CV date	1/2020

Part A. PERSONAL INFORMATION

First and Family name	Victor Guallar		
Social Security, Passport, ID number	43714250J	Age	48
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	34934137727	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

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

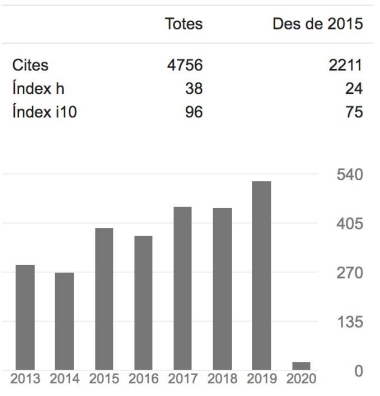
Statistics from Google Scholar:

Total number of citations: 4756

H index: 38 (24 since 2015)

I10 index: 96 (75 since 2014)

Prof Guallar has directed 14 PhD thesis (with 6 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. Full Publication list

Authors	Title	Publication	Volume	Pages	Year
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
Alonso, Sandra;	Genetically engineered proteins with two active sites for enhanced biocatalysis and synergistic chemo-and biocatalysis	Nature Catalysis		1-10	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
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
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
Linde, Dolores;et al.	Catalytic surface radical in dye-decolorizing peroxidase: a computational, spectroscopic and site-directed mutagenesis study	Biochemical Journal	466	253-262	2015
Kotev, Martin; Lecina, Daniel; Tarragó, Teresa; Giralt, Ernest; Guallar, Víctor;	Unveiling prolyl oligopeptidase ligand migration by comprehensive computational techniques	Biophysical journal	108	116-125	2015

Linde, Dolores; et al.	Basidiomycete DyPs: genomic diversity, structural–functional aspects, reaction mechanism and environmental significance	Archives of biochemistry and biophysics	574	66-74	2015
Ferreira, Patricia; et al	Aromatic stacking interactions govern catalysis in aryl-alcohol oxidase	The FEBS journal	282	3091-3106	2015
Monza, Emanuele; Lucas, M Fatima; Camarero, Susana; Alejaldre, Lorea C; Martínez, Angel T; Guallar, Victor;	Insights into laccase engineering from molecular simulations: Toward a binding-focused strategy	The journal of physical chemistry letters	6	1447-1453	2015
Babot, Esteban D; et al.	Steroid hydroxylation by basidiomycete peroxygenases: a combined experimental and computational study	Appl. Environ. Microbiol.	81	4130-4142	2015
Sáez-Jiménez, Verónica; Acebes, Sandra; Guallar, Victor; Martínez, Angel T; Ruiz-Dueñas, Francisco J;	Improving the oxidative stability of a high redox potential fungal peroxidase by rational design	PLoS One	10	e0124750	2015
Skånberg, Robin; Vazquez, Pere-Pau; Guallar, Victor; Ropinski, Timo;	Real-time molecular visualization supporting diffuse interreflections and ambient occlusion	IEEE transactions on visualization and computer graphics	22	718-727	2015
Giannotti, Marina I; Cabeza de Vaca, Israel; Artés, Juan M; Sanz, Fausto; Guallar, Victor; Gorostiza, Pau;	Direct measurement of the nanomechanical stability of a redox protein active site and its dependence upon metal binding	The Journal of Physical Chemistry B	119	12050-12058	2015
Saen-Oon, Suwipa; de Vaca, Israel Cabeza; Masone, Diego; Medina, Milagros; Guallar, Victor;	A theoretical multiscale treatment of protein–protein electron transfer: The ferredoxin/ferredoxin-NADP+ reductase and flavodoxin/ferredoxin-NADP+ reductase systems	Biochimica et Biophysica Acta (BBA)-Bioenergetics	1847	1530-1538	2015
Kopečná, Jana; et al.	Porphyrin binding to Gun4 protein, facilitated by a flexible loop, controls metabolite flow through the chlorophyll biosynthetic pathway	Journal of Biological Chemistry	290	28477-28488	2015
Edman, Karl;et al.	Ligand binding mechanism in steroid receptors: from conserved plasticity to differential evolutionary constraints	Structure	23	2280-2290	2015
Cabeza de Vaca, Israel; Lucas, Maria Fátima; Guallar, Victor;	New Monte Carlo based technique to study DNA–ligand interactions	Journal of chemical theory and computation	11	5598-5605	2015
Hermosilla, Pedro;et al.	Instant visualization of secondary structures of molecular models	VCBM 15:		51-60	2015
Lucas, Maria; Guallar, Víctor;	Protein engineering: what's next?: PI-025	Protein Science	24		2015
Hermosilla, Pedro; Guallar, Víctor; Vinacua Pla, Álvaro; Vázquez Alcocer, Pere Pau;	Adaptive on-the-fly molecular ribbons generation	EuroVis 2015: The EG/VGTC Conference on Visualization: Posters track		1-3	2015
Lucas, Maria F; et al.	Atomic level rendering of DNA-drug encounter	Biophysical journal	106	421-429	2014
Hosseini, Ali; et al.	Atomic picture of ligand migration in toluene 4-monooxygenase	The Journal of Physical Chemistry B	119	671-678	2014
Jones, Eric M; et al.	Differential control of heme reactivity in alpha and beta subunits of hemoglobin: A combined Raman spectroscopic and computational study	Journal of the American Chemical Society	136	10325-10339	2014
Gil, Víctor A; Guallar, Víctor;	pyProCT: automated cluster analysis for structural bioinformatics	Journal of chemical theory and computation	10	3236-3243	2014
Esteban-Martín, Santiago; et al.	Correlated inter-domain motions in adenylate kinase	PLoS computational biology	10	e1003721	2014

Saen-oon, Suwipa; Lee, Soon Goo; Jez, Joseph M; Guallar, Victor;	An alternative mechanism for the methylation of phosphoethanolamine catalyzed by Plasmodium falciparum phosphoethanolamine methyltransferase	Journal of Biological Chemistry	289	33815-33825	2014
Andreotti, Giuseppina;et al.	Conformational Response to Ligand Binding in Phosphomannomutase2	Journal of Biological Chemistry	289	34900-34910	2014
Fernández-Fueyo, Elena; et al.	Structural implications of the C-terminal tail in the catalytic and stability properties of manganese peroxidases from ligninolytic fungi	Acta Crystallographica Section D: Biological Crystallography	70	3253-3265	2014
Rao, Satish; et al.	Direct observation of single DNA structural alterations at low forces with surface-enhanced Raman scattering	Biophysical journal	104	156-162	2013
Lucas, M Fátima; Guallar, Víctor;	Single vs. multiple ligand pathways in globins: A computational view	Biochimica et Biophysica Acta (BBA)-Proteins and Proteomics	1834	1739-1743	2013
Hosseini, Ali; et al.	Molecular interactions of prodiginines with the BH3 domain of anti-apoptotic Bcl-2 family members	PloS one	8	e57562	2013
Wallrapp, Frank H; Voityuk, Alexander A; Guallar, Victor;	In-silico assessment of protein-protein electron transfer. A case study: cytochrome c peroxidase–cytochrome c	PLoS computational biology	9	e1002990	2013
Valdés, James J; et al.	Tryptogalinin is a tick Kunitz serine protease inhibitor with a unique intrinsic disorder	PLoS One	8	e62562	2013
Madadkar-Sobhani, Armin; Guallar, Victor;	PELE web server: atomistic study of biomolecular systems at your fingertips	Nucleic acids research	41	W322-W328	2013
Saen-Oon, Suwipa; Lucas, Maria Fatima; Guallar, Victor;	Electron transfer in proteins: theory, applications and future perspectives	Physical Chemistry Chemical Physics	15	15271-15285	2013
Gil, Víctor A; Guallar, Víctor;	pyRMSD: a Python package for efficient pairwise RMSD matrix calculation and handling	Bioinformatics	29	2363-2364	2013
Takahashi, Ryoji; Gil, Víctor A; Guallar, Victor;	Monte Carlo free ligand diffusion with Markov state model analysis and absolute binding free energy calculations	Journal of chemical theory and computation	10	282-288	2013
Spyrakis, Francesca; et al.	Comparative analysis of inner cavities and ligand migration in non-symbiotic AHb1 and AHb2	Biochimica et Biophysica Acta (BBA)-Proteins and Proteomics	1834	1957-1967	2013
Miki, Yuta; et al.	Formation of a tyrosine adduct involved in lignin degradation by Trametopsis cervina lignin peroxidase: a novel peroxidase activation mechanism	Biochemical Journal	452	575-584	2013
Masone, Diego; Cabeza de Vaca, Israel; Pons, Carles; Recio, Juan Fernandez; Guallar, Victor;	H-bond network optimization in protein–protein complexes: Are all-atom force field scores enough?	Proteins: Structure, Function, and Bioinformatics	80	818-824	2012
Espona-Fiedler, Margarita; et al.	Identification of dual mTORC1 and mTORC2 inhibitors in melanoma cells: prodigiosin vs. obatoclax	Biochemical pharmacology	83	489-496	2012
Hernández-Ortega, Aitor; et al.	Stereoselective hydride transfer by aryl-alcohol oxidase, a member of the GMC superfamily	ChemBioChem	13	427-435	2012
Cossins, Benjamin P; Hosseini, Ali; Guallar, Victor;	Exploration of protein conformational change with PELE and meta-dynamics	Journal of chemical theory and computation	8	959-965	2012
Yu, Michelle A; et al.	Two tyrosyl radicals stabilize high oxidation states in cytochrome C oxidase for efficient energy conservation and proton translocation	Journal of the American Chemical Society	134	4753-4761	2012

Lucas, M Fátima; Guallar, Víctor;	An atomistic view on human hemoglobin carbon monoxide migration processes	Biophysical journal	102	887-896	2012
Espona-Fiedler, M; Soto-Cerrato, V; Hosseini, A; Guallar, V; Perez-Tomas, R;	990 Prodigiosin, a New Bcl-2 Homology Domain-3 Mimetic Proapoptotic Drug	european journal of cancer	48	S239	2012
Hernández-Ortega, Aitor; et al.	Role of active site histidines in the two half-reactions of the aryl-alcohol oxidase catalytic cycle	Biochemistry	51	6595-6608	2012
Rousseau, Denis L; et al.	Two tyrosyl radicals stabilize high oxidation states in cytochrome c oxidase for efficient energy conservation and proton translocation	Biophysical Journal	102	466a	2012
F Lucas, Maria; Masone, Diego; Saen-oon, Suwipa; Wallrapp, Frank; Guallar, Víctor;	Using QM/MM Methods for the Exploration of Electron Transfer Pathways	Current Inorganic Chemistry	2	263-272	2012
Daskalakis, Vangelis; Farantos, Stavros C; Guallar, Victor; Varotsis, Constantinos;	Regulation of electron and proton transfer by the protein matrix of cytochrome c oxidase	The Journal of Physical Chemistry B	115	3648-3655	2011
Hernández-Ortega, Aitor; et al.	Substrate diffusion and oxidation in GMC oxidoreductases: an experimental and computational study on fungal aryl-alcohol oxidase	Biochemical Journal	436	341-350	2011
Hernández-Ortega, Aitor; et al.	Modulating O2 reactivity in a fungal flavoenzyme involvement of aryl-alcohol oxidase PHE-501 contiguous to catalytic histidine	Journal of Biological Chemistry	286	41105-41114	2011
Cossins, Benjamin P; Jacobson, Matthew P; Guallar, Victor;	A new view of the bacterial cytosol environment	PLoS computational biology	7	e1002066	2011
Lucas, M Fátima; Rousseau, Denis L; Guallar, Victor;	Electron transfer pathways in cytochrome c oxidase	Biochimica et Biophysica Acta (BBA)-Bioenergetics	1807	1305-1313	2011
Wallrapp, Frank H; Guallar, Victor;	Mixed quantum mechanics and molecular mechanics methods: Looking inside proteins	Wiley Interdisciplinary Reviews: Computational Molecular Science	1	315-322	2011
Guallar, Victor; Wallrapp, Frank H;	QM/MM methods: Looking inside heme proteins biochemisty	Biophysical chemistry	149	1-11	2010
Borrelli, Kenneth W; Cossins, Benjamin; Guallar, Victor;	Exploring hierarchical refinement techniques for induced fit docking with protein and ligand flexibility	Journal of computational chemistry	31	1224-1235	2010
Wallrapp, Frank H; Voityuk, Alexander A; Guallar, Victor;	Temperature Effects on Donor− Acceptor Couplings in Peptides. A Combined Quantum Mechanics and Molecular Dynamics Study	Journal of chemical theory and computation	6	3241-3248	2010
Rao, Satish; Bálint, Štefan; Cossins, Benjamin; Guallar, Victor; Petrov, Dmitri;	Raman study of mechanically induced oxygenation state transition of red blood cells using optical tweezers	Biophysical journal	96	209-216	2009
Guallar, Victor; Lu, Changyuan; Borrelli, Kenneth; Egawa, Tsuyoshi; Yeh, Syun-Ru;	Ligand Migration in the Truncated Hemoglobin-II from Mycobacterium tuberculosis THE ROLE OF G8 TRYPTOPHAN	Journal of Biological Chemistry	284	3106-3116	2009
Wallrapp, Frank; Voityuk, Alexander; Guallar, Victor;	Solvent Effects on Donor− Acceptor Couplings in Peptides. A Combined QM and MD Study	Journal of chemical theory and computation	5	3312-3320	2009
Pipirou, Zoi;et al.	Peroxide-dependent formation of a covalent link between Trp51 and the heme in cytochrome c peroxidase	Biochemistry	48	3593-3599	2009
Daskalakis, Vangelis; Farantos, Stavros C; Guallar, Victor; Varotsis, Constantinos;	Vibrational resonances and CuB displacement controlled by proton motion in cytochrome c oxidase	The Journal of Physical Chemistry B	114	1136-1143	2009
Rao, Satish K; Balint, Stefan; Cossins, Benjamin;	Monitoring of mechanically induced transitions in biology using Raman tweezers	Biophysical Journal	96	311a	2009

Guallar, Victor; Petrov, Dmitri;					
Rao, Satish; Balint, Stefan; Cossins, Benjamin; Guallar, Victor; Petrov, Dmitri;	Raman study of mechanically indued oxygenation state transition of red blood cells using optical tweezers.(vol 96, pg 209, 2009)	Biophysical Journal	96	2043-2043	2009
Fenosa, Anna; Fusté, Ester; Ruiz, Lidia; Veiga-Crespo, Patricia; Vinuesa, Teresa; Guallar, Victor; Villa, Tomas G; Viñas, Miguel;	Role of TolC in Klebsiella oxytoca resistance to antibiotics	Journal of antimicrobial chemotherapy	63	668-674	2009
Rao, Satish; Balint, # 138tefan; Cossins, Benjamin; Guallar, Victor; Petrov, Dmitri;	Spectroscopy, Imaging, Other Techniques-Raman Study of Mechanically Induced Oxygenation State Transition of Red Blood Cells Using Optical Tweezers	Biophysical Journal	96	209	2009
Guallar, Victor;	Heme electron transfer in peroxidases: The propionate e-pathway	The Journal of Physical Chemistry B	112	13460-13464	2008
Martí, Marcelo A; et al.	Mechanism of product release in NO detoxification from Mycobacterium tuberculosis truncated hemoglobin	Journal of the American Chemical Society	130	1688-1693	2008
Wallrapp, Frank; Masone, Diego; Guallar, Victor;	Electron transfer in the P450cam/PDX complex. The QM/MM e-pathway	The Journal of Physical Chemistry A	112	12989-12994	2008
Guallar, Victor; Wallrapp, Frank;	Mapping protein electron transfer pathways with QM/MM methods	Journal of The Royal Society Interface	5	233-239	2008
Marti, Marcelo A; et al.	Nitric oxide reactivity with globins as investigated through computer simulation	Methods in enzymology	437	477-498	2008
Wang, Qin; Xia, Jiarong; Guallar, Victor; Krilov, Goran; Kantrowitz, Evan R;	Mechanism of thermal decomposition of carbamoyl phosphate and its stabilization by aspartate and ornithine transcarbamoylases	Proceedings of the National Academy of Sciences	105	16918-16923	2008
Martı, MA; Bidon-Chanal, A; Crespo, A; Yeh, SR; Guallar, V; Luque, FJ; Estrin, DA;	Mechanism of product release in NO detoxification from Mycobacterium tuberculosis truncated hemoglobin NJ Am	Chem. Soc	130	1688-1693	2008
Alcantara, RE; Xu, C; Spiro, TG; Guallar, V;	A quantum-chemical picture of hemoglobin affinity	Proceedings of the National Academy of Sciences	104	18451-18455	2007
Guallar, Victor;	QMMM methods for the spin density in heme compound I	AIP Conference Proceedings	963	315-317	2007
Altun, Ahmet; Guallar, Victor; Friesner, Richard A; Shaik, Sason; Thiel, Walter;	The effect of heme environment on the hydrogen abstraction reaction of camphor in P450cam catalysis: A QM/MM study	Journal of the American Chemical Society	128	3924-3925	2006
Guallar, Victor; Olsen, Brett;	The role of the heme propionates in heme biochemistry	Journal of inorganic biochemistry	100	755-760	2006
Guallar, Victor; Jarzecki, Andrzej A; Friesner, Richard A; Spiro, Thomas G;	Modeling of ligation-induced helix/loop displacements in myoglobin: toward an understanding of hemoglobin allostery	Journal of the American Chemical Society	128	5427-5435	2006
Small, Yolanda A; et al	Hydrogen bonding pathways in human dihydroorotate dehydrogenase	The Journal of Physical Chemistry B	110	19704-19710	2006
Friesner, Richard A; Guallar, Victor;	Ab initio quantum chemical and mixed quantum mechanics/molecular mechanics (QM/MM) methods for studying enzymatic catalysis	Annu. Rev. Phys. Chem.	56	389-427	2005
Cho, Art E; Guallar, Victor; Berne, Bruce J; Friesner, Richard;	Importance of accurate charges in molecular docking: quantum mechanical/molecular mechanical (QM/MM) approach	Journal of computational chemistry	26	915-931	2005
Song, Yuhua; Guallar, Victor; Baker, Nathan A;	Molecular dynamics simulations of salicylate effects on the micro-and mesoscopic properties of a dipalmitoylphosphatidylcholine bilayer	Biochemistry	44	13425-13438	2005
Borrelli, Kenneth W; Vitalis, Andreas; Alcantara, Raul; Guallar, Victor;	PELE: protein energy landscape exploration. A novel Monte Carlo based technique	Journal of chemical theory and computation	1	1304-1311	2005

Guallar, Victor; Borrelli, Kenneth W;	A binding mechanism in protein–nucleotide interactions: implication for U1A RNA binding	Proceedings of the National Academy of Sciences	102	3954-3959	2005
Guallar, Victor; Friesner, Richard A;	Cytochrome P450CAM enzymatic catalysis cycle: a quantum mechanics/molecular mechanics study	Journal of the American Chemical Society	126	8501-8508	2004
Guallar, Victor; Jacobson, Matt; McDermott, Ann; Friesner, Richard A;	Computational modeling of the catalytic reaction in triosephosphate isomerase	Journal of molecular biology	337	227-239	2004
Guallar, Victor; Baik, Mu-Hyun; Lippard, Stephen J; Friesner, Richard A;	Peripheral heme substituents control the hydrogen-atom abstraction chemistry in cytochromes P450	Proceedings of the National Academy of Sciences	100	6998-7002	2003
Friesner, Richard A; Baik, Mu-Hyun; Gherman, Benjamin F; Guallar, Victor; Wirstam, Maria; Murphy, Robert B; Lippard, Stephen J;	How iron-containing proteins control dioxygen chemistry: a detailed atomic level description via accurate quantum chemical and mixed quantum mechanics/molecular mechanics calculations	Coordination Chemistry Reviews	238	267-290	2003
Guallar, Victor; Gherman, Benjamin F; Miller, William H; Lippard, Stephen J; Friesner, Richard A;	Dynamics of alkane hydroxylation at the non-heme diiron center in methane monooxygenase	Journal of the American Chemical Society	124	3377-3384	2002
Guallar, Victor; Harris, Danni L; Batista, Victor S; Miller, William H;	Proton-transfer dynamics in the activation of cytochrome P450eryF	Journal of the American Chemical Society	124	1430-1437	2002
Guallar, Victor;et al.	Quantum chemical studies of methane monooxygenase: comparision with P450	Current opinion in chemical biology	6	236-242	2002
Margulis, CJ; Guallar, V; Sim, E; Friesner, RA; Berne, BJ;	A new semiempirical approach to study ground and excited states of metal complexes in biological systems	The Journal of Physical Chemistry B	106	8038-8046	2002
Harris, DL; Batista, VS; Miller, WH; Guallar, V;	Proton transfer mechanism in the activation of P450s and thiolate heme proteins: Tole of structure, electronic state, and tunneling	BIOPHYSICAL JOURNAL	82	448A-448A	2002
Guallar, Victor; Batista, Victor S; Miller, William H;	Semiclassical molecular dynamics simulations of intramolecular proton transfer in photoexcited 2-(2′-hydroxyphenyl)–oxazole	The Journal of Chemical Physics	113	9510-9522	2000
Guallar, Victor; Batista, Victor S; Miller, William H;	Semiclassical molecular dynamics simulations of excited state double-proton transfer in 7-azaindole dimers	The Journal of chemical physics	110	9922-9936	1999
Guallar, Víctor; Douhal, Abderrazzak; Moreno, Miquel; Lluch, José M;	DNA mutations induced by proton and charge transfer in the low-lying excited singlet electronic states of the DNA base pairs: A theoretical insight	The Journal of Physical Chemistry A	103	6251-6256	1999
Organero, Juan Angel; et al.	Proton-transfer reaction in isolated and water-complexed 8-hydroxyimidazo [1, 2-a] pyridine in the S0 and S1 electronic states. A theoretical study	The Journal of Physical Chemistry A	103	5301-5306	1999
Guallar, Victor; Batista, Victor S; Miller, William H;	Gas Phase Dynamics and Structure: Spectroscopy, Molecular Interactions, Scattering, and Photochemistry-Semiclassical molecular dynamics simulations of excited state double-proton transfer in	Journal of Chemical Physics	110	9922-9936	1999
Guallar, Victor; Douhal, Abderrazzak; Moreno, Miquel; Lluch, Jose M;	MOLECULAR STRUCTURE, BONDING, QUANTUM CHEMISTRY, AND GENERAL THEORY-DNA Mutations Induced by Proton and Charge Transfer in the Low-Lying Excited Singlet Electronic States of the DNA Base	Journal of Physical Chemistry A	103	6251-6256	1999
Guallar, Víctor; Moreno, Miquel; Lluch, José M;	On the localization of the electronic excitation in supramolecules built up by equivalent units linked by hydrogen bonds	Chemical physics	228	1-7	1998
Douhal, Abderrazzak; Guallar, Victor; Moreno, Miquel; Lluch, Jose Maria;	Theoretical study of molecular dynamics in model base pairs	Chemical physics letters	256	370-376	1996

Guallar, Víctor; Moreno, Miquel; Lluch, José M; Amat-Guerri, Francisco; Douhal, Abderrazzak;	**H-Atom Transfer and Rotational Processes in the Ground and First Singlet Excited Electronic States of 2-(2 '-Hydroxyphenyl) oxazole Derivatives: Experimental and Theoretical Studies**	**The Journal of Physical Chemistry**	**100**	**19789-19794**	**1996**

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

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