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	31/01/2023

First name	IGNACIO		
Family name	TUÑÓN GARCÍA DE VICUÑA		
Gender (*)	Male	Birth date (dd/mm/yyyy)	19/10/1966
ID number	24328661C		
e-mail	ignacio.tunon@uv.es	URL Web	www.uv.es/efme
Open Researcher and Contributor ID (ORCID) (*)		0000-0002-6995-1838	

(*) Mandatory

A.1. Current position

Position	Full Professor		
Initial date	15/04/2010		
Institution	UNIVERSIDAD DE VALENCIA		
Department/Center	Química Física	Facultad de Químicas	
Country	Spain	Teleph. number	963544880
Key words	Multiscale methods, Enzymatic reactions, reaction dynamics		

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

Period	Position/Institution/Country/Interruption cause
2000-2010	Profesor Titular/Universidad de Valencia/Spain
1995-2000	PostDoc/Universidad de Valencia/Spain
1994	PostDoc/Université de Nancy/France
1990-1993	PhD fellowship/Universidad de Valencia/Spain

A.3. Education

PhD, Licensed, Graduate	University/Country	Year
Degree in Chemistry	UNIVERSIDAD DE VALENCIA	1989
PhD in Chemistry	UNIVERSIDAD DE VALENCIA	1993

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

Research Area: Physical Chemistry
Number of Positive Research Periods ('sexenios'): 5 (last one 2014-2019)
Number of Positive Teaching Periods ('quinquenios'): 6 (last one 2015-2019)

I. Tuñón got the degree in Chemistry in June 1989, obtaining the second national award. His PhD Thesis was supervised by Prof. Silla in the Department of Physical Chemistry at the University of Valencia and was devoted to the development and use of continuum models for the study of chemical processes in solution. The PhD thesis was presented in 1993 deserving the extraordinary award recognition of the University. Afterwards he engaged as a postdoctoral researcher in the laboratory of Chimie Théorique leaded by Prof. JL Rivail in the University of Nancy (France) with a fellowship of the Spanish Ministry of Education. The research work was devoted to the development of one of the first computational codes for hybrid QM/MM simulations. He came back to the University of Valencia with a reincorporation postdoctoral contract, obtaining the position of Profesor Titular in 2000 and that of Catedrático in 2010. The

scientific work carried out in the research unit leaded by I. Tuñón has been focused in the development of theories and methodologies for the study of chemical reactions in biological environments using QM/MM methods. The work included the development of techniques for the exploration of potential energy surfaces and for the calculation of free energies and other contributions to the reaction rate constant. These methodologies have been applied to reactions in solution and enzymatic processes, showing the role of electrostatic fields in catalysis. The research unit of I. Tuñón is nowadays a reference in the field of enzyme catalysis modelling as demonstrated by the publication of 205 scientific articles (including 1 in Nature Chem., 27 in J. Am. Chem. Soc, 5 in Angewandte Chemie, 2 in Proc. Nat. Acad. Sci and 4 in Chemical Sciences). These articles have received until now more than 5800 cites. Three recent articles have been recommended in the F1000Prime web (JACS, 140, 4327, 2018 and PNAS 114, 12390, 2017) and in Faculty Opinions (Angewandte Chemie Int. Ed. 60, 25933, 2021). I. Tuñón has been invited to give lectures in more than 60 international and national meetings and has been nominated visiting professor in the Université de Nancy (France), the Ecole Normale Supérieure (Paris, France) and Universidad de Talca (Chile). In 2008 Prof. Tuñón, together with coauthors, received the 'Expoquimia' research award. He also co-edited a book of the Royal Society of Chemistry entitled 'Simulating Enzymes Reactivity' (ISBN 978-1-78262-429-5). I. Tuñón also co-organized two scientific conference (Isotopes 2007 and 'DNA: Damage and Repair' 2019) and participated in the scientific committee of several of them (Isotopes, ESPA, Watoc series).

I.Tuñón has supervised 12 PhD students, including two thesis co-supervised in the Universidad de Talca (Chile). 10 of these students have continued a scientific career in Universities or Research Centers (Universidad de Valencia, Universidad Jaume I, University of Bristol, Universidad de Talca y de Concepción in Chile, IRB in Barcelona), one is the responsible of the Computational Center at the Universidad de Valencia and one is a science teacher at secondary school. I.Tuñón also actively participates in the Erasmus Mundus Master in Theoretical Chemistry and Computational Modelling, being the head at the Universidad de Valencia. He is also a member of the board of the Science Doctoral school of the Universidad de Talca (Chile).

I. Tuñón was the coordinator of the Chemistry and Material Science access commite of the Barcelona Supercomputing Center/Red Española de Supercomputación (2013-2017); member of the panel of evaluators of the Agencia Estatal de Investigación (2014, 2016, 2017 and 2021) and collaborator since 2021. He is currently the chair of the 'Chemistry and Computation' Division of the Real Sociedad Española de Química since 2018.

Part C. RELEVANT MERITS *(sorted by typology)*

C.1. Publications *(see instructions)*

1. Inhibition mechanism of SARS-CoV-2 main protease with ketone-based inhibitors Unveiled by Multiscale Simulations: Insights for Improved Designs.
C. A. Ramos-Guzmán, J. J. Ruiz-Pernía, I. Tuñón.
Angewandte Chemie Int. Ed., 60 (49), 25933-25941, **2021**

2. A microscopic description of SARS-CoV-2 main protease inhibition with Michael acceptors. Strategies for improving inhibitor design.
C. A. Ramos-Guzmán, J. J. Ruiz-Pernía, I. Tuñón.
Chemical Science, 12, 3489-3496, **2021**

3. Are Heme-Dependent Enzymes Always Using a Redox Mechanism? A Theoretical Study of the Kemp Elimination Catalyzed by a Promiscuous Aldoxime Dehydratase
S. Marti, J. Bertran, I. Tuñón, V. Moliner
ACS Catalysis, 10 (19), 11110-11119, **2020**

4. Insights on the Origin of Catalysis on Glycine *N*-Methyltransferase from Computational Modeling
K. Świderek, I. Tuñón, I.H. Williams, V. Moliner
Journal of the American Chemical Society 140 (12), 4327-4334, **2018**

5. Quantifying the limits of transition state theory in enzymatic catalysis
K. Zinovjev, I. Tuñón
Proceedings of the National Academy of Sciences 114 (47), 12390-12395, **2017**

6. Minimization of dynamic effects in the evolution of dihydrofolate reductase
J.J. Ruiz-Pernía, E. Behiry, L.Y.P. Luk, E.J. Loveridge, I. Tunón, V. Moliner, R.K. Allemann
Chemical Science 7 (5), 3248-3255, **2016**
7. Peptide bond formation mechanism catalyzed by ribosome
K. Świderek, S. Marti, I. Tuñón, V. Moliner, J. Bertran
Journal of the American Chemical Society 137 (37), 12024-12034, **2015**
8. Protein Isotope Effects in Dihydrofolate Reductase From *Geobacillus stearothermophilus* Show Entropic–Enthalpic Compensatory Effects on the Rate Constant
L.Y.P.Luk, J.J. Ruiz-Pernía, W.M. Dawson, E.J. Loveridge, I. Tuñón, V. Moliner, R.K. Allemann
Journal of the American Chemical Society 136 (49), 17317-17323, **2014**
9. Dynamics and Reactivity in *Thermus aquaticus* N6-Adenine Methyltransferase
J. Aranda, K. Zinovjev, M. Roca, I. Tuñón
Journal of the American Chemical Society 136 (46), 16227-16239, **2014**
10. Studying the role of protein dynamics in an S_N2 enzyme reaction using free-energy surfaces and solvent coordinates
R. García-Meseguer, S. Marti, J.J. Ruiz-Pernía, V. Moliner, I. Tuñón
Nature Chemistry 5 (7), 566-571, **2013**

C.2. Congress

I. Tuñón has delivered more than 30 invited talks in international meetings during the last 10 years. 10 of them are selected here:

- ACS meeting Spring 2021, on-line, March 2021. 'Computational Analysis of Catalysis and Inhibition in SARS-CoV-2 3CL Protease Using DFT/MM Free Energy Simulations'
- Pulse Investigations in Chemistry, Physics and Biology & Reaction Kinetics in Condensed Phases. Lodz (Poland), September 2018. 'Enzymatic Reaction Pathways and Transition States'
- ACS meeting Fall 2016, Phildelphia, August 2016. 'New methodological developments for the study of enzymatic chemical reactions.Exploring reactivity on Free Energy Surface'.
- Gordon Research Conference. Computational Chemistry Conference, Gerona, July 2016. 'Challenges in Computational Enzymology. Exploring Free Energy Surfaces'
- Isotopes 2015, Jerusalem (Israel) June 2015. 'Diabatic and Adiabatic Hydride Transfer in Fromate Dehydrogenase'.
- Cecam workshop: investigating fine quantum effects in biological systems, toward a synergy between experimental and theoretical approaches? Paris Junio 2014. 'Electrostatic effects and protein motions in enzymatic catalysis'
- Gordon Research Conference. Isotopes in Biological & Chemical Sciences, Galveston (USA) Febrero 2014. 'Electrostatic catalytic effects in light and heavy versions of Purine Nucleoside Phosphorylase'
- EMBO Workshop. Glycoproteins from structure to disease, Mallorca Mayo 2013. 'Protein Motions and Catalysis'
- 21st IUPAC International Conference on Physical Organic Chemistry, Durham (UK), Septiembre 2012. 'Dynamical effects in enzymatic catalysis. Do they invalidate Transition State Theory?'
- Advances in Quantum Chemistry: Interfacing Electronic Structure with Dynamics, Minneapolis (USA), Junio 2012. 'Dynamical effects in enzymatic catalysis'

C.3. Research projects

-Title of the project: Simulación Computacional de la Actividad de la Proteasa Principal del SARS-CoV-2
Financing Firm/administration: Generalitat Valenciana. Consellería de Innovación
Number of the project: GVCOV19/Decreto180/2020 Amount: 152.000,00 Period: 2020-2021
Researcher/s in charge: Ignacio Tuñón
-Title of the project: A computational study of the reactivity in the main protease of SARS-CoV-2 to guide the design of inhibitors
Financing Firm/administration: PRACE

Number of the project: COVID19-05 Amount: 23 M of CPU hours Period: 2020 (3 months)
Researcher/s in charge: Ignacio Tuñón
-Title of the project: Qmcube: Una Plataforma Universal Para Simulaciones Multiescala En Sistemas Biologicos. Simulando Procesos Enzimaticos En Condiciones Estandar y No Estandar.
Financing Firm/administration: Ministerio de Ciencia, Innovación y Universidades
Number of the project: PGC2018-094852-B-C22Amount: 101.640,00 Period: 2019-2021
Researcher/s in charge: Ignacio Tuñón
-Title of the project / contract: Caminos de Mínima Energía Libre en Reacciones Enzimáticas. Aplicación a la caspasa-1
Financing Firm/administration: Generalitat Valenciana.
Number of the project: AICO/2018/238, Period: 2018-2019. Amount:40.000 €
Researcher/s in charge: Ignacio Tuñón.
-Title of the project: Modelización Multiescala De Reacciones Químicas En Entornos Biológicos. Desarrollos Metodológicos Y Aplicaciones En Epigenética
Financing Firm/administration: MINECO. Ministerio de Economía y Competitividad
Number of the project: CTQ2015-66223-C2-2-P Amount: 114.950,00 Period: 2016-2018
Researcher/s in charge: Ignacio Tuñón
-Title of the project: Supercomputador de Arquitectura Mixta
Financing Firm/administration: Ministerio de Economía y Competitividad
Number of the project: UNLV15-EE- 3261 Amount: 500.000,00 Period: 2016-
Researcher/s in charge: Jose M. Ibáñez
-Title of the project: Simulaciones moleculares de catalizadores biológicos. Nuevas metodologías para el cálculo de potenciales de fuerza media y aplicaciones de interés biomédico.
Financing Firm/administration: Dirección General de Investigación Científica y Técnica
Number of the project: CTQ2012-36253-C03-03 Amount: 101.000,00 Period: 2013-2015
Researcher/s in charge: Ignacio Tuñón

C.4. Contracts, technological or transfer merits

- Coordinator and member of the access commite of the Barcelona Supercomputing Center/Red Española de Supercomputación. Chemistry and Material Science section. (2013-2017)
- Member of the panel for the evaluation of the Projects for the National Plan of Chemical Science and Technology (2014, 2016, 2017 and 2021)
- Collaborator of the Agencia Estatal de Investigación (2021-)
- Reviewer in more than 30 research journals including, Science, 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…
- Reviewer of Projects for national (ANEP, AGU; AGAE,..) and foreign national agencies (Chile, Israel, Argentina, Poland…)
- Head of the Master in Theoretical Chemsitry and Computational Modelling at the Universidad de Valencia (2018-)
- Chair of the Division of ‘Chemistry and Computation’ of the Real Sociedad Española de Química (2018-)