

Part A. PERSONAL INFORMATION

CV date

08/12/2020

First and Family name	F. Javier LUQUE GARRIGA		
Social Security, Passport, ID number	35047889Y	Age	58
Researcher codes	Open Researcher and Contributor ID	0000-0002-8049-3567	
	SCOPUS Author ID	23025357900	
	WoS Researcher ID	L-9652-2014	

A.1. Current position

Name of University/Institution	University of Barcelona		
Department	Nutrition, Food Science and Gastronomy		
Address and Country	Prat de la Riba 171, 08921 Santa Coloma de Gramenet		
Phone number	93 4033788	E-mail	fjluque@ub.edu
Current position	Full Professor	From	10/06/2003
Key words	Computational Biology - Physical Chemistry - Biomolecular Recognition - Drug Design		

A.2. Education

Graduate in Chemistry	Autónoma de Barcelona	1985
Máster Molecular Biology and Biotechnology	Autónoma de Barcelona	1987
PhD in Chemistry	Autónoma de Barcelona	1989

A.3. General indicators of quality of scientific production (see instructions)

No. 6-year research periods: 5 (last period: 1/1/2013 - 31/12/2018)

Supervised PhD thesis: 12

H-index: 68 (WOS), 73 (Google Scholar)

Total number of publications: 380 (WOS)

Total number of citations: 14816 (WOS), 18107 (Google Scholar)

Average citations per item: 39 (WOS)

Average citations per year (since 2015): 782 (WOS), 1008 (Google Scholar)

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

I obtained the degree in Science (Chemistry) by the Universidad Autónoma de Barcelona in 1989. My scientific career has involved post-doctoral stays in Swiss Federal Institute of Technology in Zurich (ETH, Prof. W. F. Van Gunsteren, 1992), University of Pisa (Prof. J. Tomasi, 1995) and University of Nancy (Prof. J. L. Rivail, M. F. Ruiz-López), where I was invited professor in 1999. In 1991 I was appointed Associate Professor at the University of Barcelona (UB), being currently Full Professor since 2003. Recently, I was invited professor at the University of Parma (2017). I am leading the Computational Biology and Drug Design research team at the UB, a group recognized and financed by the Generalidad de Catalunya. I am also member of the Institute of Biomedicine (IBUB) and Institute of Theoretical and Computational Chemistry (IQTUB), both pertaining to the UB.

My research is focused on the study of biomolecular systems with the aim to establish the relation between structure, dynamics and function, understand the molecular determinants involved in the recognition between biomolecules, and apply this knowledge in the design of new bioactive compounds (drugs). His research involve from molecular interactions in molecular systems of small size until the dynamic analysis of biomolecules. However, in his trajectory he has maintained his interest in the development of bioactive molecules for the treatment of neurodegenerative disease (Alzheimer), and more recently he has expended his interest to the study of targets related to infectious disease such as tuberculosis, influenza and malaria.



I have published near of 380 papers in international journals in the fields of Multidisciplinary Chemistry, Medicinal Chemistry, Physical Chemistry, Computational Chemistry and Biochemistry, with almost 15,000 citations and an index H of 68 (WOS). Moreover, I am co-author of 30 book chapters and I have co-edited one book. I am also co-inventor of 6 patents. I have (co-)supervised 25 doctoral theses along my career. I am member of the editorial board of *Theoretical Chemistry Accounts*, *Journal of Computer-Aided Molecular Design* and *Molecules*. I have been guest editor of two special issues for *Biochimica et Biophysica Acta: Protein and Proteomics*, and *Antioxidants and Redox Signalling*.

My scientific trajectory has been supported by several awards including the “Premio anual del Colegio de Químicos de Catalunya a jóvenes investigadores” (1995), “Premio Promoción de la Investigación para Jóvenes Científicos de la Generalidad de Cataluña” (2002-2006), and more recently the ICREA Academia award by ICREA foundation (2013-2017). Likewise, I has been distinguished with the award Luis Federico Leloir award granted by the Ministerio de Investigación de la República Argentina (2015), Antoni Caparros award granted by Fundació Bosch I Gimpera and the Consell Social from the University of Barcelona (2017), and Bruker/Manuel Rico award by the Sociedad Española de Biofísica in 2018.

Part C. RELEVANT MERITS (sorted by typology)

C.1. Publications (*) Corresponding author

1. Espargaró, A.; Llabrés, S.; Saupe, S.J.; Curutchet, C.; **Luque, F.J.**.* Sabaté, R. On the Binding of Congo Red to Amyloid Fibrils. *Angewandte Chemie International Edition* 2020, 21, 8104.
2. Zamora, W.J.; Campanera, J. M.; **Luque, F. J.*** Development of a Structure-Based, pH-Dependent Lipophilicity Scale of Amino Acids from Continuum Solvation Calculations. *Journal of Physical Chemistry Letters* 2019, 10, 883.
3. Estarellas, C.; Scaffidi, S.; Saladino, G.; Spyraakis, F.; Franzoni, L.; Galdeano, C.; Bidon-Chanal, A.; Gervasio, F. L.;* **Luque, F. J.*** Modulating ligand dissociation through methyl isomerism in accessory sites: Binding of retinol to cellular carriers. *Journal of Physical Chemistry Letters* 2019, 10, 7333.
4. Ginex, T.; Trius, M.; **Luque, F. J.*** Computational Study of the Aza-Michael Addition of the Flavonoid (+)-Taxifolin in Inhibition of β -Amyloid Fibril Aggregation. *Chemistry European Journal* 2018, 24, 5813.
5. Alencar, N.; Sola, I.; Linares, M.; Juárez-Jiménez, J.; Pont, C.; Viayna, A.; Vilchez, D.; Sampedro, C.; Abad, P.; Pérez-Benavente, S.; Lameira, J.; Bautista, J. M.; Muñoz-Torrero, D.; **Luque, F. J.*** First homology model of Plasmodium falciparum glucose-6-phosphate dehydrogenase: Discovery of selective substrate analog-based inhibitors as novel antimalarial agents. *European Journal of Medicinal Chemistry*. 2018, 146, 108.
6. Espargaró, A.; Ginex, T.; Vadell, M. D.; Busquets, M. A.; Estelrich, J.; Muñoz-Torrero, D.; **Luque, F. J.**.* Sabaté, R. Combined in vitro cell-based/in silico screening of naturally occurring flavonoids and phenolic compounds as potential anti-Alzheimer drugs. *Journal of Natural Products*. 2017, 80, 278.
7. Llabrés, S.; Juárez-Jiménez, J.; Masetti, M.; Leiva, R.; Vázquez, S.; Gazzarrini, S.; Moroni, A.; Cavalli, A.; **Luque, F. J.*** Mechanism of the pseudoirreversible binding of amantadine to the M2 proton channel. *Journal of the American Chemical Society*, 2016, 138, 15345.
8. Sing, S.; Thakur, N.; Oliveira, A.; Petruk, A. A.; Hade, M. D.; Sethi, D.; Bidon-Chanal, A.; Marti, M. A.; Datta, H.; Parkesh, R.; Estrin, D. A.; **Luque, F. J.**; Dikshit, K. L. Mechanistic insight into the enzymatic reduction of truncated hemoglobin N of Mycobacterium tuberculosis. Role of the CD loop and pre-A motif in electron cycling. *Journal of Biological Chemistry*. 2014, 289, 21573.

9. Forti, F.; Cavasotto, C. N.; Orozco, M.; Barril, X.; **Luque, F. J.*** A multilevel strategy for the exploration of the conformational flexibility of small molecules. *Journal of Chemical Theory and Computation*. 2012, 8, 1808.
10. Preciado, S.; Vicente-García, E.; Llabrés, S.; **Luque, F. J.**; Lavilla, R. Exploration of Forbidden Povarov processes as a source of unexpected reactivity: A multicomponent Mannich-Ritter transformation. *Angewandte Chemie International Edition* 2012, 51, 86874.

C.2. Research projects

1. Mechanisms of mutation resistance in hemagglutinin: Is the uncleaved form HA0 the right target? Project no. 2020225437. EU PRACE. 42,3 million core hours. 2020. colP: **F. J. Luque**
2. Targeting conformational changes implicated in early events of viral entry COVID-19. PRACE. 15 million core hours. IP: **F. J. Luque**
3. Reposicionament basat en lligand (LBRS) de un compost fenòlic amb activitat anti amiloidogènica: Una prova de concept. Generalitat de Catalunya. 2019LLAV00016. 2020-2021. 20.000,00 €. IP: **F. J. Luque**
4. Activadores de la proteína quinasa activada por AMP para el tratamiento de la enfermedad vascular asociada a la obesidad Fundación Eugenio Rodríguez Pascual. 11.375,00 €. 2018. IP: M. S. Fernández. Investigador: **F. J. Luque**
5. Mecanismos moleculares implicados en la inhibición de dianas para tratamientos anti-influenza: Canal de protones M2 y hemagglutina. SAF2017-881074-R. Ministerio de Economía y Competitividad. 90.750,00 €. 2018-2020. IP: **F. J. Luque**
6. Mechanism of drug binding to the S31N mutated M2 proton channel of influenza virus INFLUM2(S31N). EU PRACE. 15 million core hours. 2016-2017. IP: **F. J. Luque**
7. FRAGments training NETwork (FRAGNET). 8P1MCA - HORIZON 2020, project 675899. Unión Europea (H2020 ITN program). 421.929,92 €. 2016-2020. IP: X. Barril. Investigador: **F. J. Luque**
8. Exploración de nuevas dianas y estrategias multidiana para el diseño de compuestos contra enfermedades infecciosas y prevalentes. SAF2014-57094-R. Ministerio de Economía y Competitividad. 180.000,00 €. 2015-2017. IP: **F. J. Luque**
9. Ajuts a Grups Consolidats (Biologia Computacional i Disseny de Fàrmacs). Generalitat de Catalunya. 2017SGR1746. 65.896,00 €. 2017-2019; 2014SGR1189. 38.400,00 €. 2014-2017.
10. Explorando nuevas estrategias terapéuticas para el tratamiento de enfermedades infecciosas y parasitarias. SAF2011-27642. Ministerio de Economía y Competitividad. 140.000,00 €. 2012-2014. IP: **F. J. Luque**

C.3. Contracts, technological or transfer merits

1. Serveis en química computacional. Pharmacelera S. A.; 12.100,00 €; 2020; IP: **F. J. Luque**
2. Identificación, síntesis y evaluación toxicológica de moléculas con propiedades antidetonantes. Repsol S. A.; 98.780,49 €; 2018-2019; IP: **F. J. Luque**
3. Diseño y ejecución de un estudio mecanocuántico del proceso de solubilidad y reducción de quinonas y compuestos relacionados en diversos medios. PV Hardware Solutions; 60.000,00 €; 2017-2018; IP: **F. J. Luque**
4. Optimización de software (PharmScreen/PharmQSAR) para desarrollo de fármacos. Pharmacelera S. A.; 31.500,00 €; 2016-2018; IP: **F. J. Luque**
5. Investigació sobre edulcorants. Jorofon, S. L.; 1.200,00 €; 2017-2018; IP: **F. J. Luque**
6. Diseño y ejecución de un estudio mecanocuántico del proceso de solubilidad y reducción de quinonas y compuestos relacionados en diversos medios. Repsol S.A.; 60.000,00 €; 2015-2016; IP: **F. J. Luque**
7. Synthesis and pharmacological evaluation of new molecules with antidiabetic properties. CIDQO S.L.; 67.000,00 €; 2014-2016; IP: S. Vázquez. Investigador: **F. J. Luque**.
8. Quimiointormática (Cenit HENUFOOD). Universitat de Lleida; 5.882,00 €; 2012-2013; colP: **F. J. Luque**.
9. Búsqueda de activos en pérdida de peso del extracto EBC. Biocentury; 14.100,00 €; 2011-2012; IP: **F. J. Luque**.
10. Cribado virtual y selección de compuestos. Omnia Molecular; 9.500,00 €; 2010-2011; IP: **F. J. Luque**.

C.4. Patents

1. J. Vázquez; E. Herrero; E. Gibert, **F. J. Luque**. Calculating molecular similarity. PCT/EP2016/082850. Priority date: 29/12/2016. Exploited by Pharmacelera. S.A.
2. A. Castro; P. Sanz; S. Quesada; M. García; **F. J. Luque**; A. Bidon-Chanal. Compuestos espiránicos derivados de oxindol-pirazolo [3,4-b]piridona y sus usos terapéuticos. PCT/ES2016/070868. 09/12/2016
3. A. Castro; P. Sanz; S. Quesada; M. García; **F. J. Luque**; A. Bidon-Chanal. Compuestos espiránicos derivados de oxindol-pirazolo [3,4-b]piridona y sus usos terapéuticos. ES201531786. 10/12/2015
4. A. Samadi; J. L. Marco; I. Bolea; **F. J. Luque**; M. Unzeta. New derivatives of propargylamine having neuroprotective capacity for the treatment of Alzheimer's and Parkinson's diseases. US 13/635894. 18/09/2012.
5. A. Martínez; C. Gil; M. V. Palomo; C. Pérez; D. I. Pérez; **F. J. Luque**. Inhibidores de GSK-3 útiles en enfermedades neurodegenerativas, inflamatorias, cáncer, diabetes y en procesos regenerativos. PCT/ES2012/070119. 27/02/2012.
6. A. Samadi; J. L. Marco; I. Bolea; **F. J. Luque**; M. Unzeta. Nuevos derivados de propargilamina con capacidad neuroprotectora para el tratamiento de las enfermedades de Alzheimer y Parkinson. PCT/ES2011/070186. 18/03/2011

C.5 Editorial activity and organization of scientific events

1. Member of the editorial committee of *Theoretical Chemistry Accounts* (2002-), *Journal of Computer-Aided Molecular Design* (2011-), and *Molecules* (2016-).
2. Editor of special issues: *Protein Dynamics: Experimental and Computational Approaches* published in *Biochimica Biophysica Acta: Protein & Proteinomics* (2011), *Frontiers in Computational Chemistry for Drug Discovery* published in *Molecules* (2018), and *Antioxidants & Redox Signaling* (2019).
3. Co-organizer of scientific meetings: Summer School "Risk-benefit in food safety and nutrition" (Parma, Italia, 2019); XX O2BIP Congress 2018 (Barcelona, 2018); Summer School "In silico methods for food safety" (Parma, Italia, 2017); workshop IVth New Trends in Computational Chemistry for Industry Applications (Barcelona 2017); Summer School "In silico/in vitro approaches for food science" (Parma, Italia, 2016); Workshop 3d New Trends in Computational Chemistry for Industry Applications (Barcelona 2015)

C.6 Awards

1. ICREA Academia (2013-2017)
2. Award "Luis Federico Leloir" por el Ministerio de Ciencia de la República Argentina (2015)
3. Award Antoni Caparrós award by Fundació Bosch I Gimpera (2017)
4. Award Bruker/Manuel Rico by Sociedad Española Biofísica (2018)

C.7 Others

1. Member of the Real Academia de Farmacia de Cataluña (2011-).
2. Comissions of Trust: ERC Panel (2016; LS1 panel), HPC Europa 3 (2017-), ANEP (Spain), MIUR (Italy), FONCYT (Argentina), CONYCIT (Chile), FCT (Portugal), NSF (Poland)
3. Member of the Tu YouYou Award evaluation panel (2020).