





## **CURRICULUM VITAE ABREVIADO (CVA)- 4 pages**

#### Part A. PERSONAL INFORMATION

First name	Nuria		
Family name	Sotomayor Anduiza		Date: January 2023
Gender (*)	Female		
ID number	16040929Q		
e-mail	nuria.sotomayor@ehu.eus	https://www.ehu.eus/en/web/oms/home	
Open Researcher and Contributor ID (ORCID) (*)		0000-0003-3079-6380	

(\*) Mandatory

A.1. Current position

Position	Profesor of Organic Chemistry			
Initial date	13/12/2010			
Institution	Universidad del País Vasco/Euskal Herriko Unibertsitatea UPV/EHU			
Department/Center	Organic and Inorganic Chemistry	Faculty of Science and Technology		
Country	Spain		Teleph. No.	652701736
Key words	Organic synthesis, stereoselective synthesis, asymmetric catalysis, organometallic reagents, metalation, cross-coupling reactions, C-H activation, heterocycles, alkaloids			

A.2. Previous positions (research activity interuptions, indicate total months)

Period	Position/Institution/Country/Interruption cause
01/01/1990/31/12/93	Predoctoral Fellow (FPU), UPV/EHU, Spain
01/01/1994/13/02/1995	Postdoctoral Fellow (GV), University of Waterloo, Canada
14/02/1995/	Lecturer in Organic Chemistry, UPV/EHU, Spain
01/11/1997/12/12/2010	Reader in Organic Chemistry, UPV/EHU, Spain
13/12/2010/ actualidad	Full Professor of Organic Chemistry, UPV/EHU, Spain

### A.3. Education

PhD, Licensed, Graduate	University/Country	Year
BSc (Chemistry)	Universidad del País Vasco/EHU	1988
PhD	Universidad del País Vasco/EHU	1993

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

Obtained her B. Sc. Degree in Chemistry, and her Ph.D. Degree (1993) at the University of the Basque Country on the synthesis of isoquinoline alkaloids (protoberberine and benzo[c]phenanthridines). After post-doctoral research at the University of Waterloo (Ontario, Canada) with Prof. Victor Snieckus (1994-1995), on directed *ortho*-metalation (DoM) and cross-coupling reactions, she returned to the Department of Organic Chemistry II of the University of the Basque Country in Bilbao (1995), contributing to the development of new research lines within the group led by prof. E. Lete. Then, she was promoted to Associate professor (Prof. Titular) in 1998, and to Full Professor (CU) in 2010. Together with Prof. E. Lete, she is now leading the group "Organometalicos en Síntesis" (organometalics in synthesis), recognized as Consolidated Research Group by the Basque Government since 2000. Currently, this group is part of the Consolidated Group "Metal Catalysis and Organocatalysis" leaded by Prof. E. Lete and Prof. J. L. Vicario (2022-2025). Her initial research lines on organolithium chemistry, including ligand-mediated enantioselective variants, have evolved to transition metal catalysis. The group has developed Pd(0) catalyzed alkenylation (MH-Type) and arylation reactions, including also cascade processes. Diastereo and enantioselective variants have also been developed. More recently her interests have moved to C-H activation mediated by Pd(II), studying the arylation and alkenylation of arenes and hetreoarenes. Currently, the use of more abundant and less toxic 3d metals, such as Cobalt, is one of her research lines, in which the group has contributed studying intramolecular alkene hydroarylation reactions. As a summary, her current research interests are focused on the development of methodology based on organometallic chemistry and asymmetric catalysis, and applied to the synthesis of heterocyclic systems, potentially active compounds, natural products or



drugs. She also participates in interdisciplinary projects that involve computational chemistry and machine learning (ML) tools for reactivity prediction, and for the design of biologically active molecules.

She has taken part of research projects with public funding since 1990 (8 national projects since 1996), and she is co-Principal Investigator (co-PI) of the two last projects (CTQ2016 and PID-2019). She has also participated in contracts with chemical companies (MAXAM SA, Petronor), and also with multidisciplinary partners (Virtualware, HiB), being PI of two of these contracts.

More recently, she has also been involved in multidisciplinary projects with companies and technology centers financed by the ELKARTEK program of the SPRI agency of the Department of Industry of the Basque Government. These are multidisciplinary oriented projects mainly in the area of drug discovery, for instance for neuropsychiatric diseases, or for the discovery of drug candidates for calmodulinopathies. Also, for the synthesis and preclinical assay of Metal-Organic Frameworks drug release systems for gastrointestinal (GI) Cancer Treatment. These projects have involved the collaboration with different partners from UPV/EHU, Instituto Biofisika CSIC-UPV/EHU, BCmaterials, Instituto Biodonostia, Instituto Biocruces Bizkaia, TECNALIA, Donostia International Physics Center (DIPC), GAIKER or TEKNIKER.

As a result, she has authored over 95 publications in indexed journals, together with book chapters and reviews, and > 90 communications to conferences. Training of researchers has also been a constant, and thus, she has supervised 19 PhD thesis and >50 Master/BSc students.

Besides, she is since 2012 she is Responsible for the Master program in Synthetic and Industrial Chemistry, a joint program offered by the University of the Basque Country with the University of Valladolid and the Public University of Navarra. Her more relevant contribution in University management has been the position as Director of the Postgraduate studies and Continuing Education Section, from 2006 to 2010, when she was responsible for the implementation strategy of all Master and PhD programs at the UPV/EHU.

# Part C. RELEVANT MERITS (sorted by typology)

# **C.1. Publications** (10 publications last 10 years)

- 1. Carral, A.; Sotomayor, N.; Lete, E. Palladium-catalyzed oxidative arene C-H alkenylation reactions involving olefins. *Trends Chem.*, **2022**, 4, 495-511.
- 2. Barbolla, I.; Hernández-Suárez, Quevedo-Tumailli, V.; Nocedo-Mena, D. Arrasate, S. Dea-Ayuela, M. A.; González-Díaz, H.; Sotomayor, N.; Lete, E. Palladium-mediated Synthesis and Biological Evaluation of C-10b substituted Dihydropyrrolo[1,2-*b*]isoquinolines as Antileishmanial Agents. *Eur. J. Med. Chem.* **2021**, 113458.
- 3. Carral-Menoyo, A.; Sotomayor, N.; Lete, E Amide-Directed Intramolecular Co(III)-Catalyzed C-H Hydroarylation of Alkenes for the Synthesis of Dihydrobenzofurans with a quaternary center, *J. Org. Chem.*, **2020**, *85*, 10261-10270.
- 4. Carral-Menoyo, A.; Sotorríos, L.; Ortiz-de-Elguea, V.; Diaz-Andrés, A.; Sotomayor, N.; Gómez-Bengoa, E.; Lete, E.. Intramolecular Palladium(II)-catalyzed 6-*endo* C-H alkenylation directed by the remote *N*-protecting group. Mechanistic insight and application to the synthesis of dihydroquinolines, *J. Org. Chem.*, **2020**, *85*, 2486-2503
- 5. Santiago, C.; Rubio, I.; Sotomayor, N; Lete, E. Selective Pd(II)-catalyzed Acylation of Pyrrole with Aldehydes. Application to the Synthesis of Celastramycin analogues and Tolmetin. *Eur. J. Org. Chem.*, **2020**, 4284-4295. (Selected as Very Important Paper (VIP). Front cover)
- 6. Simón-Vidal, L.; Garcia-Calvo, O.; Oteo, U.; Arrasate, S.; Lete, E.; Sotomayor, N.; González-Díaz, H. *Perturbation-Theory and Machine Learning (PTML) Model for High-Throughput Screening of Parham Reactions: Experimental and Theoretical Studies, J. Chem. Inf. Model.* **2018**, 58, 1384-1396.
- 7. Ortiz de Elguea, V.; Sotomayor, N.; Lete, E. *Two consecutive Pd(II)-promoted C-H alkenylation reactions for the synthesis of substituted 3-alkenylquinolones, Adv. Synth. Catal.* **2015**, *357*, 463-473.
- 8. A. R. Azcargorta, E. Coya, A. M. Panaite, N. Sotomayor, E. Lete, Intramolecular Addition of Heteroaryllithiums onto Activated Alkenes. Access to Heterofused Indolizines and Pyrroloazepines, *Eur. J. Org. Chem.* **2017**, 2462-2468 (Highlighted in *SYNFACTS* **2017**, *13*, 0693-0693)
- 9. E. Coya, N. Sotomayor, E. Lete, Enantioselective palladium catalyzed Heck-Heck cascade reactions. Ready access to the tretracyclic core of lycorane alkaloids, *Adv. Synth. Catal.* **2015**, 357, 3206-3214 (Highlighted in *SYNFACTS* **2016**, *12*, 0067-0067)



10. E. Coya, N. Sotomayor, E. Lete, Intramolecular Direct Arylation and Heck reactions in the formation of medium sized rings. Selective synthesis of fused indolizine, pyrroloazepine and pyrroloazocine systems, Adv. Synth. Catal. **2014**, 356, 1853 – 1865.

## C.2. Congress

Regular participation in national and international conferences: > 90 communications (oral comunications and posters); 1 invited lecture (Spanish Italian Symposum in Organic Chemistry)

# **C.3. Research projects** (last 10 years)

1. Project: New synthetic and cheminformatic tools for the construction and diversification of drug-like heterocycles. C-H activation and Machine Learning approaches

Principal Investigator: Esther Lete, Nuria Sotomayor Code: PID2019-104148GB-I00

Funding entity: MINECO (Call 2019, State Plan for R+D+i Projetcs-PGC B Type)

Start-End date: 01/06/2020-31/05/2023 Total amount (euros): 93.000

2. Project: Grants for Consolidated Research Groups of Universities of the Basque Country Principal Investigator: Esther Lete Expósito, José Luis Vicario Code: IT1558-22

Funding entity: Basque Government (Call 2021)

Start-End date: 01/01/2022-31/12/2025

Total amount (euros): 331.800

3. Project: Transition metal-catalyzed C-H activation reactions in synthesis and functionalization of heterocyclic sytems. A joint experimental and computational study

Principal Investigator: Esther Lete, Nuria Sotomayor Code: CTO2016-74881-P

Funding entity: MINECO (Call 2015, State Plan for R+D+i Projetcs)

Start-End date: 30/12/2016-29/12/2019 Total amount (euros): 89.000

4. Project: Grants for Consolidated Research Groups of Universities of the Basque Country

Principal Investigator: Esther Lete Expósito Code: IT1045-16

Funding entity: Basque Government (Call 2015)

Start-End date: 01/01/2016-31/12/2021 Total amount (euros): 209.589

5. Project: Gas Chromatograhy Mass Spectrometer GC/Q-TOF system (Infrastructure)

Principal Investigator: Esther Lete Expósito Code: 2015UNPV15-EE-3069

Funding entity: MINECO (Call 2016 Scientific and Technical Infrastructures and Equipment Start-End date: 2016 Total amount (euros): 347.526

6. Project: Asymmetric catalysis in synthesis. New chiral ligands for transition metal-based catalysis, synthetic applications and computational models. Code: CTQ2013-41229-P

Principal Investigator: Esther Lete Expósito

Funding entity: MINECO (Call 2013 State Plan for R+D+i Projects)

*Start-End date*: 01/01/2014-31/12/2016 Total amount (euros): 94.380

7. Project: Grants for Consolidated Research Groups of Universities of the Basque Country Principal Investigator: Esther Lete Expósito Code: IT623-13

Funding entity: Basque Government (Call 2012)

Start-End date: 01/01/2013-31/12/2015 Total amount (euros): 68.100

# **C.4. Contracts, technological or transfer merits** (last 10 years)

1. Project: Artificial Intelligence Guided Platform for Experimental Synthesis and Preclinical Assay of Metal-Organic Frameworks Drug Release Systems for Gastrointestinal (GI) Cancer Treatment and Code: KK-2022/00032

Partners: UPV/EHU, BCmaterials, Instituto Biodonostia, Instituto de Investigación Sanitaria Biocruces Bizkaia, TECNALIA

Funding entity: ELKARTEK program (Basque Government, Industry Department)

Start-End date:01/01/2022-31/12/2023 Total amount subproject (euros): 99.220

Principal Investigator: O. Castillo (Subproject PI Humberto González Díaz)

2. Project: Integrated platform for the discovery of candidates for calmodulinopathies (CardiCaM) Code: KK-2020/00110

Partners: UPV/EHU, Instituto Biofisika CSIC-UPV/EHU, Donostia International Physics Center (DIPC), GAIKER, TEKNIKER

Funding entity: ELKARTEK program (Basque Government, Industry Department)

Total amount subproject (euros): 66.228 Start-End date:01/01/2020-31/12/2021

Principal Investigator: A. Villaroel (Subproject PI Humberto González Díaz)

3. Project: Computational prediction of eco-friendly alternative building-blocks for fuel blends in Petrochemistry with PTML models (CHAIN) Code: KK-2019/00037

Partners: UPV/EHU (Departments of Physical Chemistry and Organic Chemistry II), Petronor



Funding entity: ELKARTEK program (Basque Government, Industry Department), Petronor SA Start-End date:01/01/2019- 31/12/2020 Total amount subproject (euros): 58.870

Leader: Petronor SA (Subproject PI Humberto González Díaz)

4. Project: Development of a platform for the discovery of drugs for neuropsychiatric diseases (PHAIKER)

Code: KK-2017-00023

Partners: UPV/EHU, Instituto Biofisika CSIC-UPV/EHU, Asoc. Fundación Biodonostia, Fundación Tecnalia Research & Development

Funding entity: ELKARTEK program (Basque Government, Industry Department)

*Start-End date*:01/01/2017- 30/06/2018 *Total amount subproject (euros)*: 35.991

Principal Investigator: Javier Meana (Subproject PI Esther Lete)

5. Contract/project: Definition of laboratory techniques and processes for virtualization

Code: Gaitek 2011 (OTRI 2011 0627), Gaitek 2012 (OTRI 2012.0055)

Partners: UPV/EHU, High Identity Buildings SL company

Funding entity: GAITEK Program (Basque Govern. Industry Dep.), High Identity Buildings SL company

*Start-End date*: 01/10/2011-31/12/2013 *Total amount (euros)*: 13.484,00

Principal Investigator: Nuria Sotomayor

6. Contract/project: Virtualization methods for laboratory techniques and processes. Rrequirements analysis and scenarios.

Code: Gaitek 201(OTRI 2011 0629), Gaitek 2012 (2012.0055)

Partners: UPV/EHU and Virtualware, S.A company

Funding entity: GAITEK Program (Basque Government, Industry Dept.), Virtualware, S.A

*Start-End date*: 01/10/2011-31/12/2013 *Total amount (euros)*: 5.664,00

Principal Investigator: Nuria Sotomayor

## C.5. Training: Supervision of PhD Thesis, master/bachelor's degree projects:

19 PhDs supervised (7 since 2013), 5 obtained International Mention and 2 Extraodinary Doctoral awards. 5 of them achieved positions at Universities or Research Institutes in Spain [CIDETEC, (Gipuzkoa) UPV/EHU, ISCH (U. Zaragoza, CSIC)], or outside (Salahaddin University, Erbil, Iraq), 6 achieved scientific/technical positions at Pharma/Chemistry Industry: Syncom BV, (Groningen, the Netherlands), TH Company, Lucart, (Bizkaia), Pharmamar, (Madrid), Praxis Pharmaceutical (Álava), TEVA PHARMA, (Zaragoza)], 3 of them went to secondary education, 2 of them went to technical works (labour risks prevention).

Over 50 master and undergradute students supervised.

#### **C.6 Responsibility in Training Programs**

Project/Program: Interuniversity Master in Synthetic and Industrial Chemistry

Organising Universities: University of the Basque Country(UPV/EHU), Pubic University of Navarre (UPNA), University of Valladolid (UVA).

Other participating entities: CIC BioGUNE, CIC BiomaGUNE, CIC EnergiGUNE, FAES PHARMA. General Coordinator: Nuria Sotomayor (June 2012 –continues)

### C.7. Institutional responsibilities

Director of the Postgraduate studies and Continuing Education Section (2006-2010): Responsible for the implementation of Master and PhD programs at the UPV/EHU

#### C.8. Others

- 1. Editorial board (section editor: Chemical synthesis) of Curr. Top. Med. Chem. (2019-2022)
- 2. Co-Editor of the thematic issue *Enantioselective Synthesis in Organic and Medicinal Chemistry*, *Curr. Top. Med. Chem.* **2014**, *14* (*10*)
- 3. Co- President of the Advisory Committee (Experimental Sciences), annual conferences online MOL2NET: International Conference on Multidisciplinary Sciences, since 20015..
- 4. Referee of scientific journals [i.e.; *J. Org. Chem., Org. Lett. ACS Catalysis, ACS Omega*, (ACS), *Eur. J. Org. Chem., Adv. Synth. Catal., Chem. Eur. J.* (Wiley), *Synthetis* (Thieme).]
- 5. Evaluation of research projects: External reviewer for ANR (France, 2012) and FWO (Belgium, 2017).
- 6. Memberships of scientific societies: RSEQ, ACS