

1 Información personal

Nombre y Apellidos José Luis Gelpí Buchaca
Grado académico Doctor en Química

1.1 Posiciones actuales

Institución Universidad de Barcelona
Departamento Bioquímica y Biomedicina Molecular
Posición Catedrático
Inicio 25 Mayo 2021

Institución Barcelona Supercomputing Center
Dept Life Sciences
Posición Jefe de grupo
Inicio Abril 2006

2 Proyectos competitivos activos

2.1 Proyectos de investigación como IP o Co-IP

1. *EUCAIM. European Federation for Cancer Images.* DIGITAL-2022-CLOUD-AI-02-CANCER-IMAG. E.C 101100633. Importe €496,301. Período 2023-2026
2. *MDDDB. Molecular Dynamics Data Bank. The European Repository for Biosimulation Data.* HORIZON-INFRA-2022-DEV-01 E.C. 101094651. Importe €429,850. Período 2023-2026. Inv. principales. JL Gelpí. & Salvador Capella-Gutierrez (BSC)
3. *BioExcel-3 Centre of Excellence for Computational Biomolecular Research.* HORIZON-EUROHPC-JU-2021-COE-01. E. C. 101093290. Importe: €368,750. Período: 2023-2026. Inv. principales. JL Gelpí. & Salvador Capella-Gutierrez (BSC)
4. *EuroScienceGateway. leveraging the European compute infrastructures for data-intensive research guided by FAIR principles.* HORIZON-INFRA-2021-EOSC-01-04. E.C. 101057388. Importe €79,500. Período 2022-2025
5. *Disc4All. Training network to advance integrated computational simulations in translational medicine, applied to intervertebral disc degeneration.* MSCA-ITN-ETN. E.C. 955735. Importe: €501,809. Período: 2020-2025. Inv. principales: JL Gelpí & Mariano Vazquez (BSC)

2.2 Proyectos de investigación participados activos

1. *Bridging Gaps in Mental Health Support: A Comprehensive European Strategy.* 9P2CL1 - HE – Health. Importe: €575.000,00. Período: 2025-2029. Inv. principal: Karim Lekadir (UB)
2. *RadioVal. International Clinical Validation of Radiomics Artificial Intelligence for Breast Cancer Treatment Planning.* 9P2CL1 - HE – Health, Importe: €801,250. Período: 2022-2026. Inv. principal: Karim Lekadir (UB)

3. *Youth-GEMs. Gene Environment interactions in Mental health trajectories of Youth.* 9P2CL1 - HE – Health. E.C. 101057182. Importe: €708,125. Período: 2022-2027. Inv. principal: Karim Lekadir (UB)
4. *HappyMums. Understanding, predicting, and treating depression in pregnancy to improve mothers and offspring mental health outcomes.* 9P2CL1 - HE – Health. E.C. 101057390. Importe: €938,306. Período: 2022-2026. Inv. principal: Karim Lekadir (UB)
5. *DataTools4Hearth. A European Health Data Toolbox for Enhancing Cardiology Data Interoperability, Reusability and Privacy.* HORIZON-HLTH-2021-TOOL-06-03. E.C. 101057849. Importe: €1,183,750. Período: 2022-2026. Inv. principal: Karim Lekadir (UB)
6. *EuCanImage. A European Cancer Image Platform Linked to Biological and Health Data for Next-Generation Artificial Intelligence and Precision Medicine in Oncology.* HORIZON 2020. H2020-SC1-HEALTH. E.C. 9523103. Importe: €1,278,125.00. Período: 2020-2025. Inv. principal. Karim Lekadir (UB)

2.3 Otros convenios de investigación

1. Characterization of the stability of antigen constructs using high performance computing. Research agreement. Laboratorios HIPRA, S.A. 2022-23
2. Preclinical development of innovative mRNA/MVA vaccines against SARS-CoV2 (COVARNA). License Agreement. Laboratorios HIPRA, S.A. 2021-2023

3 Publicaciones (10 años)

3.1 Indicadores Bibliograficos

3.2 Web of Science

Total no. of citas: **9.888**

Promedio cit. /año (últimos 5 años): **819,6**

h-index: **39**

3.3 Google Scholar

Total no. of citas: **26.745**

Promedio cit. /año (últimos 5 años): **3.266**

h-index: **63**

3.4 Publicaciones en revista.

(* I.F. > 9, ** I.F. > 25, & Autor de correspondencia)

1. Maas, L, Contreras-Meca, C, Ghezzi S, Belmans F, Corsi A, Cant J, Vos W, Bobowicz M, Rygusik M, Laski DK, Annemans L, Hilgsmann M, **EuCanImage Working Group incl Gelpi J.L.** (2025) Cost-effectiveness analysis of artificial intelligence (AI) in earlier detection of liver lesions in cirrhotic patients at risk of hepatocellular carcinoma in Italy *J Med Econ* 28(1):1023-1036. doi: 10.1080/13696998.2025.2525006
2. ** Amaro RE et al. (2025) The need to implement FAIR principles in biomolecular simulations *Nat Methods*; 22(4):641-645. doi: 10.1038/s41592-025-02635-0.
3. Martí-Bonmatí L, Blanquer I, Tsiknakis M, Tsakou G, Martinez R, Capella-Gutierrez S, Zullino S, Meszaros J, Bron EE, **Gelpi JL**, Riklund K, Chaabane L, Schlemmer HP, Aznar M, Serrano Candelas P, Gordebeke P, Hierath M; EUCAIM Consortium; European Society of Radiology. (2025) Empowering cancer research in Europe: the EUCAIM cancer imaging infrastructure. *Insights Imaging*. 16(1):47. doi: 10.1186/s13244-025-01913-x.
4. Marcos-Villar L, Perdiguero B, López-Bravo M, Zamora C, Sin L, Álvarez E, Sorzano CÓS, Sánchez-Cordón PJ, Casasnovas JM, Astorgano D, García-Arriaza J, Anthiya S, Borrajo ML, Lou G, Cuesta B, Franceschini L, **Gelpí JL**, Thielemans K, Sisteré-Oró M, Meyerhans A, García F, Esteban I, López-Bigas N, Plana M, Alonso MJ, Esteban M, Gómez CE. Heterologous mRNA/MVA delivering trimeric-RBD as effective vaccination regimen against SARS-CoV-2: COVARNA Consortium. (2024) *Emerg Microbes Infect*. 3(1):2387906. doi: 10.1080/22221751.2024.2387906.
5. & Martin-del-Pico, E; **Gelpi J.L.**; Capella-Gutierrez, S. FAIRsoft - A practical implementation of FAIR principles for research software. 2024 *Bioinformatics* 40(8):btac464. doi: 10.1093/bioinformatics/btac464.
6. Bayarri G, Andrio P, **Gelpí JL**, Hospital A, Orozco M. Using interactive Jupyter Notebooks and BioConda for FAIR and reproducible biomolecular simulation workflows (2024) *PLoS Comput Biol* 20(6):e1012173. doi: 10.1371/journal.pcbi.1012173.
7. Marcos-Villar L, Perdiguero B, Anthiya S, Borrajo ML, Lou G, Franceschini L, Esteban I, Sánchez-Cordón PJ, Zamora C, Sorzano CÓS, Jordá L, Codó L, **Gelpí JL**, Sisteré-Oró M, Meyerhans A, Thielemans K, Martínez-Jiménez F, López-Bigas N, García F, Alonso MJ, Plana M, Esteban M, Gómez CE. Marcos-Villar L, Perdiguero B, Anthiya S, Borrajo ML, Lou G, Franceschini L, Esteban I, Sánchez-Cordón PJ, Zamora C, Sorzano CÓS, Jordá L, Codó L, Gelpí JL, Sisteré-Oró M, Meyerhans A, Thielemans K, Martínez-Jiménez F, López-Bigas N, García F, Alonso MJ, Plana M, Esteban M, Gómez CE. (2024) *NPI Vaccines* 9(1):53. doi: 10.1038/s41541-024-00838-8
8. Reinikainen J, Palosaari T, Canosa-Valls AJ, Schmidt CO, Wissa R, Chadavada S, Codó L, **Gelpí JL**, Joseph B, van der Lugt A, Pacella E, Petersen SE, Pujadas ER, Szabo L, Zeller

- T, Niiranen T, Lekadir K, Kuulasmaa K. Cohort Profile: The Cardiovascular Research Data Catalogue. (2024) *Int J Epidemiol*. 53(1):dyad175. doi: 10.1093/ije/dyad175.
9. * Salgado H, Gama-Castro S, Lara P, Mejia-Almonte C, Alarcón-Carranza G, López-Almazo AG, Betancourt-Figueroa F, Peña-Loredo P, Alquicira-Hernández S, Ledezma-Tejeida D, Arizmendi-Zagal L, Mendez-Hernandez F, Diaz-Gomez AK, Ochoa-Praxedis E, Muñiz-Rascado LJ, García-Sotelo JS, Flores-Gallegos FA, Gómez L, Bonavides-Martínez C, Del Moral-Chávez VM, Hernández-Alvarez AJ, Santos-Zavaleta A, Capella-Gutierrez S, **Gelpi JL**, Collado-Vides J. RegulonDB v12.0: a comprehensive resource of transcriptional regulation in *E. coli* K-12. *Nucleic Acids Res*. 2024 Jan 5;52(D1):D255-D264. doi: 10.1093/nar/gkad1072.
 10. * Beltrán D, Hospital A, **Gelpi JL**, Orozco M. A new paradigm for molecular dynamics databases: the COVID-19 database, the legacy of a titanic community effort (2024) *Nucleic Acids Res*. 52(D1):D393-D403. doi: 10.1093/nar/gkad991.
 11. Corvi JO, McKittrick A, Fernández JM, Fuenteslópez CV, **Gelpi JL**, Ginebra MP, Capella-Gutierrez S, Hakimi O. DEBBIE: The Open Access Database of Experimental Scaffolds and Biomaterials Built Using an Automated Text Mining Pipeline. (2023) *Adv Health Mater*. 12(25):e2300150. doi: 10.1002/adhm.202300150.
 12. Kondylakis H, Kalokyri V, Sfakianakis S, Marias K, Tsiknakis M, Jimenez-Pastor A, Camacho-Ramos E, Blanquer I, Segrelles JD, López-Huguet S, Barelle C, Kogut-Czarkowska M, Tsakou G, Siopis N, Sakellariou Z, Bizopoulos P, Drossou V, Lalas A, Votis K, Mallol P, Marti-Bonmati L, Alberich LC, Seymour K, Boucher S, Ciarrocchi E, Fromont L, Rambla J, Harms A, Gutierrez A, Starmans MPA, Prior F, Gelpi JL, Lekadir K. Data infrastructures for AI in medical imaging: a report on the experiences of five EU projects. *Eur Radiol Exp*. 2023 May 8;7(1):20. doi: 10.1186/s41747-023-00336-x.
 13. Esteban I, Pastor-Quiñones C, Usero L, Aurrecoechea E, Franceschini L, Esprit A, **Gelpi JL**, Martínez-Jiménez F, López-Bigas N, Breckpot K, Thielemans K, Leal L, Gómez CE, Sisteré-Oró M, Meyerhans A, Esteban M, Alonso MJ, García F, Plana M; COVARNA Consortium. Assessment of Human SARS CoV-2-Specific T-Cell Responses Elicited In Vitro by New Computationally Designed mRNA Immunogens (COVARNA) (2023) *Vaccines (Basel)* 12(1):15. doi: 10.3390/vaccines12010015.
 14. Suriñach A, Hospital A, Westermaier Y, Jordà L, Orozco-Ruiz S, Beltrán D, Colizzi F, Andrio P, Soliva R, Municoy M, **Gelpi JL**, Orozco M. High-Throughput Prediction of the Impact of Genetic Variability on Drug Sensitivity and Resistance Patterns for Clinically Relevant Epidermal Growth Factor Receptor Mutations from Atomistic Simulations. (2023) *J Chem Inf Model*, 63(1):321-334. doi: 10.1021/acs.jcim.2c01344.
 15. Corvi JO, McKittrick A, Fernández JM, Fuentes-lópez CV, **Gelpi JL**, Ginebra MP, Capella-Gutierrez S, Hakimi O. DEBBIE: The Open Access Database of Experimental Scaffolds and Biomaterials Built Using an Automated Text Mining Pipeline (2023) *Adv Health Mater*. 10:e2300150. doi: 10.1002/adhm.202300150.
 16. ** Nadeu F*, Royo R*, Massoni-Badosa R, Playa-Albinyana H, et al. Detection of early seeding of Richter transformation in chronic lymphocytic leukemia. (2022) *Nature Med*. 28(8):1662-1671. doi: 10.1038/s41591-022-01927-8.
 17. * Wiczór M, Genna V, Aranda J, Badia RM, **Gelpi JL**, Gapsys V, de Groot BL, Lindahl E, Municoy M, Hospital A, Orozco M. Pre-exascale HPC approaches for molecular dynamics simulations. Covid-19 research: A use case. (2022) *Wiley Interdiscip Rev Comput Mol Sci*. 30:e1622. doi: 10.1002/wcms.1622.
 18. * Royo R, Magnano L, Delgado J, Ruiz-Gil S, **Gelpi JL**, Heyn H, Taylor MA, Stankovic T, Puente XS, Nadeu F, Campo E. ATM germline variants in a young adult with chronic lymphocytic leukemia: 8 years of genomic evolution. (2022) *Blood Cancer J*. 12(6):90. doi: 10.1038/s41408-022-00686-6.

19. &* Bayarri G, Andrio P, Hospital A, Orozco M, **Gelpí JL**. BioExcel Building Blocks Workflows (BioBB-Wfs), an integrated web-based platform for biomolecular simulations. (2022) *Nucleic Acids Res.* 50(W1): W99-W107. doi: 10.1093/nar/gkac380.
20. & Bayarri G, Andrio P, Hospital A, Orozco M, **Gelpí JL**. BioExcel Building Blocks REST API (BioBB REST API), programmatic access to interoperable biomolecular simulation tools (2022) *Bioinformatics*. doi: 10.1093/bioinformatics/btac316.
21. Mariani N, Borsini A, Cecil CAM, Felix JF, Sebert S, Cattaneo A, *et al.* Identifying causative mechanisms linking early-life stress to psycho-cardio-metabolic multi-morbidity: The EarlyCause project (2021) *PLoS One*. 16(1):e0245475. doi: 10.1371/journal.pone.0245475
22. Devriendt T, Ammann C, Asselbergs F, Bernier A, Costas R, *et al.* *An agenda-setting paper on data sharing platforms: euCanSHare workshop* (2021) *Open Res Europe* 2021, 1:80 doi:10.12688/openreseurope.13860.2
23. ** Yakneen S *et al.* **PCAWG Technical Working Group incl JLGelpi**, Gertz M, Korbel JO, PCAWG Consortium. (2020) Butler enables rapid cloud-based analysis of thousands of human genomes. *Nat Biotechnol*. 38(3):288-292 doi: 10.1038/s41587-019-0360-3
24. ** **ICGC/TCGA Pan-Cancer Analysis of Whole Genomes Consortium (inc. JL Gelpi)**. (2020) Pan-cancer analysis of whole genomes. *Nature* 578(7793):82-93. doi: 10.1038/s41586-020-1969-6.
25. Zivanovic S, Bayarri G, Colizzi F, Moreno D, **Gelpí JL**, Soliva R, Hospital A, Orozco M (2020) Bioactive Conformational Ensemble Server and Database. A Public Framework to Speed Up In Silico Drug Discovery. *J Chem Theory Comput*. 6(10):6586-6597 doi: 10.1021/acs.jctc.0c00305.
26. * Hakimi O, **Gelpi JL**, Krallinger M, Curi F, Repchevsky D, Ginebra M-P (2020) The Devices, Experimental Scaffolds, and Biomaterials Ontology (DEB): A Tool for Mapping, Annotation, and Analysis of Biomaterials Data. *Avd. Funct. Mat.* 30. 1909910. Doi: 10.1002/adfm.201909910.
27. Lamprecht A-L., Garcia L, Kuzak M, Martinez C, Arcila R, Martin Del Pico E *et al.* (2019) Towards FAIR principles for research software. *Data Sci.* 3, (1), 37-59. Doi: 10.3233/DS-190026.
28. * Altenhoff AM, Garrayo-Ventas J, Cosentino S, Emms D, Glover NM, *et al.* (2020) The Quest for Orthologs benchmark service and consensus calls in 2020. *Nucleic Acids Res.* 48 (W1), W538–W545. Doi: 10.1093/nar/gkaa30.
29. * Sati S, Bonev B, Szabo Q, Jost D, Bensadoun P, Serra F, Loubiere V, *et al.* (2020) 4D Genome Rewiring during Oncogene-Induced and Replicative Senescence. *Mol Cell*. 78, 522–538. Doi: 10.1016/j.molcel.2020.03.007.
30. & Andrio P, Hospital A, Conejero J, Jordá L, Del Pino M, Codo L, Soiland-Reyes S, Goble C, Lezzi D, Badia RM, Orozco M, **Gelpi JL**. (2019). BioExcel Building Blocks, a software library for interoperable biomolecular simulation workflows. *Sci Data*.10, 6(1):169. doi: 10.1038/s41597-019-0177-4.
31. * Buitrago D, Codó L, Illa R, de Jorge P, Battistini F, Flores O, Bayarri G, Royo R, *et al.* (2019) Nucleosome Dynamics: a new tool for the dynamic analysis of nucleosome positioning. *Nucleic Acids Res.* 10, 47(18):9511-9523. doi: 10.1093/nar/gkz759.
32. Battistini F, Hospital A, Buitrago D, Gallego D, Dans PD, **Gelpí JL**, Orozco M. (2019) How B-DNA Dynamics Decipher Sequence-Selective Protein Recognition. *J Mol Biol*. 431(19):3845-3859. doi: 10.1016/j.jmb.2019.07.021.
33. * Hospital A, Battistini, F, Soliva R, **Gelpi, JL**, Orozco M (2019) Surviving the deluge of biosimulation data *Wiley Int. Reviews-Computational Molecular Science* 10(3), e1449 (Review) Doi: 10.1002/wcms.1449.

34. * Ison J, Ienasescu H, Chmura P, Rydza E, Ménager H, Kalaš M, *et al.* (2019) The bio.tools registry of software tools and data resources for the life sciences. *Genome Biol.* 20(1):164. doi: 10.1186/s13059-019-1772-6.
35. * Aterido A, Cañete JD, Tornero J, Ferrándiz C, Pinto JA, *et al.* (2019) Genetic variation at the glycosaminoglycan metabolism pathway contributes to the risk of psoriatic arthritis but not psoriasis. *Ann Rheum Dis.* 78(3). 355-364. doi: 10.1136/annrheumdis-2018-214158.
36. Delgado J, Naro D, Llorente S, **Gelpí JL**, Royo R (2018) Metadata to Describe Genomic Information. *Stud Health Technol Inform.* 247:621-625.
37. Hospital A, Candotti M, **Gelpí JL**, Orozco M (2017) The Multiple Roles of Waters in Protein Solvation. *J Phys Chem B.* 121(15):3636-3643. doi: 10.1021/acs.jpcc.6b0967.
38. Pinheiro S, Soteras I, **Gelpí JL**, Dehez F, Chipot C, Luque FJ, Curutchet C (2017). Structural and energetic study of cation- π -cation interactions in proteins. *Phys. Chem. Chem. Phys.* 12, 19(15):9849-9861. DOI: 10.1039/c6cp08448f.
39. &* López-Ferrando V, Gazzo A, de la Cruz X, Orozco M, **Gelpí JL** (2017). PMut. A web-based tool for the annotation of pathological variants on proteins, 2017 update. *Nucleic Acids Res.* 45(W1), W222-W228. DOI: 10.1093/nar/gkx313.
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41. Jiménez RC, Kuzak M, Alhamdoosh M, Barker M, Batut B, Borg M, *et al.* (2017) Four simple recommendations to encourage best practices in research software. *F1000Res.* pii: ELIXIR-876. doi: 10.12688/f1000research.11407.1.
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43. &* Hospital A, Andrio P, Cugnasco C, Codo L, Becerra Y, Dans PD, Battistini F *et al.* (2016) BIGNASim: a NoSQL database structure and analysis portal for nucleic acids simulation data. *Nucleic Acids Res.* 44(D1): D272-8.
44. **Ivani I, Dans PD, Noy A, Pérez A, Faustino I, Hospital A, Walther J, Andrio P, *et al.* (2016) ParmBSC1: A Refined Force-Field for DNA simulations. *Nat Methods.* 13(1):55-8. doi: 10.1038/nmeth.3658
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3.4.1 Publicaciones adicionales como parte del consorcio PCAWG

50. ** Rodriguez-Martin B *et al.* (Author Correction) Pan-cancer analysis of whole genomes identifies driver rearrangements promoted by LINE-1 retrotransposition (2023). *Nat Genet.* 55(6):1080. doi: 10.1038/s41588-023-01319-9.
51. ** Akdemir KC *et al.* (Author Correction) Disruption of chromatin folding domains by somatic genomic rearrangements in human cancer. (2023) *Nat Genet.* 55(6):1079. doi: 10.1038/s41588-023-01318-w.
52. ** Zapotka M *et al.* (Author Correction) The landscape of viral associations in human cancers. (2023) *Nat Genet.* 55(6):1077. doi: 10.1038/s41588-023-01316-y.
53. ** Cortés-Ciriano I *et al.* (Author Correction) Comprehensive analysis of chromothripsis in 2, 658 human cancers using whole-genome sequencing. *Nat Genet.*, 55(6):1076. doi: 10.1038/s41588-023-01315-z.
54. ** Yuan Y *et al.* (Author Correction) Comprehensive molecular characterization of mitochondrial genomes in human cancers. (2023). *Nat Genet.*, 55(6):1078. doi: 10.1038/s41588-023-01317-x.
55. ** Alexandrov LB *et al.* (Author Correction) The repertoire of mutational signatures in human cancer. (2023) *Nature.* 614(7948):E41. doi: 10.1038/s41586-022-05600-5.
56. ** Li Y *et al.* (Author Correction) Patterns of somatic structural variation in human cancer genomes. (2023) *Nature*, 614(7948):E38. doi: 10.1038/s41586-022-05597-x.
57. ** Gerstung M *et al.* (Author Correction) The evolutionary history of 2, 658 cancers. (2023) *Nature*, 614(7948):E42. doi: 10.1038/s41586-022-05601-4.
58. Rheinbay E *et al.* (Author Correction) Analyses of non-coding somatic drivers in 2, 658 cancer whole genomes. (2023) *Nature.* 614(7948):E40. doi: 10.1038/s41586-022-05599-9.
59. ** PCAWG Transcriptome Core Group *et al.* (Author Correction) Genomic basis for RNA alterations in cancer. (2023) *Nature*, 614(7948):E37. doi: 10.1038/s41586-022-05596-y.
60. Carlevaro-Fita J *et al.* (Author Correction) Cancer LncRNA Census reveals evidence for deep functional conservation of long noncoding RNAs in tumorigenesis. (2022) *Commun Biol.* , 5(1):1347. doi: 10.1038/s42003-022-03769-z.
61. * Rubanova Y *et al.* (Author Correction) Reconstructing evolutionary trajectories of mutation signature activities in cancer using TrackSig. (2022) *Nat Commun.*, 13(1):7567. doi: 10.1038/s41467-022-32336-7.
62. * Sieverling L *et al.* (Author Correction) Genomic footprints of activated telomere maintenance mechanisms in cancer. (2022) *Nat Commun.* 13(1):7574. doi: 10.1038/s41467-022-32328-7.
63. * Shuai S, *et al.* (Author Correction) Combined burden and functional impact tests for cancer driver discovery using DriverPower. (2022) *Nat Commun.* 13(1):7571. doi: 10.1038/s41467-022-32343-8.
64. * Cmero M *et al.* (Author Correction) Inferring structural variant cancer cell fraction (2022) *Nat Commun.*, 13(1):7568. doi: 10.1038/s41467-022-32338-5
65. * Jiao W *et al.* (Author Correction) A deep learning system accurately classifies primary and metastatic cancers using passenger mutation patterns. (2022) *Nat Commun.* 13(1):7573. doi: 10.1038/s41467-022-32329-6.
66. * Paczkowska M *et al.* (Author Correction) Integrative pathway enrichment analysis of multivariate omics data. (2022) *Nat Commun.* 13(1):7570. doi: 10.1038/s41467-022-32342-9.
67. * Zhang Y *et al.* (Author Correction) High-coverage whole-genome analysis of 1220 cancers reveals hundreds of genes deregulated by rearrangement-mediated cis-

- regulatory alterations. (2022) *Nat Commun.* 13(1):7572. doi: 10.1038/s41467-022-32333-w.
68. * Bhandari V *et al.* (Author Correction) Divergent mutational processes distinguish hypoxic and normoxic tumours. (2022) *Nat Commun.* 13(1):7569. doi: 10.1038/s41467-022-32339-4.
 69. ** Reyna MA *et al.* (Author Correction) Pathway and network analysis of more than 2500 whole cancer genomes. (2022) *Nat Commun.* 13(1):7566. doi: 10.1038/s41467-022-32334-9.
 70. * Bailey MH *et al.* Retrospective evaluation of whole exome and genome mutation calls in 746 cancer samples. (2020) *Nat Commun.* 11(1):4748. doi: 10.1038/s41467-020-18151-y.
 71. * Li CH *et al.* (2020) Sex differences in oncogenic mutational processes. *Nat Commun.* 11(1):4330. doi: 10.1038/s41467-020-17359-2.10.1038.

3.5 Preprints

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4 Contribuciones relevantes a conferencias. Charlas por invitación (10 años)

1. MDDb. Molecular Dynamics Data Bank. The Repository for Biosimulation Data. Pushing the frontiers of molecular dynamics simulations. CECAM Lausanne. Switzerland. Oct 2024.
2. AI modelling demo: pros & cons. Del camino de la captura del dato a la generación de conocimiento. 2nd Taulí Health Artificial Intelligence Symposium. Sabadell (Barcelona) June 2023.
3. OpenEBench. The Open Data ELIXIR benchmarking platform. ELIXIR's IDP Community Meeting Dublin August 2022
4. e-Infrastructures. Integrative approach to the theoretical study of chromatin CECAM. Zaragoza. Spain June 2022
5. ELIXIR, Infraestructura europea de para bioinformática. Encuentro de trabajo de Infraestructuras de Investigación internacionales con representación española. Spain. 2021
6. Computational Infrastructures for Bioinformatics. Disc4All Winter School. Barcelona Spain Feb. 2021

7. Software availability for computational biomedicine. BIOEXCEL. High performance Innovation Conference. Red Española de Supercomputacion. Spain. March 2020
8. Managing High-Throughput Molecular Dynamics Simulation Data. Symposium BigData4Science. Moving Research in Scientific Fields One Step Forward with Big Data Technologies. PASC'19. Zurich, Switzerland (2019).
9. Bioinformatics. Approaching cosmetics. Sociedad Española de Químicos Cosméticos. Barcelona (2019)
10. e-Infrastructure for the Multi-Scale Complex Genomics VRE 3D and 4D chromatin structure workshop. Fundació Privada Institut de Recerca Biomèdica de Barcelona (IRB). Barcelona. Spain (2019)
11. ELIXIR Software Containers Infrastructure - Human Data Use cases. ELIXIR All hands 2018. Berlin. Germany (2018)
12. e-Infrastructure for the Multi-Scale Complex Genomics Virtual Research Environment. CECAM Workshop - Epigenetic and Multiscale Genomics. Lausanne. Switzerland (2018)
13. The Multi-Scale Complex Genomics VRE. Design your e-Infrastructure workshop. EGI. Krakow. Poland (2016)

5 Tesis doctorales dirigidas (10 años)

1. Eva Martin del Pico. Towards a permanent observatory for quality of software in Life Sciences. U. Barcelona. Deposito. Oct 2025
2. Javier O. Corvi. Reaching a modular, generic and containerised development in Biomedical Natural Language Processing systems. Jul 2025
3. Luis Jorda. Protein dynamics: analysis of consensus motions in trajectory ensembles. U. Barcelona. Feb 2024
4. Romina Royo. Development and application of methodologies and infrastructures for cancer genome analysis within Personalized Medicine. U. Barcelona, 2022. Co-Director
5. Laia Codó. Computational infrastructures for biomolecular research. U. Barcelona. 2019
6. Victor López-Ferrando. Characterization of single amino acid variants. U. Barcelona. 2019
7. Dmitry Repchevsky. Ontology Based Data Integration in Life Sciences. U. Barcelona 2016

5.1 Tesis doctorales en curso

8. M Paola Ferri. Designing a scalable Cloud and HPC platform for diseases mechanisms investigation U. Barcelona Expected 2025.
9. Maria Chavero. Strategies for the optimal use of federated learning infrastructures in the life sciences. U. Barcelona. Co-Director
10. Pieter Zanders. Analysis of Allosteric Regulation in proteins through Molecular Dynamics Simulations and Artificial Intelligence approaches. U. Barcelona.