

**CURRICULUM VITAE ABREVIADO (CVA)**

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

**Part A. PERSONAL INFORMATION**

			<b>CV Date</b>	20/01/2025
Name	Javier			
Family Name	García Marín			
Sex	Male	Date of Birth	04/01/1991	
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Open Researcher and Contributor ID (ORCID) (*)			0000-0002-5883-4783	

(\*) *Mandatory*

**A.1. Current position**

Position	Assistant Professor		
Date	01/03/2023		
Affiliation	Universidad de Alcalá (UAH)		
Department	Department of Organic and Inorganic Chemistry		
Country	Spain	Phone number	(+34) 918854622
Keywords	Medicinal Chemistry, Molecular Modeling, Drug Design, Chemical Biology		

**A.2. Previous positions**

Period	Position/Institution/Country/Cause of the interruption
2022-2023	Visiting Academic - Postdoctoral Researcher (University of Bath)
2020-2022	Postdoctoral Researcher (CIB-CSIC)
2016-2020	PhD Candidate at Universidad de Alcalá (UAH)
2015-2016	Research Assistant at Universidad de Alcalá (UAH)

**A.3. Education**

Degree/Master/PhD	University/Country	Year
PhD in Medicinal Chemistry (with honors)	Universidad de Alcalá (UAH)	2020
MSc. In Drug Discovery	University Complutense of Madrid (UCM)	2015
Bachelor of Pharmacy (with honors)	University Complutense of Madrid (UCM)	2014

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

In 2014, I received a BSc in Pharmacy from the Universidad Complutense de Madrid (Rafael Fölch Extraordinary Award). My enthusiasm for research during my undergraduate studies led me to get two competitive undergraduate research fellowships. The first was at the Spanish National Cancer Research Centre (CNIO) in 2012, focusing on medicinal chemistry. The second, in 2013, was at the Department of Pharmaceutical Chemistry (Faculty of Pharmacy, UCM) with a project focused on biocatalysis.

After finishing a MSc in Drug discovery (UCM, 2014), I began a PhD at the University of Alcalá with the support of two competitive PhD Grants: FPU-UAH (2016) from the UAH and an FPU contract from the Spanish Ministry of Education (2017), both under the supervision of Prof. Juan J. Vaquero. Later, in 2018, I was awarded with a mobility grant to carry out a research stay at the University of Bristol in UK (July-September) under the supervision of Prof. Adrian Mulholland to learn computational techniques for the study of PTP1B inhibitors.

During my PhD, my work entailed two different lines, with training on organic synthesis, molecular modelling and biologic assays. On the one hand, I worked in the design synthesis and study of PTP1B inhibitors (ChemMedChem 2020, 2023, etc). On the other hand, I had the opportunity to start and lead my first research line, based on my own ideas and with the support

of my supervisors, aimed to study ILK: $\alpha$ -parvin interaction. Part of this work has been already published (ACS. Med. Chem. Lett.), as corresponding author, and two different patents (one international, registered). Thanks to this work, I also was awarded different Prizes (SEQT Young Research 2019 and 2021, BioSolveIT 2018).

After finishing my PhD in 2020 (Extraordinary Award) and motivated by my interest in computational drug design I started (June 2020) a postdoctoral position at the Centre for Biological Research Margarita Salas (CIB-CSIC) under the supervision of Dr. Sonsoles Martin-Santamaria during COVID outbreak. In this time, I worked, mainly, in the search of new drugs against SARS-CoV-2 and its study by means of computational approaches. From this period a manuscript in preparation (Garcia-Marin, J.; et al. Manuscript submitted), and a book chapter published as well as participation in a research congress and the BioSolveIT 2020 Summer Challenge Prize.

In 2021, I received the Alfonso Martin Escudero Postdoctoral Fellowship, followed by the Margarita Salas Postdoctoral Fellowship (Spanish Ministry of Universities), which enabled me to undertake second postdoctoral research stay (February 2022) at the University of Bath in the UK, under the supervision of Prof. Carmen Domene to work on ion channels and oxygenases. Regarding this, I have, at least, one manuscript in preparation (García-Marin, J.; Oakes, V.; Domene, C. Manuscript in preparation 2025.) and participation in congresses.

Finally, on March 2023 I was appointed Assistant Professor at the UAH, where I joined the Department of Organic Chemistry to start my independent scientific career. Based on my career and interests in computational chemistry and drug design, I am starting to develop my own research lines, with some outcomes published as corresponding authors in different journals (J. Biomol. Struct. Dyn 2020 and 2023, J. Comput. Aided Mol. Des. 2022). Moreover, I have started to rise some funds for my own research from UAH (PIUAH23/CC-022), Comunidad de Madrid (CM/DEMG/2024-005) and Red Española de Supercomputación.

In addition to my research experience, I teach several courses for undergraduate students in Pharmacy, Chemistry and Biology and in the Master of Drug Discovery (2023, 2025) and Investigation in Pharmacology (CSIC, 2022). I have supervised 6 TFMs (2016, 2017, 2018, 2019, 2021, 2023) and two TFGs and I usually participate in outreach activities such as 'Semana de la Ciencia' (CSIC 2020 and 2021) and 'Química en Acción' (UAH 2016, 2017, 2018, 2019). Finally, in 2024 I started to supervise my first PhD Student, Marta Duran who is funded by CAM (until 2028) with a predoctoral grant to research on ILK.

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

### C.1. Publications (CA: Corresponding Author, OA: Open Access)

- 1 **Article**. (CA) J Garcia-Marin; et al. S. Martin-Santamaria; (1/10). *Exploring SARS-CoV-2 Spike RBD Pockets as Targets for Generic Drugs. A combined computational, biophysical and biological approach. Submitted. 2025.*
- 2 **Article**. (CA) (OA) F. Maqueda-Zelaya, L Valiño-Rivas, A Milián, S Gutiérrez, JL Aceña, J Garcia-Marin, D Sánchez-Niño, JJ. Vaquero, A Ortiz; (6/9). Identification and study of new NF- $\kappa$ B-inducing kinase (NIK) ligands derived from the imidazolone scaffold. Arch. Pharm. <https://doi.org/10.1002/ardp.202400614>
- 3 **Book chapter**. E. Gomez-Rubio, A. Matamoros-Recio, J. Garcia-Marin, S. Santamaria; (3/4) Computational Simulations of Glycan Recognition by Lectins and Other Carbohydrate Binding Proteins. Comprehensive Computational Chemistry. Edited by Professors Russell Boyd and Manuel Yanez. 2024. Elsevier. 4, pp 921-941. <https://doi.org/10.1016/B978-0-12-821978-2.00084-2>
- 4 **Article**. (CA) E. Gomez-Rubio, J. Garcia-Marin; (2/2). Molecular dynamics simulations reveal the impact of NUTD15 variants in structural conformation and dynamics. 2023. J. Biomol. Struct. Dyn. 41, pp: 14812-1482. <https://doi.org/10.1080/07391102.2023.2187626>
- 5 **Article**. (OA) (CA) J. Garcia-Marin; D. Rodríguez-Puyol; Juan J. Vaquero; (1/3). 2022.

- Insight into the mechanism of molecular recognition between human Integrin-Linked Kinase and Cpd22 and its implication at atomic level. 2022. *J. Comput. Aided Mol. Des.* 36, pp 575–589. <https://doi.org/10.1007/s10822-022-00466-1>.
- 6 Article.** (OA) H. Lucio; J. Garcia-Marin; P. Sanchez-Alonso; J. C. Garcia-Soriano; Juan J. Vaquero; F. Gago; R. Alajarín; A. Jiménez-Ruiz. (2/9). 2022. Pyridazino-pyrrolo-quinoxalium salts as highly potent and selective leishmanicidal agents targeting trypanothione reductase. *Euro. J. Med. Chem. Elsevier.* pp.113915. <https://doi.org/10.1016/j.ejmech.2021.113915>.
- 7 Article.** (CA), (OA). J. Garcia-Marin; M. Griera; A. Matamoros-Recio, D. Rodriguez-Puyol. (1/8). 2021. Tripeptides as Integrin-Linked Kinase Modulating Agents Based on a Protein–Protein Interaction with  $\alpha$ -Parvin. *ACS Med. Chem. Lett.* 12-11, pp.1656-1662. <https://doi.org/10.1021/ACSMEDCHEMLETT.1C00183>. **Issue Inside Cover.**
- 8 Article.** (CA), (OA). J. Garcia-Marin; M. Griera; R. Alajarín; M. Rodriguez-Puyol; D. Rodriguez-Puyol; Juan J. Vaquero. (1/6). 2021. A computer-driven scaffold-hopping approach generating new PTP1B inhibitors from the pyrrolo[1,2-a]quinoxaline core *ChemMedChem*. Wiley. 16-18, 2895-2906. <https://doi.org/10.1002/cmdc.202100338>.
- 9 Article.** (OA). P. Sanchez-Alonso; M. Griera; J. Garcia-Marin; M. Rodriguez-Puyol; Juan J. Vaquero; D. Rodriguez-Puyol. (3/7). 2021. Pyrrolo[1,2-a]quinoxal-5-inium Salts and 4,5-dihydropyrrolo[1,2-a]quinoxalines: Synthesis, Activity and Computational Docking for Protein Tyrosine Phosphatase 1B. *Bioorg. Med. Chem. Elsevier.* 44-15, pp.116295. <https://doi.org/10.1016/j.bmc.2021.116295>.
- 10 Article.** J. Garcia-Marin; M. Griera; P. Sanchez-Alonso; et al; D. Rodriguez-Puyol. (1/ 11). 2020. Pyrrolo[1,2-a]quinoxalines: Insulin Mimetics that Exhibit Potent and Selective Inhibition against Protein Tyrosine Phosphatase 1B *ChemMedChem*. 15-1, pp.1-15. <https://doi.org/10.1002/cmdc.202000446>. **Issue Front Cover.**
- 11 Article.** (CA). J. Garcia-Marin. (1/1). 2020. Computational Insight into the Selective Allosteric Inhibition for PTP1B versus TCPTP *J. Biomol. Struct. Dyn.* Taylor and Francis. 39-15, pp.5399-5410. <https://doi.org/10.1080/07391102.2020.1790421>.

## C.2. Congress (selection from last 5 years)

1. M. Durán; M Griera; S de Frutos García; José L Aceña; L Calleros; D Rodríguez-Puyol; J García-Marin. *Modulating the pseudokinase Integrin-Linked Kinase through new small molecules*. XX Simposio de Jóvenes Investigadores Químicos de la Real Sociedad Española de Química. Ciudad Real (Spain). Flash & Poster.18/11/2024-21/11/2024.
2. M Griera; J García-Marin; A Silvestre; et al; S de Frutos García. *Aproximación terapéutica contra la resistencia a la insulina mediante el uso de una nueva molécula activadora del andamiaje celular*. 54 Congreso Nacional de la Sociedad Española de Nefrología. 2024. Valencia (Spain). Poster. 08/11/2024 - 10/11/2024.
3. J Garcia-Marin, C Domene. *Atomic Insights into the TRPM8 Activation by Small Molecules Through Computational Approaches*. VI RSEQ Chemical Biology Group Meeting (ChemBioVI). Valencia (Spain) Poster. 06/03/2023-08/03/2023.
4. J Garcia-Marin, S. Martin-Santamaria. *SARS-CoV-2 Spike Protein Receptor Binding Domain. Computational Exploration, Drug Repurposing and Beyond*. *SARS-CoV-2 Spike Protein Receptor Binding Domain. Computational Exploration, Drug Repurposing and Beyond*. MolSim 2022. Erice (Italy). Poster. 25/06/2022-29/05/2022.
5. J Garcia-Marin, C Domene. *Deciphering the role of O<sub>2</sub> molecule in oxygenases catalysis. Hybrid Quantum Mechanics / Molecular Mechanics (QM/MM) approaches to biochemistry and beyond*. Lausanne (Switzerland). Poster. 16/05/2022-20/05/2022.
6. J Garcia-Marin, M. Griera; D. Rodríguez-Puyol; M. Rodríguez-Puyol; J. Vaquero; R. Alajarín. *Strategies against chronic kidney disease: new modulators of PTP1B and ILK*. Paul Ehrlich Euro-PhD Network Virtual Meeting 2021. Paul Ehrlich Euro-PhD Network. Italy. Invited Communication. 19/07/2021-24/07/2021.

### C.3. Research projects

1. CM/DEMG/2024-005, Aproximaciones químicas y computacionales para la modulación de la quinasa ligada a integrinas. Javier García Marín. (Universidad de Alcalá). 01/01/2025-30/12/2026. Comunidad de Madrid-UAH. 15.000 €. **Principal Investigator**.
2. RD24/0004/0008, RICORS2040-RENAL, Redes de Investigación Cooperativa Orientadas a Resultados en Salud. Coor: Alberto Ortiz. PI: Manuel Ángel Rodríguez. Instituto de Salud Carlos III. 138.000 €. Researcher.
3. BCV-2024-3-0010, Computational insights into the scaffolding activation of a pseudokinase by a small molecule (II). Javier García Marín. Red Española de Supercomputación. (Universidad de Alcalá). 01/11/2024-28/02/2025. 600 kh, Marenostrum 5. **Principal Investigator**.
4. BCV-2024-2-0037, Computational insights into the scaffolding activation of a pseudokinase by a small molecule. Javier García Marín. Red Española de Supercomputación. (Universidad de Alcalá).01/07/2024-31/10/2024. 2016 kh, Marenostrum 5. **Principal Investigator**.
5. PIUAH23/CC-022, Nuevas estrategias terapéuticas en enfermedad renal crónica: Desarrollo de nuevos activadores de CPT1A. Javier García Marín. (Universidad de Alcalá). From 01/12/2023 to 30/11/2024. 6.500 €. **Principal investigator**.
6. P2022/BMD-7221, INNOREN-CM, Nuevas estrategias diagnósticas y terapéuticas en enfermedad renal crónica. PI: Santiago Lamas Peláez. (Universidad de Alcalá). 01/01/2021-31/12/2026. 818.000,0 €. Researcher.
7. SGL2103050, Plataforma de Antivirales WP9. Fondo Recuperación EU/Recovery and Resilience Facility. 2021-22. PI: Khlar. (Centre For Biological Research CIB-CSIC). From: 01/07/2021. Working team.

### C.4. Technology/Knowledge transfer and exploitation of result

- 1 **Patent.** Javier García Marín; Ramón Alajarín Ferrández; Juan José Vaquero López; Sergio de Frutos; Diego Rodríguez Puyol. PCT/ES2021/070571. Compuestos que se unen a la ILK y modulan la interacción ILK/alfa-parvina y la polimerización de actina. International. 2022/02/03. Universidad de Alcalá. Number: WO2022023612.
- 2 **Patent.** Javier García Marín; Ramón Alajarín Ferrández; Juan José Vaquero López; Mercedes Griera; Manuel Rodríguez Puyol; Sergio de Frutos; Diego Rodríguez Puyol. P202030775. COMPUESTOS QUE SE UNEN A LA ILK Y MODULAN LA INTERACCIÓN ILK/ALFA-PARVINA Y LA POLIMERIZACIÓN DE ACTINA. Spain. 2021/07/27. Universidad de Alcalá. Number: ES2892087
- 3 **Patent.** Javier García Marín; Ramón Alajarín Ferrández; Juan José Vaquero López; Mercedes Griera; Sergio de Frutos; Manuel Rodríguez Puyol; Diego Rodríguez Puyol. P202030776. COMPUESTOS MODULADORES DEL EFECTO DE LA QUINASA LIGADA A INTEGRINAS (ILK) SOBRE LA POLIMERIZACIÓN DE ACTINA. Spain. 27/07/2020. Universidad de Alcalá. Number: ES2892025.

### C.5. Awards (Last 5 years)

1. Premio Extraordinario de Doctorado de la Universidad de Alcalá (2020-2021) 2022.
2. Paul Ehrlich Award 2021 Euro-PhD Network Award (2021).
3. Premio Asisa de la Real Academia Nacional de Farmacia (2021).

### C.5. Doctoral thesis

1. Marta Durán. Medicinal Chemistry Program (UAH). *Development of new ILK modulators for highly prevalent diseases*. Expected defense: 2028. Funding: CAM Predoctoral grant.