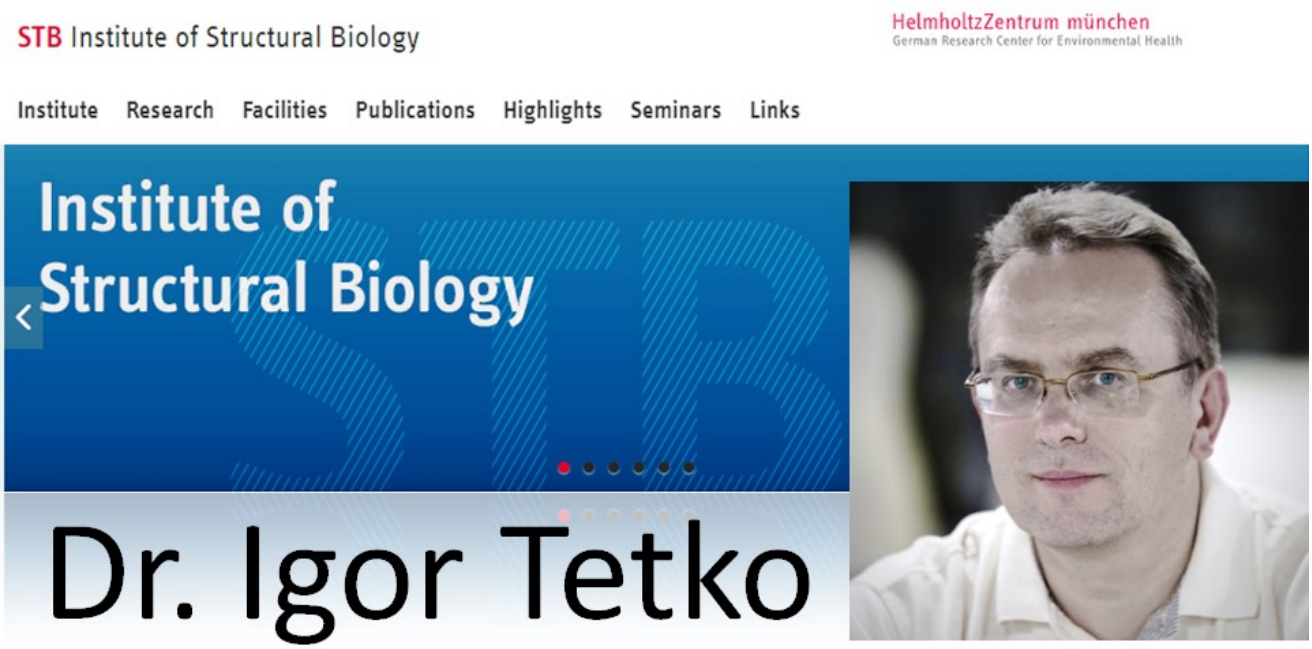


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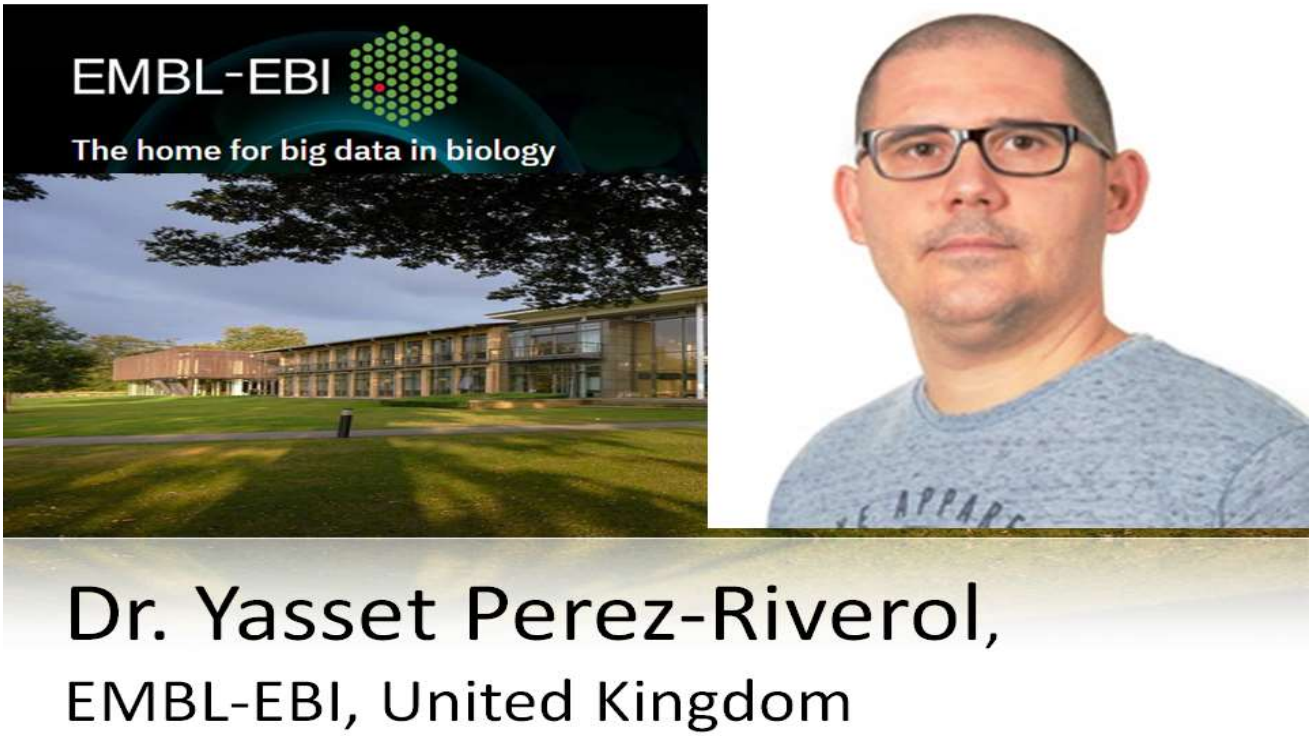


Dr. Yasset Perez-Riverol, European Bioinformatics Institute(EMBL-EBI), Cambridge, **United Kingdom.**

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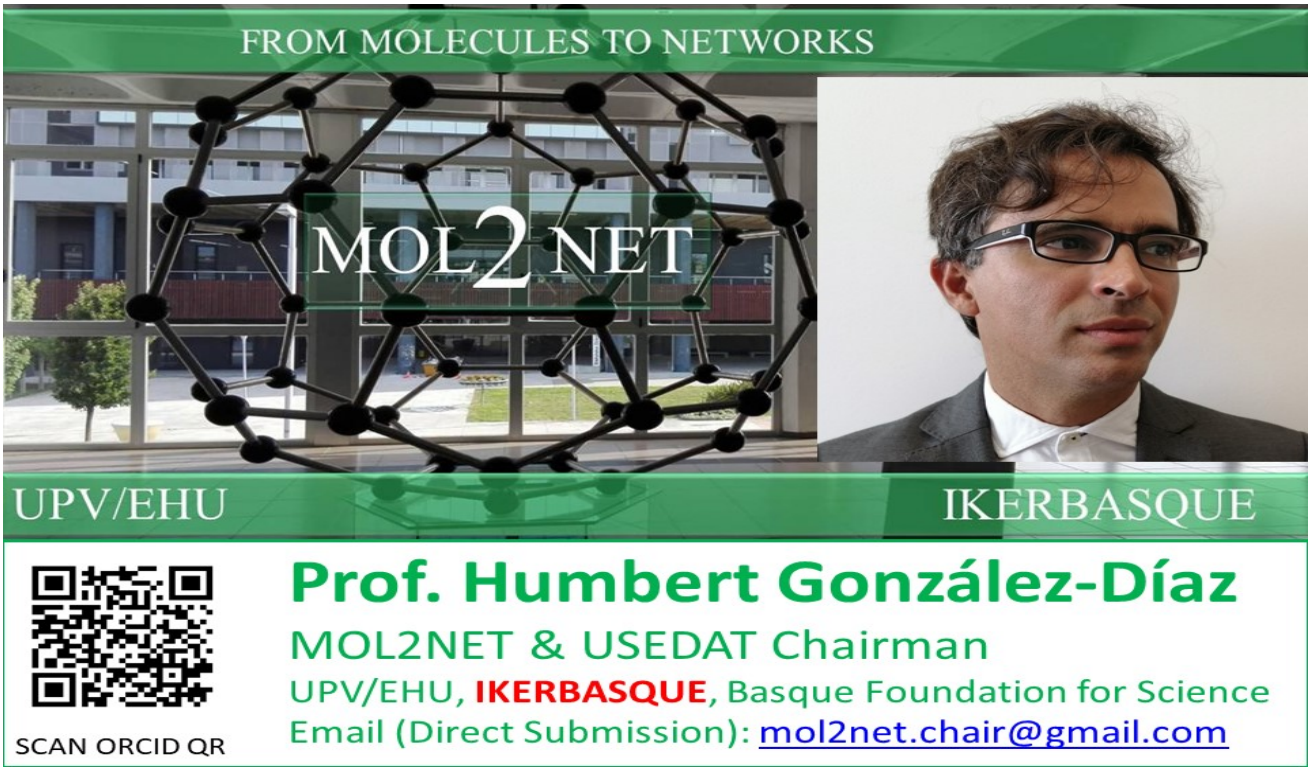


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Dr. Aliuska Duardo-Sanchez (Law.Lic., Ph.D. TICs & Legal Sciences) PANELFIT European Commission Project Manager. Research Group: Chair in Law and The Human Genome, Dept. of Public Law, University of Basque Country (UPV/EHU), Campus Biscay, **Basque Country, Spain.**

**List of Papers (37)**

| Title | Authors |
|---|---|
| permeability coefficients of antitumor drugs | Tomás Silva<br>Miguel Machuqueiro |
| Big Data Database Information Fusion Problem in AI-guided Drug Discovery Full Product Life Cycle Analysis | Viviana Quevedo<br>Bernabe Ortega-Tenezaca<br>Humbert González-Díaz |
| Bridging the gap between lactoferrin and V-ATPase through a multi-stage computational approach | Cátia Santos-Pereira<br>Juliana Rocha<br>Henrique Fernandes<br>Lígia Rodrigues<br>Manuela Côrte-Real<br>Sérgio Sousa |
| Computational Screening and Design of G-quadruplex Ligands Targeting c-MYC in Breast Cancer | Israa Alakhras Aljnadi<br>Bruno L. Victor<br>Alexandra Paulo |
| Design of Indoloisoquinoline derivatives as potential inhibitors of the interaction between c-MYC:G4 and helicase | Bárbara Bruni<br>Alexandra Paulo<br>Bruno Victor |
| Development of new computational workflow for the identification of hAQP5 modulators | Jésssica Marques<br>Bruno L. Victor<br>Graça Soveral |
| Domination, γ-Domination Topological Indices, and φ P-polynomial of Some Chemical Structures Applied for the Treatment of COVID-19 Patients | Hanan Ahmed<br>Anwar Alwardi<br>Ruby Salestina.M<br>Nandapa N.Soner |
| Extension of the stochastic CpHMD method to the CHARMM36m force field | João Sequeira<br>Filipe Rodrigues<br>Telmo Silva<br>Pedro Reis<br>Miguel Machuqueiro |
| First steps towards the identification of a new hybrid antimalarial therapeutic agent targeting PfAQP | Marta S. P. Batista<br>Paulo J. Costa<br>Bruno L. Victor |

| Title | Authors |
|---|---|
| HTVS protocol to identify non-covalent inhibitors of CRM1 | João Sequeira<br>Wolfgang Link<br>Miguel Machuqueiro |
| Identification of membrane PAINS via an optimized computational protocol | Pedro Rafael Magalhães<br>Pedro Reis<br>Diogo Vila-Viçosa<br>Miguel Machuqueiro<br>Bruno Victor |
| Impact of halogen radii in the prediction of hydration free energies using PBSA calculations | Andreia Fortuna<br>Paulo Costa |
| In silico Identification of Potential Sesquiterpene Lactones from SistematX Database against *Schistosoma mansoni* | Chonny Herrera-Acevedo<br>Renata Barros de Menezes<br>Luciana Scotti<br>Ericsson Coy-Barrera<br>Marcus Tullius Scotti |
| *In silico* study of peptidic dendrimers as transfection agents in DNA/RNA vaccines | Filipe E. P. Rodrigues<br>Tamis Darbre<br>Miguel Machuqueiro |
| Ligand-Based and Structure-based virtual screening for the discovery of natural larvicidal against *Aedes aegypti* | Renata Priscila Barros de Menezes<br>Chonny Herrera-Acevedo<br>Luciana Scotti<br>Marcus Tullius Scotti |
| Machine Learning and drug repositioning | Carlos Santolaria |
| Multi-objective screening of non-small cell lung cancer drug candidates | Nhung NGUYEN<br>Nghia TRAN<br>Quang LE<br>Oanh NGUYEN<br>Hai PHAM |
| | Francisco Romero- |

| Title | Authors |
|---|---|
| NEURODAT'21 IBRO-PERC Lecture on Databases in Neurosciences | Duran |
| New antitumor Ru-based compound derivatives optimized using in silico methods | Inês Pires<br>Tânia Morais<br>Miguel Machuqueiro |
| Obtaining QSPR models for the prediction of physicochemical properties of topical antimicrobials | Quan Tran<br>Juan Polo<br>Luis Gomez |
| Opinion on the use of artificial intelligence in drug design | LAURA Acosta<br>Aliuska Sanches |
| Prediction in infection of Helicobacter Pylori with machine learning | Maxim Belii |
| Predictive models as a useful tool for preclinical assay optimization in antimalarial compounds. | Viviana Quevedo<br>Bernabe Ortega-Tenezaca |
| Protein ligand complexation: a computational and experimental approach | Ramon Rial<br>Michael Gonzalez-Durruthy<br>Juan Ruso Beiras |
| PyBindE: Development of a Simple Python MM-PBSA Implementation for Estimating Protein-Protein and Protein-Ligand Binding Energies | João Vitorino<br>Pedro Reis<br>Miguel Machuqueiro |
| *QSARINS Based* Computational Identification of Sars-Cov-2 Main Protease Inhibitors | Juan Castillo-Garit<br>Yudith Cañizares-Carmenate<br>Hai Pham-The<br>Francisco Torrens<br>Facundo Pérez-Giménez |
| Repurposing Drugs to Find HIV-1 Protease Inhibitors: A | Raphael Onuku |

| Title | Authors |
|---|---|
| Virtual Study | Ngozi Nwodo Akachukwu Ibezim |
| Summary for PTML Chemoinformatics Linear Discriminant Analysis classification model for enantioselective reactions | Shan He |
| Summary of Software Testing for Chemoinformatics | Shan He |
| The Catalytic Mechanism of the SARS-Cov-2 Main Protease | Henrique Fernandes, Sérgio Sousa, Nuno Cerqueira |
| Towards a framework to unify in silico methods for endocrine disruptors identification: the inhibition of thyroid peroxidase | Bruno Calçada, Andrea Sartini, Adrian Fowkes, Bruno L. Victor, Paulo Costa |
| Virtual screening based on covalent docking and MM-PBSA calculations predict the drugs neratinib, sacubitril, alprostadil, trandolapril, and florbetapir as promising cruzain inhibitors useful against Chagas disease. | Lucas Costa, Thiago Aquino, Igor Nascimento |