Xavier Barril
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Summary
Computational chemist with broad experience in drug discovery and a track record of achievement both in industrial and academic environments. My main research interests are the chemical validation of new therapeutic targets, the integration of experimental and computational methods and the development of computational techniques for drug design.

Key figures: 11 patents; 58 original papers; 12 reviews; 9 book chapters; 1 Edited Book; 35 invited talks in conferences. Cited 3700 times; H-index=33 (source: Web of Science)

Education
- B. S. Biochemistry. University of Barcelona. (June 1996)
- M. S. Chemistry. University of Barcelona. (September 1997)
- Ph. D. Biochemistry. University of Barcelona. (November 2001)
  Key facts. PhD supervisors: Profs. M. Orozco and F.J. Luque. Research stays in the groups of Prof. W.F. van Gunsteren (ETH, Zurich; 3 months) and Prof. I. D. Kuntz (UCSF, San Francisco; 6 months).

Professional Experience
- Computational Chemist, Vernalis - UK (01/2002-09/2005).
  Key facts. Contributed to the discovery and optimization of new lead series against a variety of therapeutic targets, mainly in the oncology area. Some of those compounds were out-licensed to Novartis and underwent clinical trials. Gained a sound knowledge of the drug discovery process, a better understanding of the merits and limitations of computer-aided and structure-based drug design, and – above all – a passion for collaborative research. Played a pivotal role in establishing a fragment-based drug discovery approach, was repeatedly promoted (Senior Scientist grade 1 03/2004, Senior Scientist grade 2 01/2005), co-authored 6 patents and 10 papers.

- ICREA Research Professor, Barcelona University - Spain (10/2005-present).
  Key facts. This post is equivalent to tenure, but does not involve start-up funds. Coming from industry, I had to start from scratch, establishing a line of research, attracting PhD students and obtaining resources. At present, I lead a group of 10 people, have active collaborations with several academic groups and pharmaceutical companies, publish regularly and have achieved peer recognition, as evidenced by invitations to conferences, to edit books and journal issues, to collaborate in funded projects, to write reviews and book chapters or to act as referee for prestigious journals.

- Co-founder Minoryx Therapeutics (12/2011-12/2017)
- CSO Gain Therapeutics (01/2018-present)
  Key facts. Companies devoted to the discovery of new treatments for rare diseases with unmet medical needs. Minoryx in-licensed the technology developed in my group and applied it to the discovery of non-competitive pharmacological chaperones. In 2018 this research line was transferred to Gain Therapeutics where I act as CSO.

- Rector's delegate for Research Personnel Policies, UB (01/2017-present).
  Key facts. Lead the implementation of the European Charter & Code for Researchers in the policies and practices of the university through the Human Resources Strategy for Researchers (HRS4R) (https://www.ub.edu/web/ub/en/recerca_innovacio/hr_excellence)

Patents

1. Inhibitors of ERK nuclear translocation
   Seger, Rony; Flores, Karen; **Barril Alonso, Xavier**; Galdeano Cantador, Carlos. X (Yeda Research and Development Co. Ltd; Universitat de Barcelona; ICREA)
   USPTO Patent Application (**2018**). Serial No. 62/774,360.

2. Heteroaryl compounds and their use.
   García Collazo, Ana Maria; **Barril Alonso, Xavier**; Cubero Jorda, Elena; Revés Vilaplana, Marc; Roberts, Richard Spurring (Minoryx Therapeutics S.L., Spain).
   PCT Int. Appl. Filed (**2017**). PCT/US2017/058477. Priority: EP 2016-382672

3. Isoquinoline compounds, methods for their preparation, and therapeutic uses thereof.
   García Collazo, Ana Maria; Martinell Pedemonte, Marc; Cubero Jorda, Elena; **Barril Alonso, Xavier**; Rodriguez Pascau, Laura; (Minoryx Therapeutics S.L., Spain).
   PCT Int. Appl. Filed (**2017**). PCT/US2017/058438. Priority: EP 2016-382660

4. Di(hetero)arylamides and sulfonamides, methods for their preparation and therapeutic uses thereof.
   García, A.M.; **Barril, X**.; Aymamí, J.; Revés, M.; Lavilla, R.; Martinell, M. (Minoryx Therapeutics S.L.)
   European Patent Application (**2013**) EP13382314

5. Method of binding site and binding energy determination by mixed explicit solvent simulations.
   Barril-Alonso, X.; Alvarez-Garcia, D.; Schmidtke, P. (University of Barcelona & ICREA)
   PCT Int. Appl. (**2013**), WO 2013/092922

6. Preparation of aryl and heteroaryl purine compounds as HSP90 protein inhibitors for the treatment of cancer.
   Brough. P. A.; Drysdale, M.J.; **Barril-Alonso, X**.
   PCT Int. Appl. (**2007**), WO 2007/034185

7. Preparation of pyrimidothiophene derivatives for use as HSP90 inhibitors.
   Barril-Alonso, X.; Brough. P. A.; Drysdale, M.J.; Webb, P. (Vernalis (Cambridge) Ltd; Cancer Research Technology Ltd; The Institute Of Cancer Research).
   PCT Int. Appl. (**2006**), WO 2006/008503

8. Pyridothiophene compounds
   Drysdale, M.J.; Dymock, B.W.; **Barril-Alonso, X**. (Vernalis (Cambridge) Ltd).
   PCT Int. Appl. (**2005**), WO 2005/034950

9. Pyrimidothiophene compounds
   Barril-Alonso, X.; Dymock, B.W.; Drysdale, M.J.; Fromont, C.; Jordan, A. (Vernalis (Cambridge) Ltd; Cancer Research Technology Ltd; The Institute Of Cancer Research).
   PCT Int. Appl. (**2005**), WO 2005/021552

10. Pyrazole compounds as hsp90 inhibitors for the treatment of cancer
Barril-Alonso, X.; Dymock, B.W.; Drysdale, M.J. (Vernalis (Cambridge) Ltd; Cancer Research Technology Ltd; The Institute Of Cancer Research).
PCT Int. Appl. (**2004**), WO 2004/096212

11. Preparation of 3,4-diarylpyrazoles as inhibitors of heat shock protein 90 (HSP90) and their use in the therapy of cancer.
Drysdale, M. J.; Dymock, B. W.; **Barril-Alonso, X.**; Workman, P.; Pearl, L. H.; Prodromou, C.; MacDonald, E. (Ribotargets Limited, UK; Cancer Research Technology Ltd.; The Institute of Cancer Research).
PCT Int. Appl. (**2003**), WO 2003/055860

Publications

Original Papers

1. Are protein-ligand complexes robust structures?
Majewski M, Carmona SR, **Barril X**
bioRxiv, 454165
https://www.biorxiv.org/content/biorxiv/early/2018/10/26/454165

2. Biophysical approach reveals a novel allosteric ligand binding site of SMYD3 histone methyltransferase
Talbot VO, Faibini E, FitzGerald EA, Mihalic F, Talu MJ, Rachman MM, Bartolini M, Del Rio A, **Barril X**, Dobritzsch D, Danielson H
Submitted

3. Computer-aided drug design: time to play with novel chemical matter (Editorial)
Barril X.
Expert Opinion on Drug Discovery, **2017**;12(10):977-980

4. Binding mode prediction and MD/MMPBSA-based free energy ranking for agonists of REV-ERBα/NCoR
Westermaier Y, Ruiz-Carmona S, Theret I, Perron-Sierra F, Poissonnet G, Dacquet C, Boutin JA, Ducrot P, **Barril X**
Journal of Computer-Aided Molecular Design. **2017**; 31(8):755-775

5. LigQ: a WebServer to select and prepare ligands for virtual screening
Radusky LG, Ruiz-Carmona S, Modenutti C, **Barril X**, Turjanski AG, Martí MA.
Journal of Chemical Information and Modelling. **2017**; 57(8):1741−1746

6. Molecular Dynamics in Mixed Solvents Reveals Protein-Ligand Interactions, Improves Docking, and Allows Accurate Binding Free Energy Predictions
Arcon JP, Defelipe LA, Modenutti CP, López ED, Alvarez-Garcia D, **Barril X**, Turjanski AG, Martí MA.
Journal of Chemical Information and Modelling. **2017**; 57(4):846-863

7. Identification and characterization of a secondary sodium-binding site and the main selectivity determinants in the human Concentrative Nucleoside Transporter 3
   Arimany-Nardi C, Claudio-Montero A, Viel-Oliva A, Schmidtke P, Estarellas C, **Barril X**, Bidon-Chanal A, Pastor-Anglada M.
   Molecular Pharmacology, **2017**; 14(6):1980-1987

8. Detecting similar binding pockets to enable systems polypharmacology.
   Duran-Frigola X, Siragusa L, Persi E, Ruppin E, **Barril X**, Cruciani G, Aloy P.
   PLOS Computational Biology, **2017**; 13(6):e1005522

9. Dynamic Undocking and the Quasi-Bound State as Tools for Drug Design
   Ruiz-Carmona S, Schmidtke P, Luque FJ, Baker L, Matassova N, Davis B, Roughley S, Murray J, Hubbard R, **Barril X**.
   Nature Chemistry, **2017**; 9:201-206.

10. Docking-undocking combination applied to the D3R Grand Challenge
    Ruiz-Carmona S, **Barril X**.
    Journal of Computer-Aided Molecular Design, **2016**; 30(9):805-815.

11. Inherent conformational flexibility of F1-ATPase alpha-subunit
    Hahn-Herrera O, Salcedo G, **Barril X**, García-Hernández E.
    BBA-Bioenergetics, **2016**; 1857 (9):1392-1402

12. Combined Use of Oligopeptides, Fragment Libraries, and Natural Compounds: A Comprehensive Approach To Sample the Druggability of Vascular Endothelial Growth Factor
    Bayó-Puxan N, Rodríguez-Mias R, Goldflam M, Kotev M, Ciudad S, Hipolito CJ, Varese M, Suga H, Campos-Olivas R, **Barril X**, Guallar V, Teixidó M, García J, Giralt E.
    ChemMedChem, **2016**; 11:928-939

13. Binding Kinetics in Drug Discovery (Editorial)
    Barril X., Danielsson H.
    Drug Discovery Today: Technologies, **2015**; 17:35-36

14. In Silico/In Vivo Insights into the Functional and Evolutionary Pathway of Pseudomonas aeruginosa Oleate-Diol Synthase. Discovery of a New Bacterial Di-Heme Cytochrome C Peroxidase Subfamily
    Estupiñán M, Álvarez-García D, **Barril X**, Diaz P, Manresa A.
    PLoS One, **2015**; 10(7):e0131462.

15. Assessing the Suitability of the Multilevel Strategy for the Conformational Analysis of Small Ligands
    Juárez-Jiménez J, **Barril X**, Orozco M, Pouplana R, Luque FJ.
    J Phys Chem B, **2015**; 119(3):1164-72.

16. Molecular simulations with solvent competition quantify water displaceability and provide accurate interaction maps of protein binding sites
    Alvarez-Garcia D, **Barril X**
    Journal of Medicinal Chemistry, **2014**; 57(20):8530–8539

17. Binding of Calix[4]pyrroles to Pyridine N-oxides Probed with Surface Plasmon Resonance
    Adriaenssens L, Acero-Sánchez JL, **Barril X**, O´Sullivan CK, Ballester P
    Chemical Science. **2014**; 5(11):4210–4215

18. Ligand discovery: Docking points *(NEWS & VIEWS)*
    Barril X.
    Nat Chem. **2014**, 6(7):560-561

19. Relationship between protein flexibility and binding: lessons for structure-based drug design
    Alvarez-Garcia D, **Barril X**
    J. Chem. Theory Comput., **2014**, 10 (6):2608–2614

20. VAV3 mediates resistance to breast cancer endocrine therapy.
    Aguilar H, Urruticoechea A, Halonen P, Kiyotani K, Mushiroda T, **Barril X**, Serra-Musach J, Islam A, Caizzi L, Di Croce L, Nevedomskaya E, Zwart W, Bostner J, Karlsson E, Tenorio GP, Fornander T, Sgroi DC, Garcia-Mata R, Jansen MP, García N, Bonifaci N, Climent F, Soler MT, Rodríguez-Vida A, Gil M, Brunet J, Martrat G, Gómez-Baldó L, Extremera AI, Figueras A, Balart J, Clarke R, Burnstein KL, Carlson KE, Katzenellenbogen JA, Vizoso M, Esteller M, Villanueva A, Rodríguez-Peña AB, Bustelo XR, Nakamura Y, Zembutsu H, Stål O, Beijersbergen RL, Pujana MA.
    Breast Cancer Res. **2014**,16(3):R53

21. TuberQ: a Mycobacterium tuberculosis protein druggability database.
    Radusky L, Defelipe LA, Lanzarotti E, Luque J, **Barril X**, Marti MA, Turjanski AG.
    Database (Oxford). **2014**, 2014(0):bau035.

22. rDock: A Fast, Versatile and Open Source Program for Docking Ligands to Proteins and Nucleic Acids
    Ruiz-Carmona S, Alvarez-Garcia D, Foloppe N, Garmendia-Doval AB, Juhos S, Schmidtke P, **Barril X**, Hubbard RE, Morley SD
    PLOS Computational Biology **2014**, 10(4):e1003571

23. On the transferability of fractional contributions to the hydration free energy of amino acids.
    Campanera JM, **Barril X**, Luque FJ.
    Theoretical Chemistry Accounts. **2013**, 132:1343

24. A Multilevel Strategy for the Exploration of the Conformational Flexibility of Small Molecules.
    Forti F, Cavasotto CN, Orozco M, **Barril X**, Luque FJ.
    Journal of Chemical Theory and Computation, **2012**; 8(5); 1808–1819

25. Allosteric Regulation of PKCθ: Understanding Multistep Phosphorylation and Priming by Ligands in AGC Kinases
    Seco J, Ferrer-Costa C, Campanera JM, Soliva R, **Barril X**.
    Proteins: Structure, Function, and Bioinformatics, **2012;** 80(1):269-280

26. Shielded Hydrogen Bonds as Structural Determinants of Binding Kinetics. Application in Drug Design.
Schmidtke P, Luque FJ, Murray JB, **Barril X**.
Journal of the American Chemical Society, **2011;** 133(46):18903-18910

27. MDpocket: Open Source Cavity Detection and Characterization on Molecular Dynamics Trajectories.
Schmidtke P, Bidon-Chanal A, Luque FJ, **Barril X**.
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Schmidtke P, **Barril X**.
Journal of Medicinal Chemistry, **2010**; 53(15); 5858–5867
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29. Ensemble docking from homology models
Novoa EM, Ribas de Pouplana L, **Barril X**, Orozco M.
Journal of Chemical Theory and Computation, **2010**; 6(8); 2547–2557

30. Combining Hit Identification Strategies: Fragment-Based and in Silico Approaches to Orally Active 2-Aminothieno[2,3-d]pyrimidine Inhibitors of the Hsp90 Molecular Chaperone
Brough PA, **Barril X**, Borgognoni J, Chene P, Davies NG, Davis B, Drysdale MJ, Dymock B, Eccles SA, Garcia-Echeverria C, Fromont C, Hayes A, Hubbard RE, Jordan AM, Jensen MR, Massey A, Merrett A, Padfield A, Parsons R, Radimerski T, Raynaud FI, Robertson A, Roughley SD, Schoepfer J, Simmonite H, Sharp SY, Surgenor A, Valenti M, Walls S, Webb P, Wood M, Workman P, Wright L.
Journal of Medicinal Chemistry, **2009**; 52(15); 4794-4809

31. Tacripyrines, the First Tacrine-Dihydropyridine Hybrids, as Multi-Target-Directed Ligands for the Treatment of Alzheimer´s Disease
León R, de los Ríos C, Marco-Contelles J, Bartolini M, Andrisano V, Huertas O, **Barril X**, Luque FJ, Rodríguez-Franco MI, López B, López MG, García AG, Careiras MC, Villarroya M.
Journal of Medicinal Chemistry, **2009**; 52(9); 2724-2732

32. Binding site detection and druggability index from first principles
Seco J., Luque F.J., **Barril X.**
Journal of Medicinal Chemistry, **2009**; 52(8); 2363-2371
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33. Towards accurate energy predictions of the bioactive conformation of drugs.
Butler, K.T., Luque, F.J., **Barril, X.**
Journal of Computational Chemistry. **2009;** 30(4), 601-610

34. New tacrine-dihydropyridine hybrids that inhibit acetylcholinesterase, calcium entry, and exhibit neuroprotection properties.
León R, de los Ríos C, Marco-Contelles J, Huertas O, **Barril X**, Luque FJ, López MG, García AG, Villarroya M.
Bioorganic Medicinal Chemistry Letters. **2008**; 16(16), 7759-7769

35. NVP-AUY922: A Novel Heat Shock Protein 90 Inhibitor Active against Xenograft Tumor Growth, Angiogenesis, and Metastasis.
Eccles SA, Massey A, Raynaud FI, Sharp SY, Box G, Valenti M, Patterson L, de Haven Brandon A, Gowan S, Boxall F, Aherne W, Rowlands M, Hayes A, Martins V, Urban F, Boxall K, Prodromou C, Pearl L, James K, Matthews TP, Cheung KM, Kalusa A, Jones K, McDonald E, **Barril X**, Brough PA, Cansfield JE, Dymock B, Drysdale MJ, Finch H, Howes R, Hubbard RE, Surgenor A, Webb P, Wood M, Wright L, Workman P.
Cancer Research, **2008**; 68(8), 2850-2860

36. 4,5-Diarylisoxazole Hsp90 Chaperone Inhibitors: Potential Therapeutic Agents for the Treatment of Cancer
Brough P.A., Aherne W., **Barril X.**, Borgognoni J., Boxall K., Cansfield J.E., Cheung K.M., Collins I., Davies N.G., Drysdale M.J., Dymock B., Eccles S.A., Finch H., Fink A., Hayes A., Howes R., Hubbard R.E., James K., Jordan A.M., Lockie A., Martins V., Massey A., Matthews T.P., McDonald E., Northfield C.J., Pearl L.H., Prodromou C., Ray S., Raynaud F.I., Roughley S.D., Sharp S.Y., Surgenor A., Walmsley D.L., Webb P., Wood M., Workman P., Wright L.
Journal of Medicinal Chemistry, **2008**; 51(2), 196-218

37. Extension of the MST continuum solvation model to the RM1 semiempirical Hamiltonian
Forti, F., **Barril, X**., Orozco, M., Luque, F.J.
Journal of Computational Chemistry. **2008;** 29(4), 578-87

38. Inhibition of the HSP90 molecular chaperone in vitro and in vivo by novel, synthetic, potent resorcinylic pyrazole/isoxazole amide analogs
Sharp, S.Y., Prodromou, C., Boxall, K., Powers, M.V., Holmes, J., Box, G., Matthews, T.P., Cheung, K.M.J., Kalusa, A., James, K., Hayes, A., Hardcastle, A., Dymock, B., Brough, P.A., **Barril, X.**, Cansfield, J.E., Wright, L., Surgenor, A., Foloppe, N., Hubbard, R.E., Aherne, W., Pearl, L.H., Jones, K., McDonald, E., Raynaud, F., Eccles, S., Drysdale, M., Workman P.
Molecular Cancer Therapeutics. **2007;** 6(4), 1198-211.

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Journal of Molecular Modelling. **2007**; 13(2), 357-365

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Howes, R., **Barril, X.**, Dymock, B.W., Grant, K., Northfield, C.J., Robertson, A.G.S., Surgenor, A., Wayne, J., Wright, L., James, K., Matthews, T., Cheung, K.-M., McDonald, E., Workman, P., Drysdale, M.J.
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41. 4-Amino Derivatives of the HSP90 Inhibitor CCT018159
Barril, X., Beswick, M., Collier, A., Drysdale, M.J., Dymock, B.W., Fink, A., Grant, K., Howes, R., Jordan, A.M., Massey, A., Surgenor, A., Wayne, J., Workman, P., Wright, L.
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48. Adenosine Derived Inhibitors of the Molecular Chaperone HSP90 – SAR explained through multiple x-ray structures.
Dymock, B., **Barril, X.**, Beswick, M., Collier, A., Davies, N., Drysdale, M., Fink, A., Fromont, C., Hubbard, R.E., Massey, A., Surgenor, A., Wright, L.
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Reviews

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3. Virtual screening: An in silico tool for interlacing the chemical universe with the proteome
   Westermaier Y, **Barril X**, Scapozza L.
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   WIREs Comput Mol Sci **2013**; 3(4): 327–338

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9. Virtual Screening in Structure-Based Drug Discovery
   Barril, X., Hubbard, R.E., Morley M.D.
   Mini Reviews in Medicinal Chemistry, **2004**; 4(7):779-791.

10. Rational Design of Reversible Acetylcholinesterase Inhibitors.
    Barril, X., Kalko, S.G., Orozco, M., Luque, F.J.
    Mini Reviews in Medicinal Chemistry. **2002**; 2(1):27-36

11. Towards Improved Acetylcholinesterase Inhibitors: A Structural and Computational Approach.
    Barril, X., Orozco, M., Luque, F.J.
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12. Theoretical Methods for the representation of solvent
Orozco, M. ,Alhambra, C., **Barril, X.**, Lopez ,J., Busquets, M., Luque, F.J.
Journal of Molecular Modelling,2: 1-15, **1996**.

Book Chapters

1. Dynamic Undocking: A Novel Method for Structure-Based Drug Discovery
Majewski M, Ruiz-Carmona S, **Barril X**
Rational Drug Design. Edited by Mavromoustakos T., Kellici T. Series Methods in Molecular Biology, volume 1824.
Humana Press, New York, NY. **2018**. pp. 195-215

2. Molecular dynamics: A tool to understand nuclear receptors
Spyrakis F, **Barril X**, Luque FJ.
Computational Approaches to Nuclear Receptors. Edited by P. Cozzini & G.E. Kellogg.
Royal Society of Chemistry. **2012**. pp. 60-83

3. Expanding the Target Space: Druggability Assessments
Schmidtke P, Alvarez-Garcia D, Seco J, **Barril X**.
In Physico-Chemical and Computational Approaches to Drug Discovery. Edited by X. Barril & FJ. Luque. Series "Drug Discovery".
Royal Society of Chemistry. **2012**. pp. 312-318

4. Druggability Prediction.
Alvarez-Garcia D, Seco J, Schmidtke P, **Barril X**.
Protein-Ligand Interactions. Edited by H. Gohlke. Series "Methods and Principles in Medicinal Chemistry", Eds. R. Mannhold, H. Kubinyi & G. Folkers.
Wiley-VCH. **2012**. pp. 267-282

5. In silico Screening.
Luque, F.J., **Barril, X.**
Protein Surface Recognition: Approaches for the Inhibition of Protein-protein Interactions for Drug Discovery. Edited by E. Giralt, M. Peczuh & X. Salvatella.
John Wiley & Sons. **2010**; pp. 211-235

6. Molecular Modelling
Barril X., Soliva R.
Structure-Based Drug Design. Edited by Hubbard, R.E.,
Royal Society of Chemistry, London (UK) **2006**; pp.52-94

7. Partitioning of free energies of solvation into fragment contributions: Applications in drug design.
Muñoz, J., **Barril, X.**, Luque, F.J., Gelpí, J.L., Orozco, M.
Fundamentals of Molecular Similarity. Edited by Carbó-Dorca et al.. Kluwer Academic/Plenum Publishers, New York **2001**; 143-168.

8. On the use of SCRF methods in drug design studies.
Orozco, M., Colominas, C., **Barril, X.**, Luque, F.J.

Molecular Modeling and Prediction of Bioactivity. K. Gundertofte and F.S. Jorgensen (Editors), Kluwer/Plenum, New York, **2000**, pp.129-134

9. Nucleic Acid Bases in Solution.
   Orozco, M., Cubero, E., **Barril, X.**, Colominas, C., Luque, F.J.
   Computational Molecular Biology. Theoretical Computational Chemistry. J. Leszcynski (Editor). Elsevier Science. Chapter 4, 119-166, **1999**.

Invited Conferences

1. Structure-based discovery of novel allosteric ligands: methods and applications
   X Meeting of the Spanish Drug Discovery Network
   Bilbo (Spain), 22-23 November 2018

2. Structural stability: a design principle for protein-ligand complexes?
   ISQBP President's Meeting 2018
   Barcelona (Spain), 19-21 June 2018

3. Targeting novel allosteric sites with confidence: Advanced SBDD methods make it possible
   EMBL-EBI Industry Workshop 'Target Tractability Assessment'
   Hinxton-Cambridge (UK), 3-4 May 2017

4. The Quasi-Bound state of protein-ligand complexes. Implications in drug discovery
   CECAM Workshop "Water at interfaces: from proteins to devices"
   Vienna (Austria), 29 November to 2 December 2016

5. Estabilidad estructural de los complejos ligando-proteína: Aplicaciones en cribado virtual
   1er workshop latinoamericano de modelado molecular y simulación computacional
   Buenos Aires (Argentina), 15 June 2016

6. Structural stability of protein-ligand complexes: Applications in virtual screening
   3rd NovAliX Conference - Biophysics in Drug Discovery 2016
   Strasbourg (France), 7-10 June 2016

7. Kinetic stability of protein-ligand complexes: Applications in virtual screening
   251st ACS National Meeting
   San Diego, California (USA), 13-17 March 2016

8. Dynamic Undocking, a new tool for virtual ligand screening
   BSC-RES Symposium
   Barcelona (Spain), 22 February 2016

9. Moving in water: molecular simulations as enabling tools for hit and lead generation
   SMi Advances and Progress in Drug Design

London (UK), 15-16 February 2016

10. High-Throughput Virtual Dissociation Experiments: Application to Fragment Screening
    Gordon Research Conference on Computer-Aided Drug Design
    Mount Snow - West Dover, VT (USA), 19-24 July 2015

11. SEE-Tx: strategies to identify and exploit novel allosteric sites for the development of non-competitive pharmacological chaperones – application to beta-galactosidase
    AffyMSLifeChem: International Workshop
    Rüsselsheim, 24th November 2014

12. Understanding the role of water molecules in the drug-target binding process: Advances in structure-based drug discovery
    WaterEurope, Interdisciplinary Conference about Water
    Zaragoza (Spain), 12-14 June 2014

13. Protein flexibility in solvation studies: striking the right balance between accuracy and precision
    Cutting Edge Approaches to Drug Design 2014: Modelling water in biological systems
    London (UK). 28 March 2014

14. Mecanismos de acción farmacológica no convencionales: Oportunidades y aproximaciones computacionales
    Simposio Interno UNAM en Homenaje al Dr. Alfonso Romo de Vivar
    Mexico DF (Mexico). 29 January 2014

15. Targeting non-standard binding sites in drug discovery: Challenges and Opportunities
    SFB 630 3rd International Symposium: "Novel Agents Against Infectious Diseases – An Interdisciplinary Approach"
    Würzburg (Germany). 22 November 2013

16. Druggability assessment: an essential tool to choose the optimal therapeutic approximation
    Cardio-Facio-Cutaneous (CFC) meeting; strategies to study RASopathies and other rare diseases.
    Haifa (Israel). 22 June 2013

17. Improvements in docking performance with a new type of scoring functions derived from molecular dynamics simulations of mixed solvents.
    Advances and Progress in Drug Design
    London (UK). 18 February 2013

18. Water-Shielded Hydrogen Bonds: A Handle on Binding Kinetics of Protein-Ligand Complexes
    CHI & Bio-IT World's 12th Annual Structure-Based Drug Design Conference
    Boston (USA). 8 June 2012

19. Water-shielded hydrogen bonds as structural determinants of binding kinetics

Noordwijkerhout-Camerino-Cyprus Symposium 2012
Amsterdam (Netherlands). May 2012

20. Improvements in docking scoring functions: the physics-based perspective
Select Biosciences Discovery Chemistry Congress 2012
Munich (Germany). March 2012

21. Improvements in docking scoring functions: the physics-based perspective
7th German Conference on Chemoinformatics
Goslar (Germany). November 2011

22. Shielded Hydrogen Bonds as Structural Determinants of Binding Kinetics. Application in Drug Design.
CECAM Workshop: Innovative Approaches to Computational Drug Discovery
Laussane (Switzerland). October 2011

23. Binding site detection and druggability predictions: the solvent's perspective
New Approaches in Drug Design & Discovery
Rauischholzhausen (Germany). March 2010

24. Use of Molecular Dynamics Simulations to Predict Druggability
XRQTC Workshop - New Trends in Computational Chemistry for Industry Applications
Barcelona (Spain). July 2009

25. Use of Molecular Dynamics to Detect Binding Sites on Protein Surfaces
Journées Nationales de Chémoinformatique
Montpellier (France). June 2009

26. Binding Site Detection and Druggability Index from First Principles
CHI's 9th Annual Structure-Based Drug Design Conference - Sophisticated Approaches to Drug Discovery
Cambridge, MA (US). 5 June 2009

27. Binding site detection and druggability index from first principles
CCPB - Biomolecular Simulation 2009
York (UK). January 2009

28. Detection of druggable sites with an explicit solvation method
Grand Challenges in Computational Biology. Joint BSC - IRB Barcelona Conference.
Barcelona (Spain). June 2008

29. Mejoras en los metodos de virtual screening
XXX Congreso de la SEBBM
Malaga (Spain). September 2007

30. Assessing the druggability of protein-protein interactions.
AIMECS07 - 6th AFMC International Medicinal Chemistry Symposium.
Istanbul (Turkey). July 2007

31. Bioactive conformations of drugs: how much strain have they?

7th Spanish Symposium on Bioinformatics and Computational Biology
Zaragoza (Spain). November 2006

32. Handling protein flexibility in structure-based drug design
Next Generation Tools in Virtual Screening and Lead Identification.
London (UK). December 2005

33. The Issue of Protein Flexibility in Docking-Based Virtual Screening
eCheminfo Autumn 2005 InterAction Meeting
Basel (Switzerland). November 2005

34. Consideraciones farmacogenómicas en el diseño de fármacos.
Reunión del Grupo de Biología Molecular Teórica - XXVIII Congreso de la SEBBM.
Zaragoza (Spain). September 2005.

35. Screening virtual basado en Docking: Aplicaciones y Direcciones Futuras
II Reunión de Modelización Molecular y Quimioinformática
Barcelona (Spain). June 2005.

Courses and Seminars

1. Structure-based discovery of allosteric ligands: Applications and methodological developments
Lecture series on modern drug Discovery, TU Dortmund
Dortmund (Germany), 6 June 2018

2. Biología computacional orientada al diseño de fármacos 3 (11h)
Centro Latinoamericano de Formación Interdisciplinaria (CELFI)
Buenos Aires (Argentina), 14-18 May 2018

3. From scientist to entrepreneur: What does it take?
10th Summer School on Medicines Medicines: from Target to Market
Ribeirão Preto (Brazil), 16-23 March 2018

4. Diseño de fármacos mediante métodos computacionales (30h)
Instituto de Química – UNAM
Mexico City (Mexico), 17-21 October 2016

5. Escuela de simulación computacional avanzada en Química (8h)
Centro Latinoamericano de Formación Interdisciplinaria (CELFI)
Buenos Aires (Argentina), 9-16 July 2016

6. A fresh view on molecular recognition: the dynamic perspective (4h)
Advances and Progress in Drug Design - SMi
London (UK), 17th February 2016

Books (Edited)

Physico-Chemical and Computational Approaches to Drug Discovery
Editors: Javier Luque, Xavier Barril
RSC Drug Discovery Series No. 23
The Royal Society of Chemistry 2012
Cambridge, UK
ISBN: 978-1-84973-537-7
DOI:10.1039/9781849735377

Research Projects as PI (Public Funds)

1. "A novel hybrid platform to generate chemical probes. Application to the Fbw7 E3 ligase"
   Ministerio de Economía y Competitividad (Proyectos I+D). 2016-2018
   SAF2015-68749-R
   € 170,000.00

2. "FRAGNET – FRAGments training NETwork"
   EU Marie Curie Innovative Training Network. 01/03/2016-01/03/2020
   Call H2020-MSCA-ITN-2015. Project 675899
   € 495745.92 (XB); € 3,842,481.96 (Total)

3. "DIGITAL – DIagnóstico, seGuImiento y Tratamiento de pacientes con enfermedades genéticas incluídas en programas de cribado neonatAL y otras enfermedades raras metabólicas"
   Ministerio de Economía y Competitividad (Proyectos RETOS). 2014-2016
   RTC-2014-2412-1
   € 65,000.00

4. "Expanding the druggable genome: new tools to tackle new targets"
   Ministerio de Economía y Competitividad (Proyectos I+D). 2013-2015
   SAF2012-33481
   € 100,000.00

5. "Chaperons-4-neurons: Desarrollo de chaperonas farmacológicas para el tratamiento de enfermedades raras neurometabólicas"
   Ministerio de Economía y Competitividad (Proyectos INNPACTO). 2013-2015
   IPT2012-0561
   € 56,960.00

6. "LightScreening: a technique for faster and more effective drug discovery"
   Ministerio de Ciencia e Innovación (Acciones Complementarias). 2011-2012
   BIO2010-11453-E
   € 50,000.00

7. "Expanding the druggable genome: Protein-protein interfaces as a new target class"
   Ministerio de Ciencia e Innovación (Proyectos I+D). 2010-2012

SAF2009-08811
€ 120,000.00

8. "Optimizacion y desarrollo de inhibidores de proteinas metiladoras de histonas"
   Ministerio de Educación y Ciencia (Proyectos PETRI). 2008-2010
   PET2007-0319
   € 264,554.40

Contract Research as PI (Private Funds)

1. "Asesoramiento en diseño computacional de dianas terapéuticas relacionadas con la adenosina"
   Palobiofarma, S.L.
   € 10,573.00

2. "Desenvolupament de llibreria virtual d'anàlegs de nucleòsids"
   Plasmia Biotech, S.L. 18/11/2013-17/11/2014
   € 28.823.00

3. "Investigation on the stability of a protein complex using molecular dynamics approach"
   Institut de Recherches Servier. 01/06/2013-30/03/2015
   € 92,560.00

4. "Identification of bioactive compounds"
   Minoryx Therapeutics. 01/01/2012 -31/12/2014
   € 81,206.00

5. "Identificación de nuevas entidades químicas por métodos de virtual screening (Proyecto DENDRIA)"
   Brainco Biopharma; Programa CENIT. 26/10/2011-31/12/2013
   € 42,500.00

6. "Optimization and implementation of a new druggability method"
   Sanofi-Aventis recherche & développement. 01/10/2009-30/09/2010
   € 60,000.00

7. "Abordaje multidisciplinar en la enfermedad de Alzheimer (Proyecto MIND)"
   Oryzon Genomics; Programa CENIT. 2008-2011
   € 80,224.00

8. "Construction & Exploitation of an integrated VS platform"
   GRUPO J. URIACH, S.L., Programa CENIT. 2006-2009
   € 127,600.00

Doctoral Theses

1. Sergio Ruiz-Carmona
   Virtual screening for novel mechanisms of action: applications and methodological developments.
   20/01/2017
   Director
   Extraordinary Doctorate Award

2. Montserrat Pujadas Lorente
   Protein-protein interfaces: A new type of therapeutic target
   20/02/2015
   Director

3. Daniel Álvarez García
   Protein solvation preferences: applications to drug discovery
   18/12/2014
   Director

4. Mousumi Bhattacharyya
   Conformational Variability: Implications for Biomolecular Activity and in Drug Design
   21/05/2012
   Director

5. Peter Schmidtke
   Protein-ligand binding sites Identification, characterization and interrelations
   14/10/2011
   Director
   Extraordinary Doctorate Award

6. Flavio Forti
   Flexibilidad conformacional de moléculas bioactivas: Implicaciones en diseño de fármacos y función de globinas
   06/09/2011
   Co-director

7. Jesus Seco
   Aproximaciones Computacionales en el Desarrollo Racional de Fármacos
   06/07/2011
   Director

Master Theses

1. Marina Miñarro
   A Computational Pipeline for Participation in CELPP
   15/07/2018
   Director – MSc Bioinformatics (UPF / UB)

2. Serena Gaetana Piticchio
   A Computational Platform for Fragment Evolution

15/07/2016
Director – MSc Bioinformatics (UPF / UB)

3. Kevin Pinto Gil
   Solvent extension of the MDmix methodology and its impact on the quality of the predictions
   18/07/2013
   Director – MSc Biotechnology (UB)

4. Sergio Ruiz Carmona
   Expanding the druggable genome: Protein-protein interfaces as a new target class
   17/07/2012
   Director – MSc Bioinformatics (UPF / UB)

5. Daniel Álvarez García
   Novel prospective MD-based scoring function: MDMixSF
   17/07/2012
   Director – MSc Bioinformatics (UPF / UB)