CV date	Jan/2025

Part A. PERSONAL INFORMATION

First and Family name	Victor Guallar			
Social Security, Passport, ID number	43714250J		Age	53
Researcher numbers		Researcher ID	B-1579-2013	
		Orcid code	0000-0002-4580-1114	

A.1. Academic position

Name of University/Institution	Barcelona Supercomputing Center		
Department	Life Sciences		
Address and Country	Jordi Girona 29, 08034 Barcelona (Spain)		
Phone number	34934137727	E-mail	Victor.guallar@bsc.es
Current position	ICREA Professor	From	07 / 2006
Espec. cód. UNESCO	*230226*		

Synergistic positions:

Since 2020: **CSO** at **Nostrum Biodiscovery**

Since 2016: 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 Berkeley	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

200 publications in international peer-reviewed journals (~90% in Q1)

Statistics from Google Scholar (at 1/25):   Total number of citations: 9640

H index: 53 (34 since 2020)   I10 index: 164 (113 since 2020)

Prof Guallar has directed 21 PhD thesis (with 12 more ongoing)
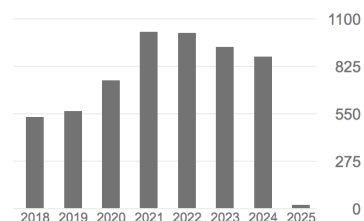
Part B. CV SUMMARY *(max. 3500 characters, including spaces)*

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 an advanced ERC). 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* 2020, *Nature Catalysis* 2023).

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 six EU-consortiums, and obtained two ERC grants. Overall Prof Guallar has guaranteed over 7 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. Publications (representative ones for the last 3 years)

Authors	Title	Publication	Volume	Pages	Year
Ana Barajas, Pep Amengual-Rigo, Anna Pons-Grífols, Raquel Ortiz, et al.	**Virus-like particle-mediated delivery of structure-selected neoantigens demonstrates immunogenicity and antitumoral activity in mice**	**Journal of Translational Medicine**	**22**	**14**	**2024**

Authors	Title	Journal	Vol	Pages	Year
C Ávila-Nieto, J Vergara-Alert, P Amengual-Rigo, wt al.	Immunization with V987H-stabilized Spike glycoprotein protects K18-hACE2 mice and golden Syrian hamsters upon SARS-CoV-2 infection	Nature Communications	15	2349	2024
A Morales-Pastor, L Malo, I Filella-Merce, V Guallar, A Molina	Scoreformer: A Surrogate Model For Large-Scale Prediction of Docking Scores	ICML'24			2024
Carles Perez-Lopez, Alexis Molina, Estrella Lozoya, Victor Segarra, Marti Municoy, Victor Guallar	Combining machine-learning and molecular-modeling methods for drug-target affinity predictions	Wiley Interdisciplinary Reviews: Computational Molecular Science	13	e1653	2023
Díaz-Rovira, Anna M; Martin, Helena; Beuming, Thijs; Díaz, Lucía; Guallar, Victor; Ray, Soumya S;	Are deep learning structural models sufficiently accurate for virtual screening? Application of docking algorithms to AlphaFold2 predicted structures	Journal of Chemical Information and Modeling	63	1668-1674	2023
Robles-Martín, Ana; Amigot-Sánchez, Rafael; Fernandez-Lopez, Laura	Sub-micro-and nano-sized polyethylene terephthalate deconstruction with engineered protein nanopores	Nature Catalysis	12	1	2023
Xu, Xiaomin; van Hengst, Jacob MA; Mao, Yejia; Martinez, Mireia; Roda, Sergi; Floor, Martin; Guallar, Victor; Paul, Caroline E; Alcalde, Miguel; Hollmann, Frank;	Peroxygenase-Catalysed Selective Oxidation of Silanes to Silanols	Angewandte Chemie International Edition	62	e202302844	2023
Roda, Sergi; Fernandez-Lopez, Laura; Benedens, Marius; Bollinger, Alexander; Thies, Stephan; Schumacher, Julia; Coscolín, Cristina; Kazemi, Masoud; Santiago, Gerard; Gertzen, Christoph GW;	A plurizyme with transaminase and hydrolase activity catalyzes cascade reactions	Angewandte Chemie	134	e202207344	2022
Rodon, Jordi; Muñoz-Basagoiti, Jordana; Perez-Zsolt, Daniel; Noguera-Julian, Marc; Paredes, Roger; Mateu, Lourdes; Quiñones, Carles; Perez, Carles; Erkizia, Itziar; Blanco, Ignacio;	Identification of plitidepsin as potent inhibitor of SARS-CoV-2-induced cytopathic effect after a drug repurposing screen	Frontiers in pharmacology	12	646676	2021
Amengual-Rigo, Pep; Fernández-Recio, Juan; Guallar, Victor;	UEP: an open-source and fast classifier for predicting the impact of mutations in protein–protein complexes	Bioinformatics	37	334-341	2021
Roda, Sergi; Fernandez-Lopez, Laura; Canadas, Ruben; Santiago, Gerard; Ferrer, Manuel; Guallar, Victor;	Computationally driven rational design of substrate promiscuity on serine ester hydrolases	ACS Catalysis	11	3590-3601	2021
Amengual-Rigo, Pep; Guallar, Victor;	NetCleave: an open-source algorithm for predicting C-terminal antigen processing for MHC-I and MHC-II	Scientific reports	11	13126	2021

C.2 Top Recent Representative Conference Oral presentations

- *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)

- <u>Victor Guallar</u>, "Adaptive Monte Carlo Techniques for Drug Design", 2019 Structure based Drug design (SBDD), Sestri Levante, Italy (2019)
- <u>Victor Guallar</u>, "Tailored AI&MM modelling for Enzyme Engineering and Bioprospecting", CLIB International conference, Dusseldorf, Germany (2022)
- <u>Victor Guallar</u>, "Artificial Intelligence for Early Drug Discovery", 2022 Drug Discovery Chemistry, San Diego, USA (2022)
- <u>Victor Guallar</u>, "Combining Machine Learning and Molecular Modeling in Drug Discovery", 2022 Drug on Target, Boston, USA (2022)
- <u>Victor Guallar</u>, "Adaptive Learning for the Next Generation of Molecular Screening, a Tasting Recipe", 2023 Discovery on Target, Boston, USA (2023)
- <u>Victor Guallar</u>, "Active Learning Processes in Biomolecular Modelling", 24th EuroQSAR, Barcelona, SPAIN (2024)
- <u>Victor Guallar</u>, "GlueE3, A Modelling Platform for True Rational MG Screening", 4th TPD Europe, London, UK (2024)

C.3. Recent Representative Research projects and grants
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: 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

Title: Technologies of the Future for Low-Cost Enzymes for Environment-Friendly Products
Project Number: 101000327 Agency:EU-2020/FNR-16-2020   PI: Manuel Ferrer (CSIC)
Lenght: 2021-2025   Amount-BSC: 330.000 euros

Title: Transition towards environment-friendly consumer products by co-creation of an oxidoreductase foundry
Project Number: 101000607-2 Agency:EU-2020/FNR-16-2020   PI: Gro Elin Kjæreng (NORCE)
Lenght: 2021-2025   Amount-BSC: 420.000 euros (PI BSC: Victor Guallar)

Title: Enzymatic Synthesis and Recycling of Biobased Furanic Polymers. Project Number: PDC2021-121117-I00
Agency: Ministerio de Economia y Competividad   Academic-PI: Angel Martinez (CSIC)
Lenght: 10/2021-11/2024   Amount: 117.000 euros (BSC budget)

Title: Title: Robust industrial biocatalysts with peroxygenase, phenol-oxidase or furfuryl-oxidase activities from bacterial and fungal hosts. Project Number: CIRCBIO-01 – 101135119
Agency: EU-HORIZON-CL6-2023   PI: SUSANA CAMARERO (CSIC)
Lenght: 1/2024-12/2027   Amount-BSC: 418.750 euros (PI BSC: Victor Guallar)

Title: Synthetic proteins for sustainable animal feeding. Project Number: PATHFINDEROPEN-01 -101186580
Agency: EU-2024/EIC   PI: Juanjo Pascual (UDV)
Lenght: 2/2025-01/2029   Amount-BSC: 468.125 euros (PI BSC: Victor Guallar)

C.4. Contracts
Type: Subcontract within a MIsiones grant for Vaccine development
Financing Company: Nostrum Biodiscovery (with HIPRA the grant coordinator)
Duration: 2021 – 2023   PI: Victor Guallar

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