Curriculum vitae

Personal data

Name : Daura Ribera, Xavier
Date of birth : May 1, 1966
Place of Birth : Barcelona, Spain
Nationality : Spanish

Current work address

Institute of Biotechnology and Biomedicine (IBB)
Mòdul B de Recerca, Campus UAB
Universitat Autònoma de Barcelona
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E-mail : Xavier.Daura@uab.cat

Education

Graduation studies:

- Graduated in Biological Sciences (Biochemistry, 5-year degree)
  Universitat Autònoma de Barcelona (UAB), Barcelona, Spain (June 1991).

Post-graduation studies:

- Master in Biotechnology
  Universitat Autònoma de Barcelona (UAB), Barcelona, Spain (September 1993).
- Doctor in Biological Sciences
  Universitat Autònoma de Barcelona (UAB), Barcelona, Spain (February 1996).
  Title: Structural and thermodynamic properties of biomolecules from molecular dynamics simulations. Application to the study of the protein inhibitor of carboxypeptidases, PCI.
  Supervisors: Prof. Francesc X. Avilés and Prof. Enrique Querol, Department of Biochemistry and Molecular Biology.

Positions

From November 2005:
Adjunct Professor at Universitat Autònoma de Barcelona.

From May 2002:
Research Professor at the Catalan Institution for Research and Advanced Studies (ICREA). Head of the Computational Biology Group at the Institute of Biotechnology and Biomedicine of UAB.

April 1996 - April 2002:
Postdoctoral research assistant in the group of Prof. Wilfred F. van Gunsteren, Laboratory of Physical Chemistry, ETH Zürich, Switzerland.

Institutional and academic responsibilities

June 2017 - January 2024:
Coordinator of the Doctoral Program in Bioinformatics of Universitat Autònoma de Barcelona, Universitat de Barcelona, Universitat de Girona, Universitat de Lleida, Universitat Oberta de Catalunya, Universitat Politècnica de Catalunya, Universitat Rovira i Virgili and Universitat de Vic - Universitat Central de Catalunya.

February 2011 - February 2017:
Director of the Institute of Biotechnology and Biomedicine (IBB) of UAB.

January 2005 - January 2011:
Vice-director of the Institute of Biotechnology and Biomedicine (IBB) of UAB.

Commissions and panels

- Memeber of UAB's Permanent Board for Doctorate, 2021 - 2024.
- Member of the working group for the development of a "Strategic and action plan to reduce the risks of selection and dissemination of antimicrobial resistance", National Plan on Antibiotic Resistance, Spain, 2015-2021.
- Coordinator of the Panel for Biomedicine and Life Sciences of the Access Committee of Barcelona Supercomputing Center – Centro Nacional de Supercomputación, 2015-2019.
- Member of three Delegate Commissions of UAB's Governing Council: Research (2011-2017), Knowledge Transfer and Strategic Projects (2012-2017) and Doctorate (2013-2017).
- Member of the Scientific Committee of the Health Sciences Research Institute of the "Germans Trias i Pujol" Foundation (IGTP), 2011-2013.
- Member of the Direction Board of the Spanish Biophysical Society, 2008 - 2012.

Fellowships

- **Fellowship:** CIRIT travel bursary for studies in Fine Chemistry.
  Awarded by: Direcció General de Recerca, Catalan Autonomic Government.
  For: A stay of 3 months in the group of Prof. Dr. Wilfred F. van Gunsteren, ETH Zurich, Switzerland (October - December 1994).
- **Fellowship:** Supercomputing fellowship.
  Awarded by: Fundació Catalana per a la Recerca and CRAY Research, Inc.
  For: A stay of 2 months in the group of Dr. John Carpenter, Cray Research, Inc. Corporate Software Training Center, Minnesota (USA) (October - December 1993).
- **Fellowship:** Support for scientific cooperation with Swedish Institutions.
  Awarded by: Dirección General de Relaciones Culturales y Científicas, Ministerio de Asuntos Exteriores, Spanish Government.
  For: A stay of 3 months in the group of Prof. Dr. Orlando Tapia, Fysikalisk Kemiska Institutionen, Uppsala University, Sweden (June - September 1993).
- **Fellowship:** CIRIT doctoral fellowship for the formation of research personnel in the area of Fine Chemistry.
  Awarded by: Direcció General de Recerca, Catalan Autonomic Government.
  For: Pre-doctoral research (May 1993 - February 1996).
- **Fellowship:** Support for scientific cooperation with Swedish Institutions.
  Awarded by: Dirección General de Relaciones Culturales y Científicas, Ministerio de Asuntos Exteriores, Spanish Government.
  For: A stay of 3 months in the group of Prof. Dr. Orlando Tapia, Fysikalisk Kemiska Institutionen, Uppsala University, Sweden (May - August 1992).

Main project grants as group leader

- **Title:** Quorum sensing regulatory networks in *Stenotrophomonas maltophilia* as targets for therapeutic alternatives to current antibiotics. (StenoQS)
  Funding body: Ministerio de Ciencia, Innovación y Universidades, Spain (Ref. PID2019-111364RB-I00)
  Participant entities: Universitat Autònoma de Barcelona
  Duration: 01.06.2020 - 31.05.2024
  Principal Investigators: Xavier Daura, Daniel Yero
- **Title:** AMB Advanced Therapeutics: Potentiating current antibiotics against life-threatening resistant hospital-acquired infections
  Funding body: "la Caixa" Foundation & Caixa Capital Risk (CaixaImpulse, ref. CI17-00021).
  Participant entities: Universitat Autònoma de Barcelona
  Duration: 01.07.2017 - 31.12.2019
  Principal Investigator: Xavier Daura

- **Title:** Non-essential biological processes in *Stenotrophomonas maltophilia* as targets for the design of new antimicrobial strategies
  Funding body: Ministerio de Ciencia e Innovación, Spain (Ref. BIO2015-66674-R)
  Participant entities: Universitat Autònoma de Barcelona
  Duration: 01.01.2016 - 31.12.2019
  Principal Investigators: Xavier Daura, Isidre Gibert

- **Title:** Proteomic approximation to the determination and analysis of virulence factors in *Stenotrophomonas maltophilia*
  Funding body: Ministerio de Ciencia e Innovación, Spain (Ref. BFU2010-17199)
  Participant entities: Universitat Autònoma de Barcelona
  Duration: 01.01.2011 - 30.06.2014
  Principal Investigator: Isidre Gibert

- **Title:** From genome to antigen: a multidisciplinary approach towards the development of an effective vaccine against *Burkholderia pseudomallei*, the etiological agent of melioidosis – GtA
  Funding body: Fondazione Cariplo, Italy (Contract no. 2009-3577)
  Participant entities: Università degli Studi di Milano (IT), Consiglio Nazionale delle Ricerche (IT), University of Exeter (UK), Fondazione Centro San Raffaele del Monte Tabor (IT), Universitat Autònoma de Barcelona (ES)
  Duration: 01.11.2010 - 30.10.2014
  Principal Investigator at UAB: Xavier Daura

- **Title:** Identification and validation of novel drug targets in Gram-negative bacteria by global search: a trans-system approach – AntiPathoGN
  Funding body: European Commission, Seventh Framework Programme (Contract no. HEALTH-F3-2009-223101)
  Participant Entities: Universitat Autònoma de Barcelona (ES), Institut de Recerca Biomèdica (ES), Infociencia (ES), Microbionta (ES), Proteros Biostructures (DE), InterMed Discovery (DE), Bio-Xtal (F), Fundació Clínic per a la Recerca Biomèdica (ES), Deutsches Krebsforschungszentrum Heidelberg (DE), Anaxomics Biotech (ES), Helmholtz-Zentrum für Infektionsforschung (DE)
  Duration: 01.02.2009 - 31.07.2013
  Project Coordinator: Xavier Daura

- **Title:** Identificación de dianas secundarias y diseño de fármacos para enfermedades relacionadas con el envejecimiento mediante análisis estructural y funcional de rutas biológicas – DrugsForAgeing
  Funding body: Ministerio Educación y Ciencia, Spain (Ref. PSE-010000-2007-1 and PSE-010000-2009-8)
  Participant entities: Infociencia S. L., Infociencia Clinical Research S. L., Universitat Pompeu Fabra, Institut de Recerca Biomèdica de Barcelona, Universitat Autònoma de Barcelona, Consejo Superior de Investigaciones Científicas
  Duration: 01.01.2007 - 31.12.2008 and 01.10.2009 - 30.06.2011
  Principal Investigator at UAB: Xavier Daura

- **Title:** Biologia computacional de polipeptidos: Simulacion de procesos de plegamiento y analisis de interacciones polipeptido-MHC II
  Funding body: Ministerio de Educación y Ciencia, Spain (Ref. BIO2007-62954)
  Participant entities: Universitat Autònoma de Barcelona
  Duration: 01.12.2007 - 30.11.2010
  Principal Investigator: Xavier Daura

- **Title:** Assessment of Structural Requirements in Complement-Mediated Bactericidal Events: Towards a Global Approach to the Selection of New Vaccine Candidates – BacAbs
  Funding body: European Commission, Sixth Framework Programme (Contract no. LSHB-CT-2006-037325)
  Participant entities: Universitat Autònoma de Barcelona (ES), Novartis Vaccines and Diagnostics Srl (IT), ASLA Biotech Ltd. (LV), Bio-Xtal S. A. (FR), Consiglio Nazionale delle Ricerche (IT), Jacobs University Bremen (DE), Università degli Studi di Milano (IT), Universiteit Utrecht (NL), Infociencia S. L. (ES)
  Duration: 01.01.2007 - 30.06.2010
  Project Coordinator: Xavier Daura

- **Title:** Estudio computacional y espectroscópico de los mecanismos de plegamiento y agregación de polipéptidos
  Funding body: Ministerio de Ciencia y Tecnología, Spain (Ref. BIO2003-02848)
  Participant entities: Universitat Autònoma de Barcelona
  Duration: 01.12.2003 - 30.11.2006
  Principal Investigator: Xavier Daura

Teaching experience

Universitat Autònoma de Barcelona, Spain:

- Courses 2019 – 2020 to 2023 – 2024:
  MSc in Bioinformatics (http://mscbioinformatics.uab.cat); lecturer for module 4 (Structure and Function of Proteins and Drug Design).
- Courses 2012 – 2013 to 2018 – 2019:
  MSc in Bioinformatics (http://mscbioinformatics.uab.cat); lecturer for modules 2 (Core Bioinformatics) and 4 (Structure and Function of Proteins and Drug Design).
- Courses 2004 - 2005 to 2008 – 2009:
  Estructura y Función de Proteínas, inter-university doctoral program, Mention of Quality of the Ministerio de Educación y Ciencia, Spanish Government; coordinator and lecturer of the course on "Análisis bioinformático y modelado molecular".

VIII Escuela de Química Teórica de la Universitat de les Illes Balears (http://www.uibcongres.org/congresos/ficha.es.html?cc=262):

- July 9-13, 2012, Palma (Mallorca), Spain. Simulación de Dinámica Molecular; lecturer.

NCCR, Switzerland (http://www.structuralbiology.unizh.ch/):

- 6th, 8th and 10th NCCR Practical Course (January 6-11, 2008; January 10-15, 2010; January 8-13, 2012), Kandersteg, Switzerland. Biomolecular Modelling; lecturer.

Collaborative Computational Project 5 (http://www.ccp5.ac.uk/):

- The CCP5 Methods in Molecular Simulation Summer School 2002 (July 8-16) and 2003 (July 7-15), King's College London, England; 2004 (July 9-17), 2005 (July 11-19) and 2006 (July 17-25), University of Cardiff, Wales; 2007 (July 9-17), 2008 (July 7-15) and 2009 (July 6-14), University of Sheffield, England; 2010 (July 18-27) and 2011 (July, 17-26) Queens University Belfast, Northern Ireland: Advanced Course on Simulation of Organic and Bio Molecules; coordinator and lecturer.

Universitat Pompeu Fabra, Spain:

- Course 2004 - 2005:
  MSc Bioinformatics for Health Sciences; lecturer for the course on Advanced Molecular Simulations.

ETH Zurich, Switzerland.

- Courses 2000 - 2001 and 2001 - 2002:
  Informatikgestützte Chemie III, Computer Simulation in Chemistry and Physics (Chemistry, 7th semester); lecturer.
- Courses 1998 - 1999 to 2001 - 2002:
  Informatikgestützte Chemie III, Computer Simulation in Chemistry and Physics (Chemistry, 7th semester); assistant for practical exercises.
- Courses 1996 - 1997 to 2001 - 2002:
  Informatik I (Chemistry, 1st semester); assistant for practical exercises.

Direction of PhD theses

- Valentin P. Junet. Machine Learning techniques in bioinformatics: From data integration to the development of application-oriented tools. Universitat Autònoma de Barcelona, February 1, 2022. Co-director: José M. Mas.
- Pau M. Muñoz. Bioinformatic study of the antigenic presentation by HLA class II. Universitat Autònoma de Barcelona, January 13, 2014. Co-director: Juan A. Cedano.
- Alejandro Panjkovich. Structure and evolution of protein allosteric sites. Universitat Autònoma de Barcelona, November 7, 2013.

- Güzin Tunca. A virtual screening procedure combining pharmacophore filtering and molecular docking with LIE method. Universitat Autònoma de Barcelona, July 26, 2012.

Organisation of workshops and conferences

- Chair of the Organising Committee of the International Congress of the Spanish Biophysical Society – SBE Barcelona 2012, Barcelona, Spain, July 3-6, 2012 (http://www.sbe-bcn2012.org/).

Oral presentations at workshops and congresses

- One Health Perspectives on Infection and Immunity: Humans, Animals and the Environment, Chiang Mai, Thailand (October 21-22, **2019**). **Invited Address**: *Non-essential functions in Stenotrophomonas maltophilia as targets for therapeutic alternatives to current antibiotics*.
- Learning from each other: Clinical Management and Prevention of Major and Hidden Health Care Problems in Greater Mekong Subregion, Khon Kaen, Thailand (February 12-13, **2018**). **Invited Address**: *Exploring the pan-genome of pathogenic bacteria for the identification of novel antimicrobial targets and vaccine candidates.*
  http://amsoffice.kku.ac.th:50140/file/GYYT440LPA17.pdf
- EFSA Workshop on *Xylella fastidiosa*: knowledge gaps and research priorities for the EU, Brussels, Belgium (November 12-13, **2015**). **Communication**: *Decoding the DSF quorum-sensing system in Xanthomonadaceae: lessons from Stenotrophomonas maltophilia.*
  http://www.efsa.europa.eu/en/events/event/151112a
- 4th Workshop on biomaterials and their interactions with biological and model membranes 2015, Salou, Spain (October 19-21, **2015**). **Invited address**: *Hydroxylation of glycerol dialkyl glycerol tetraethers may enhance membrane fluidity in Archaea adapted to cold environments*.
  http://meeting.softmat.net/program
- XV Congress of the Spanish Biophysical Society, Granada, Spain (June 10-12, **2015**). **Invited address**: *Exploiting protein flexibility to predict the location of allosteric sites*.
  http://www.sbe.es/granada2015/Detailed-program.asp
- IUPAB Congress 2014, Brisbane, Australia (August 3-7, **2014**). **Invited address**: *Exploiting protein flexibility to predict the location of allosteric sites.*
  http://www.iupab2014.org/invited-speakers/xavier-daura/
- EFPIA-IMI-JPIAMR Workshop on Antibiotics and their alternatives – fixing and feeding the pipeline, Brussels, Belgium (April 4, **2014**). **Invited address:** *Identification and validation of novel drug targets in Gram-negative bacteria by global search: a trans-system approach*.
  http://ec.europa.eu/research/health/events-18_en.html
- The 50th Khon Kaen University and 36th Faculty of Associated Medical Sciences Anniversary Celebration Conference. 2013 Infection & Immunity: From Basic to Translational Research, Hua Hin, Thailand (September 21-23, **2013**). **Invited address:** *A bioinformatics approach to the identification of vaccine candidates in the genome of Burkholderia pseudomallei.*
- 4th Congress of the Spanish Proteomics Society, Segovia, Spain (February 8-11, **2011**). **Invited address:** *Computer-aided identification of potential drug targets and vaccine candidates in bacterial proteomes.*
- CESGA HPCN Workshop 2010, Santiago de Compostela, Spain (November 25, **2010**). **Invited address:** *Cribado computacional de compuestos mediante técnicas de dinámica molecular*.
- UNIA Workshop - Pseudomonas aeruginosa: opportunistic pathogen and human infections, Baeza, Spain (November 7-10, **2010**). **Communication:** *Comparative proteomic analysis of collection and clinical-isolate strains of Pseudomonas aeruginosa.*
- CCP5 visitor tour 2010: Invited by the Collaborative Computational Project 5 (CCP5) to give a series of seminars in the UK during a week, at CCLRC Daresbury Laboratory, University of Nottingham, University of Bradford and University of Leeds, October 11-15, **2010**.

- IV Spanish-Portuguese Biophysical Congress, Zaragoza, Spain (July 7-10, **2010**). **Invited address:** *Assessing the structural conservation of protein pockets to study functional and allosteric sites: implications for drug discovery*.
  http://bifi.es/events/biophysics2010/program.html
- ESF Workshop: Novel Approaches in Protein Engineering, Istanbul, Turkey (April 22-25, **2010**). **Invited address:** *Assessing the structural conservation of protein pockets to study functional and allosteric sites: implications for drug discovery.*
  http://www.functionalgenomics.org.uk/sections/activitites/2010/Sezerman/info.htm
- II Xornada Galega de Bioinformática, Santiago de Compostela, Spain (December 4, **2009**). **Invited address:** *Addressing functionally relevant large-scale motions in proteins by molecular-dynamics simulation: The ArtJ case*.
- BSC - IRB Barcelona Conference: Expanding the frontiers of molecular dynamics simulations in biology, Barcelona, Spain (November 23-25, **2009**). **Invited address:** *Polypeptide folding on a conformational-space network*.
  http://mmb.pcb.ub.es/md2009/
- Tyndall/ICHEC/IBM ACAM HPC workshop: Towards microscale molecular simulations with high-performance computing, Dublin, Ireland (October 14-16, **2009**). **Invited address:** *Addressing functionally relevant largescale motions in polypeptides by moleculardynamics simulation*.
- Conference on New Frontiers in Microbiology and Infection: From microbial pathogenesis to the discovery of antivirulence drugs, Les Diablerets, Switzerland (October 4-8, **2009**). **Communication:** *AntiPathoGN: a FP7 project for the discovery of new drug targets in Gram-negative bacteria*.
  http://www.unil.ch/cnfmi/page71825.html
- 1st Portuguese-Spanish-British Joint Biophysics Congress 2008, Lisboa, Portugal (July 10-13, **2008**). **Invited address:** *Polypeptide folding on a conformational-space network: dependence of network topology on the structural discretization procedure*.
- DEISA Symposium: Advancing Extreme Computing in Europe, Edinburgh, UK (April 28-29, **2008**). **Invited address:** *Simulation of Protein Dynamics in Vaccine Research*.
  http://www.deisa.eu/news_events/symposium/Edinburgh2008/
- PepCon2008, Shenzhen, China (April 22-24, **2008**). **Invited address:** *Investigating the Role of Antigen Structure and Dynamics in Complement-Mediated Bactericidity*.
  http://www.bitlifesciences.com/Pepcon2008/Program.htm
- DEISA Training Session, Bologna, Italy (October 29-31, **2007**). **Invited address**: *BacAbsMS: Molecular Simulation in Vaccine Research.*
- MMS06: Methods of Molecular Simulation 2006, Heidelberg, Germany (September 20-22, **2006**). **Invited address**: *Peptide-folding networks.*
- 367. WE-Heraeus-Seminar. Biomolecular Simulation: From Physical Principles to Biological Function, Bad Honnef, Germany (May 22-24, **2006**). **Invited address**: *Aspects of β-peptide folding from molecular-dynamics simulation*.
- eCheminfo Autumn 2005 InterAction Meetings: Protein Folding and Dynamics, Basel, Switzerland (November 8-10, **2005**). **Invited address**: *Aspects of β-peptide folding from molecular-dynamics simulation.*
- 2o Simposio sobre proteínas: Plegamiento, México D. F., Mexico (October 19-21, **2005**). **Invited address**: *Simulaciones por dinámica molecular del plegamiento de polipéptidos.*
  http://bq.unam.mx/~simposio/sspm.html
- XV International BIOMOS Meeting on Biomolecular Simulation, Burg Arras, Germany (August 31-September 2, **2005**). **Invited address**: *The Jarzynski equation: correct; but useful?*
- II Reunión Nacional de Modelización Molecular y Quimioinformática, Barcelona, Spain (June, **2005**). **Invited address**: *Modeling of short protein segments and side chains by fast-growth molecular dynamics*.

- IV Jornadas sobre Procesamiento y Presentación de Antígenos, Sant Andreu de Llavaneres, Spain (June, **2005**). **Invited address**: *Estudios computacionales de MHC clase II.*
- 3rd Portuguese-Spanish Biophysics Congress, Lisboa, Portugal (October 29-November 1, **2004**). **Communication**: *Entropy and free-enthalpy differences from molecular-dynamics simulation and integration over temperature.*
- III Jornadas sobre Procesamiento y Presentación de Antígeno, Segovia, Spain (April, **2004**). **Invited address**: *Modelado de complejos HLA-DR4/péptido mediante simulación molecular: Método y primeros tests.*
- SIMU Workshop: Self organization in (bio)molecular systems, Lyon, France (October 20-22, **2003**). **Invited address**: *Molecular dynamics simulation of peptide folding and aggregation.*
- ICREA-FCR Conference on Bioinformatics. Bioinformatics: Present applications and future challenges, Barcelona, Spain (May 19-21, **2003**). **Invited address**: *Peptide folding: What have we learned from molecular dynamics simulatios?*
- II Jornadas sobre Procesamiento y Presentación de Antígeno, Les Avellanes, Spain (March, **2003**). **Invited address**: *Predicción de interacciones proteína-péptido mediante métodos computacionales.*
- I Reunió de la Xarxa Catalana de Bioinformàtica, Les Avellanes, Spain (November, **2002**). **Invited address**: *The driving force for peptide folding.*
- CECAM Workshop on the Dynamics of Proteins on a Continuous Energy Landscape, Lyon, France (May 21-24, **2002**). **Invited address**: *The driving force for peptide folding*.
- I Reunión Nacional de Modelización Molecular y Quimioinformática, Barcelona, Spain (March, **2002**). **Invited address**: *Plegamiento de péptidos: Sensibilidad de observables experimentales a la distribución de conformaciones subyacente.*
- First KIAS Conference on Protein Structure and Function: Protein Folding in Post-Genome Era, Seoul, Korea (November 28-30, **2001**). **Invited address**: *New perspective on peptide folding from molecular dynamics simulations.*
- XXII Congreso de la Sociedad Española de Bioquímica y Biología Molecular, Pamplona, Spain (September, **1999**). **Communication**: *Simulación Molecular y Plegamiento de Proteínas. Una cuestión de tiempo.*
- 2nd International Workshop on Structural Characterization of Proteins by NMR, X-Ray Diffraction and Computational Methods, Verona, Italy (February 17-20, **1999**). **Invited address**: *Peptide Folding: When Simulation Meets Experiment.*
- C4 Workshop on Use of Fast Computers in Molecular Chemistry, Zurich, Switzerland (November, **1998**). **Invited address**: *Peptide Folding: When Simulation Meets Experiment.*
- 1998 Conference on Computational Physics, Granada, Spain (September 2-5, **1998**). **Communication:** *Reversible Peptide Folding in Solution by Molecular Dynamics Simulation.*

Patents

- **Title:** Enhanced antibiotic composition
  Inventors: I. Gibert, X. Daura, D. Yero, M. Indarte, O. Conchillo
  Applicant: Universitat Autònoma de Barcelona, Institució Catalana de Recerca i Estudis Avançats
  Priority date: 14.05.2015
  International application No.: PCT/EP2016/060664
  International filing date: 12.05.2016
  Publication number: WO/2016/180919 A1
  Publication date: 17.11.2016
  European Patent No.: EP 3294317
  Publication date: 09.12.2020

- **Title:** Klotho fusion protein and uses thereof
  Inventors: M. Chillón, J. Esandi, B. Almolda, A. Bosch, O. Conchillo-Solé, X. Daura, J. Giraldo, P. V. Renault
  Applicant: Universitat Autònoma de Barcelona, Fundació Hospital Universitari Vall d'Hebron - Institut de Recerca, Institució Catalana de Recerca i Estudis Avançats
  EU application No.: EP23382593.4
  Filing date: 15.06.2023

ID in databases

ResearcherID: C-9275-2009

ORCID: 0000-0001-9235-6730

Scopus Author ID: 6701320814

Research articles and reviews in peer-reviewed journals

123. A. C. Gómez, C. Horgan, D. Yero, M. Bravo, **X. Daura**, M. O'Driscoll, I. Gibert*, T. P. O'Sullivan*. Synthesis and evaluation of aromatic BDSF bioisosteres on biofilm formation and colistin sensitivity in pathogenic bacteria. *Eur. J. Med. Chem.* **2023**, 261: 115819 (doi: 10.1016/j.ejmech.2023.115819).
122. P. Coto-Segura, C. Segú-Vergés, A. Martorell*, D. Moreno-Ramírez, G. Jorba, V. Junet, F. Guerri, **X. Daura**, B. Oliva, C. Cara, O. Suárez-Magdalena, S. Abraham, J. M. Mas. A quantitative systems pharmacology model for certolizumab pegol treatment in moderate-to-severe psoriasis. *Front. Immunol.* **2023**, 14: 1212981 (doi: 10.3389/fimmu.2023.1212981).
121. X. Coves, M. Bravo, P. Huedo, O. Conchillo-Solé, A. C. Gómez, A. Esteve-Codina, M. Dabad, M. Gut, **X. Daura**, D. Yero*, I. Gibert*. A *Stenotrophomonas maltophilia* TetR-Like Transcriptional Regulator Involved in Fatty Acid Metabolism Is Controlled by Quorum Sensing Signals. *Appl. Environ. Microbiol.* **2023**, 89(6): e00635-23 (doi: 10.1128/aem.00635-23).
120. V. Junet, P. Matos-Filipe, J. M. García-Illarramendi, E. Ramírez, B. Oliva, J. Farrés*, **X. Daura***, J. M. Mas, R. Morales. A decision support system based on artificial intelligence and systems biology for the simulation of pancreatic cancer patient status. *CPT-Pharmacometrics & Systems Pharmacology* **2023**, 12(7): 916–928 (doi: 10.1002/psp4.12961).
119. **X. Daura***, O. Conchillo-Solé. On Quality Thresholds for the Clustering of Molecular Structures. *J. Chem. Inf. Model.* **2022**, 62, 5738−5745 (doi: 10.1021/acs.jcim.2c01079).
118. A. C. Gómez, T. Lyons, U. Mamat, D. Yero, M. Bravo, **X. Daura**, O. Elshafee, S. Brunke, C. G. M. Gahan, M. O'Driscoll, I. Gibert*, T. P. O'Sullivan*. Synthesis and evaluation of novel furanones as biofilm inhibitors in opportunistic human pathogens. *Eur. J. Med. Chem.* **2022**, 242, 114678 (doi: 10.1016/j.ejmech.2022.114678).
117. V. Junet, **X. Daura***. CNN-PepPred: An open-source tool to create convolutional NN models for the discovery of patterns in peptide sets. Application to peptide-MHC class II binding prediction. *Bioinformatics* **2021**, 37(23): 4567-4568 (doi: 10.1093/bioinformatics/btab687).
116. N. Serna, J. V. Carratala, O. Conchillo-Solé, C. Martinez-Torro, U. Unzueta, R. Mangues, N. Ferrer-Miralles, **X. Daura***, E. Vazquez, A. Villaverde*. Antibacterial Activity of T22, a Specific Peptidic Ligand of the Tumoral Marker CXCR4. *Pharmaceutics* **2021**, 13(11): 1922 (doi: 10.3390/pharmaceutics13111922).
115. J. R. Gutierrez-Casares*, J. Quintero, G. Jorba*, V. Junet, V. Martinez, T. Pozo-Rubio, B. Oliva, **X. Daura**, J. M. Mas, C. Montoto. Methods to Develop an in silico Clinical Trial: Computational Head-to-Head Comparison of Lisdexamfetamine and Methylphenidate. *Front. Psychiatry* **2021**, 12: 741170 (doi: 10.3389/fpsyt.2021.741170).
114. V. Junet, J. Farrés, J. M. Mas*, **X. Daura***. CuBlock: a cross-platform normalization method for gene-expression microarrays. *Bioinformatics* **2021**, 37(16): 2365-2373 (doi: 10.1093/bioinformatics/btab105).
113. D. Yero, M. Diaz-Lobo, L. Costenaro, O. Conchillo-Solé, A. Mayo, M. Ferrer-Navarro, M. Vilaseca, I. Gibert*, **X. Daura***. The *Pseudomonas aeruginosa* substrate-binding protein Ttg2D functions as a general glycerophospholipid transporter across the periplasm. *Communications Biology* **2021**, 4(1): 448 (doi: 10.1038/s42003-021-01968-8).

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