| **CV date** | 1/2020 |
|---|---|

## Part A. PERSONAL INFORMATION

| First and Family name | Victor Guallar | | |
|---|---|---|---|
| Social Security, Passport, ID number | | Age | |
| Researcher numbers | Researcher ID | B-1579-2013 | |
| | Orcid code | 0000-0002-4580-1114 | |

### A.1. Current position

| Name of University/Institution | Barcelona Supercomputing Center | | |
|---|---|---|---|
| Department | Life Sciences | | |
| Address and Country | Jordi Girona 29, 08034 Barcelona (Spain) | | |
| Phone number | | E-mail | Victor.guallar@bsc.es |
| Current position | ICREA Professor | From | 07 / 2006 |
| Espec. cód. UNESCO | *230226* | | |

Synergistic positions:
2016-present: Head of Advisory board and founder at Nostrum Biodiscovery
2006-present: Advice editor for the journal Biophysical Chemistry, Elsevier Group.

### A.2. Education and research positions

| Grade | University | Year |
|---|---|---|
| Bachelor in Chemistry | University Autonomous of Barcelona | 1994 |
| PhD in Theoretical Chemistry | University Autonomous of Barcelona and UC Berkley | 1995-1999 |
| Postdoctoral Studies | Columbia University | 2000-2003 |
| Assistant Professor | Washington University School of Medicine | 2003-2006 |

### A.3. Indicators of Quality in Scientific Production (source google scholar April/2020)

153 publications in international peer-reviewed journals (~95 in the Q1)

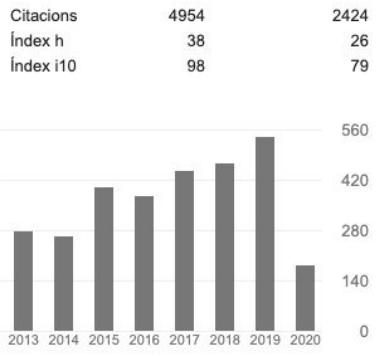
Statistics from Google Scholar:

Total number of citations: 4954

H index: 38 (26 since 2015)

I10 index: 98 (79 since 2015)

Prof Guallar has directed 14 PhD thesis (with 5 more ongoing)



**Part B. CV SUMMARY** *(max. 3500 characters, including spaces)*

Dr. Guallar was assistant professor at Washington University School of Medicine before moving with his group to the Barcelona Supercomputing Center in 2006, after he was offered a Professor permanent position by ICREA (Catalan Institute for Research and Advanced Studies). In the last 13 years the group has grown considerably, keeping a productive international character.

The PI's main scientific achievements relate with the improvement of methodologies for molecular computation. Important contributions in biophysical modelling include development of PELE, one of the best techniques to map protein-ligand induced fit (developed through a 2009 Advanced ERC grant to Prof. Guallar, the youngest researcher in Spain to receive and advanced ERC). Its public server, https://pele.bsc.es, with ~25000 visitors from 75 different countries, was underlined (top 5%) by the editors in the prestigious special server issue in Nucleic Acid Research. Other recent biophysical studies of high impact include: the first molecular level evidence on hemoglobin two tertiary state (TTS) model (*JACS* 2014); drug development in BCL-2 and mTOR kinases (*Biochem. Pharm.* 2012, *PLoS One* 2013); the first public molecular predictor of drug resistance in HIV-1 protease (JCIM 2016); the first microsecond molecular dynamics study of the non-covalent association of a DNA-drug compound (*Biophys. J* 2014); non-biased comprehensive studies on ligand-binding in Nuclear Hormone Receptors (*Structure* 2016, *Biophys. J* 2017) and *JCTC* 2019. At the biochemical level, our main contributions include computational algorithms to study long-range electron transfer processes and enzyme engineering. In this line, we have produced: one of the most complete protein-protein electron transfer studies to date (*Plos Comp. Biol.* 2013); engineering a peroxidase for a la carte substrate oxidation (*ACS Catalysys* 2016); the first *in silico* directed evolution enzyme engineering study (*Catalysis Science & Technology* 2017, and *ACS Catalysis* 2019); the development of the first Plurizyme, and enzyme with two active sites (*Biochemistry*, 2018 & *Nature Catalysis* 2019).

In addition to algorithms development (and their application), we have recently placed importance in adding interdisciplinary fields to our research: user-experience (UX), visualization and virtual reality (*SciVis* 2015) and machine learning (*Scientific Reports* 2017).

In the last 10 years at BSC, the lab has formed part of two EU-consortiums, and obtained two ERC grants (An Advanced and a PoC one). Overall Prof Guallar has guaranteed over 6 million euros in external funding

Finally we want to underline our efforts in transfer of technology. Prof Guallar is one of the two founders of Nostrum Biodiscovery (NBD), the first spin-off company of the Barcelona Supercomputing Center (started operations in September 2016). With investment from the Marcelino Botin foundation, NBD aims at providing state of the art molecular computational modeling and supercomputer power for biotechnology industries, with emphasis in *in silico* drug design (the enzyme engineering division started operations in January 2019). Moreover, a new idea from the lab, PELE-e: evolving PELE for therapeutic enzyme engineering, has been founded through the 2016 CaixaImpulse program.

## Part C. RELEVANT MERITS

### C.1. Publication list last 5 years

| Authors | Title | Publication | Volume | Pages | Year |
|---|---|---|---|---|---|
| Carles Perez, Daniel Soler, Robert Soliva, Victor Guallar | FragPELE: Dynamic Ligand Growing within a Binding Site. A Novel Tool for Hit-To-Lead Drug Design | Journal of Chemical Information and Modeling | 60 | 1728-1736 | 2020 |
| Alonso et al. | Genetically engineered proteins with two active sites for enhanced biocatalysis and synergistic chemo-and biocatalysis | Nature Catalysis | 3 | 319–328 | 2020 |
| Diaz et al | Monte Carlo simulations using PELE to identify a protein–protein inhibitor binding site and pose | RSC Advances | 10 | 7058-7064 | 2020 |
| Viña-Gonzalez, Javier; Martinez, Angel T; Guallar, Victor; Alcalde, Miguel; | Sequential oxidation of 5-hydroxymethylfurfural to furan-2, 5-dicarboxylic acid by an evolved aryl-alcohol oxidase | Biochimica et Biophysica Acta (BBA)-Proteins and Proteomics | 1868 | 140293 | 2020 |
| Gilabert, Joan F; Lecina, Daniel; Estrada, Jorge; Guallar, Victor; | Monte Carlo Techniques for Drug Design: The Success Case of PELE | Biomolecular Simulations in Drug Discovery | | | 2019 |
| Serrano, Ana; Sancho, Ferran; Viña-González, Javier; Carro, Juan; Alcalde, Miguel; Guallar, Victor; Martínez, Angel T; | Switching the substrate preference of fungal aryl-alcohol oxidase: towards stereoselective oxidation of secondary benzyl alcohols | Catalysis Science & Technology | 9 | 833-841 | 2019 |
| Aranda, Carmen;et al. | Selective synthesis of 4-hydroxyisophorone and 4-ketoisophorone by fungal peroxygenases | Catalysis Science & Technology | 9 | 1398-1405 | 2019 |
| Viña-Gonzalez, Javier; et al.; | Structure-Guided Evolution of Aryl Alcohol Oxidase from Pleurotus eryngii for the Selective Oxidation of Secondary Benzyl Alcohols | Advanced Synthesis & Catalysis | 361 | 2514-2525 | 2019 |
| Mateljak, Ivan;et al. | Increasing Redox Potential, Redox Mediator Activity, and Stability in a Fungal Laccase by Computer-Guided Mutagenesis and Directed Evolution | ACS Catalysis | 9 | 4561-4572 | 2019 |
| Carro, Juan; et al. | Modulating Fatty Acid Epoxidation vs Hydroxylation in a Fungal Peroxygenase | ACS Catalysis | 9 | 6234-6242 | 2019 |
| De Salas, Felipe;et al. | Engineering of a fungal laccase to develop a robust, versatile and highly-expressed biocatalyst for sustainable chemistry | Green Chemistry | 21 | 5374-5385 | 2019 |
| De Salas, Felipe; et al.; | Structural and biochemical insights into an engineered high-redox potential laccase overproduced in Aspergillus | International journal of biological macromolecules | 141 | 855-866 | 2019 |
| Gilabert, Joan F;et al. | PELE-MSM: a Monte Carlo based protocol for the estimation of absolute binding free energies | Journal of chemical theory and computation | 15 | 6243-6253 | 2019 |
| Saen-Oon, Suwipa; Lozoya, Estrella; Segarra, Victor; Guallar, Victor; Soliva, Robert; | Atomistic simulations shed new light on the activation mechanisms of RoRγ and classify it as type iii nuclear hormone receptor regarding ligand-binding paths | Scientific reports | 9 | | 2019 |
| Santiago, Gerard; et al. | Rational engineering of multiple active sites in an ester hydrolase | Biochemistry | 57 | 2245-2255 | 2018 |
| Gomez de Santos, Patricia; et al. | Selective synthesis of the human drug metabolite 5′-hydroxypropranolol by an evolved self-sufficient peroxygenase | ACS Catalysis | 8 | 4789-4799 | 2018 |

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| Iglesias, Jelisa; Saen-oon, Suwipa; Soliva, Robert; Guallar, Victor; | Computational structure-based drug design: Predicting target flexibility | Wiley Interdisciplinary Reviews: Computational Molecular Science | 8 | e1367 | 2018 |
| Carro, Juan; et al. | Multiple implications of an active site phenylalanine in the catalysis of aryl-alcohol oxidase | Scientific reports | 8 | 8121 | 2018 |
| Vázquez, P; Hermosilla, Pedro; Guallar, Víctor; Estrada, Jorge; Vinacua, Alvar; | Visual Analysis of protein-ligand interactions | Computer Graphics Forum | 37 | 391-402 | 2018 |
| Kotev, Martin; Pascual, Rosalia; Almansa, Carmen; Guallar, Victor; Soliva, Robert; | Pushing the Limits of Computational Structure-Based Drug Design with a Cryo-EM Structure: The Ca2+ Channel α2δ-1 Subunit as a Test Case | Journal of chemical information and modeling | 58 | 1707-1715 | 2018 |
| Fernández-Fueyo, Elena; et al. | Description of a Non-Canonical Mn (II)-Oxidation Site in Peroxidases | ACS Catalysis | 8 | 8386-8395 | 2018 |
| Robert, Viviane; et al. | Corrigendum: Probing the Surface of a Laccase for Clues towards the Design of Chemo-Enzymatic Catalysts | ChemPlusChem | 83 | 831-831 | 2018 |
| Liu, Qing;et al. | Kauniolide synthase is a P450 with unusual hydroxylation and cyclization-elimination activity | Nature communications | 9 | 4657 | 2018 |
| Khersonsky, Olga;et al. | Automated design of efficient and functionally diverse enzyme repertoires | Molecular cell | 72 | 178-186. e5 | 2018 |
| Sancho, Ferran; Santiago, Gerard; Amengual-Rigo, Pep; Guallar, Victor; | Modeling O2-dependent Heme Enzymes: A Quick Guide for Non-experts | Dioxygen-dependent Heme Enzymes | | 222-248 | 2018 |
| Giacobelli, Valerio Guido; et al. | Repurposing designed mutants: a valuable strategy for computer-aided laccase engineering–the case of POXA1b | Catalysis Science & Technology | 7 | 515-523 | 2017 |
| Robert, Viviane; et al. | Probing the Surface of a Laccase for Clues towards the Design of Chemo-Enzymatic Catalysts | ChemPlusChem | 82 | 607-614 | 2017 |
| Lucas, Maria Fátima; et al. | Simulating substrate recognition and oxidation in laccases: from description to design | Journal of chemical theory and computation | 13 | 1462-1467 | 2017 |
| Monza, Emanuele; Acebes, Sandra; Lucas, M Fátima; Guallar, Victor; | Molecular Modeling in Enzyme Design, Toward In Silico Guided Directed Evolution | Directed Enzyme Evolution: Advances and Applications | | 257-284 | 2017 |
| Grebner, Christoph;et al. | Exploring binding mechanisms in nuclear hormone receptors by Monte Carlo and X-ray-derived motions | Biophysical journal | 112 | 1147-1156 | 2017 |
| Acebes, Sandra; et al. | Mapping the long-range electron transfer route in ligninolytic peroxidases | The Journal of Physical Chemistry B | 121 | 3946-3954 | 2017 |
| Fatima Lucas, Maria; et al. | Simulating Substrate Recognition and Oxidation in Laccases: From Description to Designa | JOURNAL OF CHEMICAL THEORY AND COMPUTATION | 13 | 1462-1467 | 2017 |
| Hermosilla, Pedro; Krone, Michael; Guallar, Victor; Vázquez, Pere-Pau; Vinacua, Àlvar; Ropinski, Timo; | Interactive GPU-based generation of solvent-excluded surfaces | The Visual Computer | 33 | 869-881 | 2017 |
| Martínez, Angel T; et al. | Oxidoreductases on their way to industrial biotransformations | Biotechnology advances | 35 | 815-831 | 2017 |
| Kotev, Martin; et al. | Inhibition of human enhancer of zeste homolog 2 with tambjamine analogs | Journal of chemical information and modeling | 57 | 2089-2098 | 2017 |
| Lecina, Daniel; Gilabert, Joan F; Guallar, Victor; | Adaptive simulations, towards interactive protein-ligand modeling | Scientific reports | 7 | 8466 | 2017 |

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| Peccati, Francesca; et a;. | Binding of Thioflavin T and Related Probes to Polymorphic Models of Amyloid-β Fibrils | The Journal of Physical Chemistry B | 121 | 8926-8934 | 2017 |
| Monza, Emanuele; Blouin, George; Spiro, Thomas G; Guallar, Victor; | Allosteric signalling paths in hemoglobin: a protein dynamics network analysis | BioRxiv | | 134288 | 2017 |
| Gygli, Gudrun; Lucas, Maria Fátima; Guallar, Victor; van Berkel, Willem JH; | The ins and outs of vanillyl alcohol oxidase: Identification of ligand migration paths | PLoS computational biology | 13 | e1005787 | 2017 |
| Martínez-Martínez, Mónica; et al. | Determinants and prediction of esterase substrate promiscuity patterns | ACS chemical biology | 13 | 225-234 | 2017 |
| Hermosilla, Pedro; Guallar, Víctor; Vinacua, Alvar; Vázquez, Pere-Pau; | High quality illustrative effects for molecular rendering | Computers & Graphics | 54 | 113-120 | 2016 |
| Lucas, Fátima;et al. | Molecular determinants for selective C 25-hydroxylation of vitamins D 2 and D 3 by fungal peroxygenases | Catalysis Science & Technology | 6 | 288-295 | 2016 |
| Bayó-Puxan, Núria; et al. | Combined use of oligopeptides, fragment libraries, and natural compounds: a comprehensive approach to sample the druggability of vascular endothelial growth factor | ChemMedChem | 11 | 928-939 | 2016 |
| Molina-Espeja, Patricia; et al. | Synthesis of 1-Naphthol by a Natural Peroxygenase Engineered by Directed Evolution | ChemBioChem | 17 | 341-349 | 2016 |
| Pardo, Isabel;et al. | Re-designing the substrate binding pocket of laccase for enhanced oxidation of sinapic acid | Catalysis Science & Technology | 6 | 3900-3910 | 2016 |
| Acebes, Sandra; et al. | Rational enzyme engineering through biophysical and biochemical modeling | ACS Catalysis | 6 | 1624-1629 | 2016 |
| López, Abraham; et al. | Active-Site-Directed Inhibitors of Prolyl Oligopeptidase Abolish Its Conformational Dynamics | Chembiochem | 17 | 913-917 | 2016 |
| Hosseini, Ali; et al. | Computational prediction of HIV-1 resistance to protease inhibitors | Journal of chemical information and modeling | 56 | 915-923 | 2016 |
| Sáez-Jiménez, et al. | Unveiling the basis of alkaline stability of an evolved versatile peroxidase | Biochemical Journal | 473 | 1917-1928 | 2016 |
| Cabeza de Vaca, Israel; Acebes, Sandra; Guallar, Victor; | Ecoupling server: A tool to compute and analyze electronic couplings | Journal of computational chemistry | 37 | 1740-1745 | 2016 |
| Linde, Dolores; et al. | Asymmetric sulfoxidation by engineering the heme pocket of a dye-decolorizing peroxidase | Catalysis Science & Technology | 6 | 6277-6285 | 2016 |
| Gil, Victor A; Lecina, Daniel; Grebner, Christoph; Guallar, Victor; | Enhancing backbone sampling in Monte Carlo simulations using internal coordinates normal mode analysis | Bioorganic & medicinal chemistry | 24 | 4855-4866 | 2016 |
| Santiago, Gerard; et al. | Computer-aided laccase engineering: toward biological oxidation of arylamines | ACS Catalysis | 6 | 5415-5423 | 2016 |
| Hermosilla, Pedro; Estrada, Jorge; Guallar, Victor; Ropinski, Timo; Vinacua, Alvar; Vazquez, Pere-Pau; | Physics-based visual characterization of molecular interaction forces | IEEE transactions on visualization and computer graphics | 23 | 731-740 | 2016 |
| Deri, Batel; et al. | The unravelling of the complex pattern of tyrosinase inhibition | Scientific reports | 6 | 34993 | 2016 |

## C.2 Top Recent Representative Conference Oral presentations

- Frank Wallrap and Victor Guallar, "QM/MM e-pathway: mapping Electron transfer processes in proteins", ACS National Meeting –San Franciscisco, USA (2010)
- Victor Guallar, "Induced Fit Modelling with Monte Carlo techniques: protein Energy Landscape Exploration", 11th Structure based Drug design (SBDD), Boston, USA (2011)
- Victor Guallar, "Mapping ligand dynamics pathways in globin systems ", II International BIC Symposium, University of Canterbury, ChristChurch, New Zealand (2012)
- *Victor Guallar* "QM and MM methods: Obtaining an electronic and atomic view of nature", 2nd Synthetic Biology Minisymposium, National University of Singapore, Singapore (2013)
- *Victor Guallar* "*Coupling Protein Dynamics with Active Site Chemistry: a MM and QM tale*" ICPP8 International Conference on Porphyrins and Phtalocyanines, Istanbul, Turkey (2014)
- *Victor Guallar* "On the Fly Molecular Simulations for a Visual Interactive Use". 1st Symposium: Molecular Visualization. ULM, Germany (2015)
- *Victor Guallar* ""Mapping oxidoreductases biochemistry by computational tools", 8th Oxizymes meeting. Wageningen, The Netherlands (2016)
- *Victor Guallar* "PELE Studio: the next generation interactive and smart molecular design software", 7th Visegrad Symposium on Structural Systems Biology. Nove Hrady, Czech Republic (2017)
- *Victor Guallar* "Got Enzymes?A la Carte Design through Molecular Modeling", Industrial Biotechnology Forum (IBF) 2018. Munich, Germany (2018)
- Victor Guallar, "Adaptive Monte Carlo Techniques for Drug Design", 2019 Structure based Drug design (SBDD), Sestri Levante, Italy (2019)

### C.3. Recent Research projects and grants

Title: COMPUTATIONAL RATIONAL DESIGN OF OXIDOREDUCTASES FOR INDUSTRIAL AND TECHNOLOGICAL APPLICATIONS Project Number CTQ2013-48287-R
Agency: Ministerio de Educación i Ciencia PI: Victor Guallar
Length: 2014-2017 Amount: 131.000 euros

Title: "PELE, A la carte drug design" Project Number: 250277-PELE
Agency: European Research Council. ERC-2009-AdG , PI: Victor Guallar
Length: 06/2010- 06/2015 Amount: 1.400.000 euros

Title: "*Drug eDesign: Building the next generation of software solutions for drug design*" Project Number: H2020 - ERC-2014-PoC
Agency: European Research Council. PI: Victor Guallar
Length: 01/2015 06/2016 Amount: 150.000 euros

Title: "INDOX, Optimized oxidoreductases for medium and large scale industrial biotransformations" Project Number: KBBE- 613549
Agency: European Union PI: Angel Martinez
Length: 11/2013- 11/2016 Amount awarded to Guallar's lab: 349.200 euros

Título del proyecto: PELE-e a new platform for enzime engineeging Project Number: ISETE
Agency: La Caixa (CaixaImpulse program) PI: Victor Guallar
Lenght: 2017-2018 Amount: 70.000 euros

Title: VMUTATE: UNA PLATAFORMA PARA LA INGENIERIA DE ENZIMAS Project Number: CTQ2016-79138-R
Agency: Ministerio de Economia y Competividad PI: Victor Guallar
Lenght: 2017-2020 Amount: 144.000 euros

Title: SilicoDerm: Desarrollo de nuevas metodologías computacionales aplicadas a dianas terapéuticas dermatológicas para acelerar la identificación y optimización de entidades químicas Project Number: RTC-2017-6295-1
Agency: Ministerio de Economia y Competividad Academic-PI: Victor Guallar
Lenght: 2018-2021 Amount: 198.000 euros

Title: Using PELE for personalized Medicine Project Number: NA
Agency: IBM-Deep learning center Academic-PI: Victor Guallar
Lenght: 2017-2019 Amount: 150.000 euros

Title: Diseño de antivirales para SARS basados en polifarmacologia Project Number: COV20/00505
Agency:Ministerio de Economia y Competividad Academic-PI: Victor Guallar
Lenght: 2020-2021 Amount:196.000 euros

### C.4. Contracts

Type: Consultant and software development
Financing Company: Schrodinger Inc. (USA)
Duration: Since 2003 (annually renewed) PI: Victor Guallar

Type: Knowledge transfer between BSC and Anaxomics, within the project FP7-KBBE-2013-7-613549
Financing Company: ANAXOMICS BIOTECH S.L.
Duration: 2013 – 2016 PI: Victor Guallar

Type: Methods development on ligand binding
Financing Company: AstraZeneca and NBD (since 2016)
Duration: Since 2014 (annually renewed) PI: Victor Guallar

### C.5. Patents

Notary register and transfer of the PELE technology to Nostrum Biodiscovery