MINISTERIO DE CIENCIA E INNOVACIÓN

Cofinanciado por la Unión Europea

AGENCIA ESTATAL DE INVESTIGACIÓN

CURRICULUM VITAE (CVA)

IMPORTANT – The Curriculum Vitae cannot exceed 4 pages. Instructions to fill this document are available in the website.

Part A. PERSONAL INFORMATION

CV date	08/09/2023

First name	Moliner Ibáñez		
Family name	Vicente		
Gender (*)	male	Birth date	14/01/1965
ID number	25388050Y		
e-mail	moliner@uji.es	URL Web	www.biocomp.uji.es
Open Researcher and Contributor ID (ORCID) (*)		0000-0002-3665-3391	

(*) Mandatory

A.1. Current position

Position	Full Professor		
Initial date	31/08/2009		
Institution	Universitat Jaume I		
Department/Center	Institute of Advanced Materials (INAM)		
Country	Spain	Phone number	609625383
Key words	Computational Chemistry, Multiscale Methods, Enzymatic Catalysis, Reaction Dynamics, Inhibitors Design, Enzyme Design		

A.2. Previous positions (research activity interuptions, art. 14.2.b))

Period	Position/Institution/Country/Interruption cause
1990-92	Principal Investigator of the R&D Laboratory of Thermosets. Ferro Enamel Spain / Spain
1994 – 1995	Assistant Professor (*Profesor Ayudante de Universidad*). Departamento de Química Física y Analítica / Universitat Jaume I/ Spain
1998 – 2009	Associate Professor (Profesor Titular de Universidad) / Departamento de Química Física y Analítica / Universitat Jaume I/ Spain
2009-2010	Visiting Professor / Technical University of Lodz / Lodz / Poland
2017	"David Parkin Visiting Professor" / University of Bath / Bath / United Kingdom.

A.3. Education

PhD, Licensed, Graduate	University/Country	Year
Bachelor Degree in Chemistry	Universidad de Valencia	1988
MSc in Chemistry	Universidad de Valencia	1991
PhD in Chemistry	Universitat Jaume I	1993

Part B. CV SUMMARY *(max. 5000 characters, including spaces)*

V. Moliner graduated in Chemistry from the University of Valencia in 1988. After a brief experience in the industry as a principal investigator in the R & D laboratory of the Thermosets Division of the company Ferro Enamel Spain S.A., he received his doctorate from the University Jaume I (UJI) in 1993, under the direction of Prof. J. Andrés. The thesis was oriented to the study of the enzymatic reactivity by means of quantum methods. In 1996 he obtained a scholarship from The Leverhulme Trust to carry out a post-doctoral stay with Prof. I. H. Williams

at the University of Bath (1996/97) to work on the development of hybrid QM/MM algorithms to locate and characterize transition state structures in large systems. They published the first transition structure for an enzymatic reaction, characterized as such, by QM/MM methods (Chem. Comm. 1997). He obtained the position of Assoc. Prof. in 1998 and that of Full Prof. in 2009, both at UJI. Since then, he has carried out numerous stays in other universities, with periods from one month to a year and a half, including the 2009-2010 stay at the Lodz University of Technology (Poland) thanks to a mobility grant from the Spanish Ministry of Education, Culture and Sports; and 2017 at the University of Bath (United Kingdom) thanks to a prize awarded by the same university (David Parkin Visiting Professor), and a mobility grant from the Spanish Ministry of Education, Culture and Sports.

The interest of V. Moliner during the last years focuses on the development of QM/MM methods and the study of enzymatic reactions. Among other algorithms, he has worked on the development of QM/MM methods that allow the correction of the quantum region at a high level (JCTC 2005), or the use of global coordinates associated with the environment to describe the specific behavior of the medium (protein or solvent) in chemical reactions (JCTC 2012, Nat. Chem. 2013). The development of such methods opened the possibility to study enzyme catalyzed reactions and applications such as the design of biocatalysts (ACS Catal. 2021) or enzymatic inhibitors (Chem. Sci 2021). In these lines of research, he has fruitful collaborations with researchers, both theoretical and experimentalists. His articles (221 articles in research journals, including 1 Nature Chem., 2 Nature Commun., 28 J. Am. Chem. Soc., 3 Proc. Nat. Acad. Sci. USA, 6 Angew. Chem., 2 Chem. Soc. Rev., 5 Chem. Sci., 7 Chem. Comm., 23 ACS Catal. etc) have been continuously recognized, being selected as cover for several journals (Nat. Chem. 2013, JACS 2011 and 2018, ACS Catal. 2020 and 2021, Chem. Sci. 2020, etc), as Hot Papers (Chem. Soc. Rev. 2008, Chem. Sci. 2020), VIP paper (Angew. Chem. 2015), Spotlight in JACS (2018), ACS Editors' Choice (2020) or paper of the month in Biophys. Magazine (Febr. and Mar. 2018). V. Moliner is co-author of 9 book chapters.

V. Moliner has supervised 19 Master Thesis and 15 PhD Thesis, and is now co-supervising 3. Regarding his contributions in the research and development management, he has been the Coordinator of the access committee of the “Spanish Supercomputing network” in the area of Chemistry and Material Science section, from 2017 to 2021. He is active reviewer for more than 35 research journals (including, Nature Chemistry, Proc. Nat. Acad. Sci. USA, Chem. Rev., J. Am. Chem. Soc., J. Phys. Chem. B., ACS Catalysis, Chem. Comm., PCCP, Chem. Sci., Angew. Chem. Int. Ed., etc.) and for national and foreign agencies, including the European Research Council. V. Moliner is member (“*gestor*”) of the area of “Bioscience and Biotechnology” of the Spanish *Agencia Estatal de Investigación* from 2021.

V. Moliner has organized four international conferences (Isotopes 2007 in Benicassim, CECAM 2014 in Paris, and TrEnCa 2018 and 2019 in Benicàssim). He has been invited to give conferences in numerous international congresses (35 in the last 10 years) and national and international research centers. He was invited to write an opinion article in the journal Proc. Nat. Acad. Sci. USA ("Eppur si muove" PNAS 2011). He is member of the editorial board of Arch. Biochem. Biophys. and Int. J. Mol. Sci., guest editor of three issues of different journals (Arch. Biochem. Biophys. in 2015, Phys. Chem. Chem. Phys. in 2015, and Frontiers in Chemistry in 2019), co-editor of a book edited by the British Royal Society of Chemistry ('Simulating Enzyme Reactivity') and member of the Advisory Board of Chem. Sci. from 2023. V. Moliner received the “Excellence in Research Award 2019” from the Spanish Royal Society of Chemistry.

Part C. RELEVANT MERITS in the last 10 years.

C.1. Publications

1. *K. Świderek, S. Velasco-Lozano, M. À. Galmés, I. Olazabal, H. Sardon, F. López-Gallego, V. Moliner "Mechanistic studies of a lipase unveil effect of pH on hydrolysis products of small PET modules" Nat. Commun. 2023, 14:3556.*
2. *MA Galmés, AR Nödling, K He, LYP Luk, K Świderek, V Moliner. “Computational design of an amidase by combining the best electrostatic features of two promiscuous hydrolases” Chem. Sci. 2022, 13, 4779-4787.*

3. *M.A. Galmés, A.R. Nödling, L. Luk, K. Świderek,* V. Moliner* "Combined Theoretical and Experimental Study to Unravel the Differences in Promiscuous Amidase Activity of Two Nonhomologous Enzymes" ACS Catal. 2021, 11, 8635–8644.*
4. *K. Arafet, N. Serrano-Aparicio, A. Lodola, A.J. Mulholland, F.V. González, K. Świderek,* V. Moliner,* "Mechanism of inhibition of SARS-CoV-2 M pro by N3 peptidyl Michael acceptor explained by QM/MM simulations and design of new derivatives with tunable chemical reactivity" Chem. Sci. 2021, 12, 1433–1444.*
5. *N. Serrano-Aparicio, V. Moliner,* K. Świderek* "Nature of Irreversible Inhibition of Human 20S Proteasome by Salinosporamide A. The Critical Role of Lys–Asp Dyad Revealed from Electrostatic Effects Analysis" ACS Catal. 2021, 11, 3575–3589. Cover of Vol. 11, issue 6.*
6. *K. Świderek,* V. Moliner* "Revealing the Molecular Mechanisms of Proteolysis of SARS-CoV-2 Mpro from QM/MM Computational Methods." Chem. Sci. 2020, 11, 10626–10630. Featured on the Front Cover Issue 39, 2020, and part of The Themed Collection: 2020 Chemical Science HOT Article Collection and Celebrating 10 Years of Chemical Science*
7. *D. De Raffele, S. Martí,* V. Moliner* "Understanding the Directed Evolution of de novo Retro-Aldolases from QM/MM Studies." ACS Catal. 2020, 10, 7871–7883. Cover of Vol. 10, issue 14.*
8. *S. A. Kholodar,* A. K. Ghosha, K. Świderek, V. Moliner,* A. Kohen "Parallel reaction pathways and noncovalent intermediates in thymidylate synthase revealed by experimental and computational tools. Proc. Natl. Acad. Sci. USA. 2018, 115, 10311–10314.*
9. *K. Świderek, I. Tuñón, I. H. Williams, V. Moliner* "Insights on the origin of catalysis on glycine N-methyltransferase from computational modelling" J. Am. Chem. Soc. 2018, 140, 4327–4334. JACS Highlights, Biofisica Highlights, F1000Prime Highlights. Journal Cover.*
10. *A. Krzemińska, V. Moliner,* K. Świderek* "Dynamic and Electrostatic Effects on the Reaction Catalyzed by HIV-1 Protease." J. Am. Chem. Soc. 2016, 138, 16283–16298.*

C.2. Congress: More than 35 conferences in in the last 10 years, of which the following 10 have been selected:

1. ACS Spring 2023 "Towards the Computation-Assisted Design of New Enzymes for the Hydrolysis of Synthetic Polymers". Mineapolis, USA, 2023. Invited talk.
2. 10th International Symposium on Isotopomers (ISI) 12th Isotopes Conference. "Towards the design of an improved Retro-Aldolase based on QM/MM studies of the reaction catalyzed by different protein scaffolds". Zürich, Switzerland. 2022. Keynote.
3. 12th Congress on Electronic Structure, Principles and Applications. "Towards the computation-assisted design of new enzymes" Vigo, 2022. Invited talk.
4. ACS Fall 2021 "QM/MM computational studies of the main protease of SARS-CoV-2: towards the design of new inhibitors": Session: "Computational Chemistry of COVID-19: Lessons Learned and Future Directions" and selected by the division program chairs for the Sci-Mix session as one of the most exceptional abstracts submitted. Atlanta, USA, 2021 (virtual communications).
5. 11th International Conference on Chemical Kinetics, Conference: "Revealing the origin of the catalytic power of enzymes by merging computational studies and experiments". Orleans, France. 2019. Keynote talk.
6. 8th Modeling and Design of Molecular Materials, MDMM, Conference: "DAD's not in charge of Me". Polanica Zdroj, Poland. 2018. Plenary talk.
7. 5th Annual CCP-BioSim Conference: Frontiers of Biomolecular Simulation: "Revealing the Origin of Enzyme Catalysis from Computational Studies". Southampton, United Kingdom. 2017. Plenary talk.

8. 251st American Chemical Society National Meeting & Exposition: “Theoretical studies of enzyme catalysis: towards the design of new biocatalysts” San Diego, California, USA. 2016. Invited talk.
9. 10th World Congress of Theoretically Oriented Chemists; WATOC 2014. “Theoretical studies of enzyme dynamics and their implication in the design of new biocatalysts” Santiago de Chile, Chile. 2014. Invited talk.
10. Gordons Research Conferences: Isotopes in Biological & Chemical Sciences: “Role of Protein Motions to Catalysis. Computational Studies on Wild Type and Heavy Isotope Labelled DHFRs” Galveston, USA. 2014. Plenary talk.

C.3. Research projects

1. *Computational Biocatalysis: An Approach to the Rational Design of Enzyme Inhibitors and Biocatalysts with Biomedical Applications* (Ref. PGC2018-094852-B-C21) Spanish Ministry of Science, Research and Universities – European Regional Development Fund. 2022–2025. 157,300.00 €. PI: V. Moliner
2. A combined theoretical and experimental approach to the rational design of high value chemicals with implications for biotherapeutic engineering *(Ref. PROMETEO CIPROM/2021/079 /2021/027)*. Generalitat Valenciana – European Regional Development Fund. 2022–2026. 561,269.00 €. PI: V. Moliner
3. *Computer assisted design of compounds for the treatment of COVID-19 by means of QM/MM and Machine Learning methods (Ref. IDIFEDER/2021/027)*. Generalitat Valenciana – European Regional Development Fund. 2021–2022. 394,904.00 €. PI: V. Moliner
4. *Consolidation of the Scientific Computing Center: servers, storage and network equipment (Ref. EQC2019-006018-P)*. Spanish Ministry of Science, Research and Universities – European Regional Development Fund. 2020–2021. 399,999.38 €. PI: V. Moliner
5. *QMcube: a universal platform for multiscale simulations in biological systems* (Ref. PGC2018-094852-B-C21). Spanish Ministry of Science, Research and Universities. 2019–2021. 104,000.00 €, PI: V. Moliner
6. *Designing Multifunctional Organocatalytic Artificial Enzymes* (Ref. RPG-2017-195). The Leverhulme Trust. United Kingdom. 2017–2020. 176,847.00 £. PI: LYP Luk (Cardiff University, UK) and V. Moliner
7. *Modelización Multiescala de Reacciones Químicas en Entornos Biológicos (*CTQ2015-66223-C2-1-P). Spanish Ministry of Economy and Competitivity. 2016–2018. 95,000.00 €. PI: V. Moliner
8. *Tunneling and dynamics in enzyme catalyzed reactions*. National Institute of Health (USA). NIH R01GM065368. 2014–2018. Assigned to V. Moliner: 136,524.00 USD (122,875.00 €). PI. Amnon Kohen (University of Iowa, USA).
9. *Molecular Simulations of Catalytic Processes. Developments and applications in biomedicine and biotechnology (Ref.* CTQ2012-36253-C03-01). Spanish Ministry of Science and Innovation. 2013–2015. 91,260.00 €. PI: V. Moliner.
10. *Binding isotope effects as a new, unique tool for studies of receptor - ligand interactions (Ref.* 2011/02/A/ST4/00246)*.* Polish National Center for Science. 2012–2017. 742,070.00 €. PI: Piotr Paneth (Lodz University of Technology, Poland).