CURRICULUM VITAE ABREVIADO (CVA) 4 pages

Part A. PERSONAL INFORMATION

First name	M. Esther		
Family name	Lete Expósito		
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Open Researcher and Contributor ID (ORCID)		0000-0001-8624-6842	

A.1. Current position

Position	Profesor of Organic Chemistry		
Initial date	07-07-1997		
Institution	Universidad del País Vasco/Euskal Herriko Unibertsitatea UPV/EHU		
Department/Center	Organic and Inorganic Chemistry	Faculty of Science and Technology	
Country	Spain		
Key words	Organic synthesis, stereoselective synthesis, asymmetric catalysis, aromatic lithiation, transition-metal catalyzed cross-coupling, C-H activation, α-amidoalkylation, heterocycles, alkaloids		

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

Period	Position/Institution/Country
01-01-1979/31-12-81	Predoctoral Fellow (FPU), UPV/EHU, Spain
01-04-1981 / 31-12-1981	Teaching Assistant, UPV/EHU, Spain
01-01-1982 / 13-01-1985	Lecturer in Organic Chemistry, UPV/EHU, Spain
14-01-1985 / 06-07-1997	Reader in Organic Chemistry, UPV/EHU, Spain
07-07-1997 / actualidad	Full Professor of Organic Chemistry, UPV/EHU, Spain

A.3. Education

PhD, Licensed, Graduate	University/Country	Year
BSc	University of Bilbao	1978
PhD	University of the Basque Country UPV/EHU	1982

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

Esther Lete is Professor of Organic Chemistry at the Department of Organic and Inorganic Chemistry, Faculty of Science and Technology, UPV/EHU. She obtained a first class honors degree in Chemistry at the University of Bilbao in 1978. She received a PhD degree (doctoral award) at the University of the Basque Country in 1982 with a thesis on synthesis of 3.-arylisoquinolines (supervisor. E. Domínguez). After a stay with P. J. Garratt at University College London, studying the chemistry and synthetic applications of carbanions, she took up a lectureship in organic chemistry at the University of the Basque Country (1985) and was promoted to Full Professor in 1997. Together with Prof. Nuria Sotomayor, she leads the research group Organometallics in synthesis (www.ehu.es/oms).

She has a wide experience in synthetic organic chemistry. At the beginning of her research career, she worked on heterocyclic chemistry, in particular, on the application of classical methodologies to the synthesis of alkaloids (isqouinolines, protoberberines, benzophenanthridines) with particular emphasis on the Bischler-Napieralski reaction (*J. Org. Chem*. **1996**, *61*, 4062). In the 90's, she started her independent career opening a new research line on organolithium chemistry, and her most outstanding achievements in this field are collected in *Science of Synthesis* (Thieme). Among them are the works on Parham cyclization (an anionic equivalent of Friedel-Crafts reaction) and the development of tandem Parham cyclization–α-amidoalkylation reactions, including diastereoselective variants (*J. Org. Chem*. **1997**, *62*, 2080; *J. Org. Chem.* **2004**, *69*, 3875; *J. Org. Chem.* **2005,** *70*, 10368; *J. Org. Chem.* **2006**, *71*, 6776) and more recently enantioselective versions using CPAs (*J. Org. Chem.* **2012**, *77*, 2986). Another milestone was the enantioselective intramolecular carbolithiation reactions for the synthesis of enantiopure 4-substituted tetrahydroquinolines (*Org. Lett.* **2009**, *11*, 1237). Within the last 10 years, her research has been focused on transition-metal-catalyzed cross-coupling reactions, including diasteroselective and enantioselective and even domino reactions (Heck-Heck, Heck-Suzuki, and Heck-anion trap cascades) (*Adv. Synth. Catal* **2009**, *351*, 2460; *Adv. Synth. Catal.* **2014**, *356,* 1853; *Adv. Synth. Catal.* **2015**, 357, 3206; *J. Org. Chem.* **2019**, *84*, 10183). Afterwards, her interests have moved to the C-H activation reactions, specifically to Pd(II)-catalyzed C(sp^2)-H activation reactions, where her contributions on oxidative C-H acylations and C-H alkenylations (including the atroposelective variant

to construct C-C chiral heterobiaryls) stand out (*Trends Chem.* **2022,** 4, 495; *Org. Biomol. Chem.* **2022**, 20, 852*; J. Org. Chem.* **2020**, *85*, 2486). More recently, she began studying the use of earth-abundant and non-toxic 3d-transition-metals, in particular, high-valent Cobalt catalysis in the synthesis and functionalization of (hetero)arenes (*J. Org. Chem.* **2020**, *85*, 10261; *Eur. J. Org. Chem.* **2024**, *27*, e202301090). She also participates in interdisciplinary projects that involve computational chemistry and machine learning for reaction prediction and design of new catalysts (*Eur. J. Med. Chem*. **2021,** *220,* 113458; *J. Chem. Inf. Model.* **2022**, *29*, 3928; *J. Chemoinform. 6*, 9 (**2024**)).

She has been Principal Investigator of 9 projects of the State Research Plan since 1996, and previously she was PI of projects of the Basque Government and UPV / EHU. She is co-author of more than 120 articles in JCR journals and 9 book chapters (reviews). He has presented >130 communications and delivered around 20 invited conferences at national and international conferences, universities and / or research centers. She has got 6 research sexenios and the maximum level of regional recognition (A2). She has also some experience in technology transfer, she has participated in projects/contracts with chemical-pharmaceutical companies, such as MAXAM SA, and Petronor. She is also involved in multidisciplinary projects with Technology Centers and companies.
From the management perspective, she was Academic Secretary of the Faculty of Science and Technology of the UPV/EHU (1994-1999) and Head of the Department of Organic Chemistry II of the same Institution (2007-2011). She has been coordinator of the Master in Synthetic and Industrial Chemistry (2007-2012) and the various doctoral Programs: Advanced Studies in Fundamental and Applied Organic Chemistry (2001-2007) and Synthetic and Industrial Chemistry (2007-present). In this period she achieved the Mentions of Quality and Excellence, the highest distinctions in doctoral programs for Spanish Universities. Besides managing her research group, with 22 PhD students and 10 postdocs supervised, as well as Master's (>40) and bachelor's (>10) students.

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

C.1. Publications *(10 selected publications, last 10 years)*

1. A. Carral-Menoyo, I. Barbolla, C. Santiago, M. Espinel, N. Sotomayor, E. Gómez-Bengoa, E. Lete Título: Directed C–H Allylation of Aromatic Carboxamides with Allyl Aryl Ethers under Cp*Co(III)-Catalysis*. Eur. J. Org. Chem.* **2024***, 27*, e202301090 (Highlighted in *Chemistry Views)*
2. A. Carral, N. Sotomayor, E. Lete. Palladium-catalyzed oxidative arene C-H alkenylation reactions involving olefins. *Trends Chem.* **2022,** 4, 495-511.
3. C. Santiago, B. Ortega-Tenezaca, I. Barbolla, B. Fundora, S. Arrasate, H. González-Díaz, N. Sotomayor, E. Lete. Prediction of Antileishmanial Compounds: General Model, Preparation, and Evaluation of 2-Acylpyrrole Derivatives. *J. Chem. Inf. Model.* **2022**, *29*, 3928-3940.
4. C. Santiago, X. Jiménez-Aberasturi, E. Leicea, Marta G. Lete, N. Sotomayor, E. Lete. Microwave-assisted Palladium catalysed C-H acylation with aldehydes. Synthesis and diversification of 3-acylthiophenes. *Org. Biomol. Chem.* **2022**, 20, 852-961.
5. I. Barbolla, L. Hernández-Suárez, V. Quevedo-Tumailli, D. Nocedo-Mena, S. Arrasate, M. A. Dea-Ayuela, H. González-Díaz, N. Sotomayor, E. Lete. Palladium-mediated Synthesis and Biological Evaluation of C-10b substituted Dihydropyrrolo[1,2-*b*]isoquinolines as Antileishmanial Agents. *Eur. J. Med. Chem*. **2021**. 113458.
6. A. Carral-Menoyo, N. Sotomayor, E. Lete. 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.
7. I. Barbolla, N. Sotomayor, E. Lete, Carbopalladation/Suzuki Coupling Cascade for the Generation of Quaternary Centers. Access to Pyrrolo[1,2-*b*]isoquinolines, *J. Org. Chem.* **2019**, *84*, 10183−10196.
8. V. Ortiz de Elguea, N. Sotomayor, E. Lete, Two consecutive Pd(II)-promoted C-H alkenylation reactions for the synthesis of substituted 3-alkenylquinolones, *Adv. Synth. Catal.* **2015***, 357,* 463-473.
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: > 120 communications (oral comunications and posters). Around 20 invited lectures at symposia and institutions in the last ten years. I have been invited to scientific meetings related to my contributions to chemical synthesis and catalysis. Plenaries or Keynote/Invited include: CiQUS lecture (Santiago de Compsotela, 2022), Sixth Barluenga Lectureship (Oviedo, 2019), 12th Spanish Italian Symposium on Organic Chemistry (SISOC XII) (Ferrara, 2018), XX Semana Científica Antonio Gónzalez (La Laguna, 2016), 3rd US-Spain Symposium on Asymmetric Catalysis and Chemical Synthesis (Bilbao, 2016), Bioheterocycles 2015-XVI International Conference on Heterocycles in Bioorganic Chemistry (Metz, 2015), 6th Spanish Portuguese Japanese Organic Chemistry Symposium – 6SPJ-OCS (Lisbon, 2012), 9th International Symposium on Carbanion Chemistry (ISCC-9) (Florence, 2010).

C.3. Research projects (*selected projects, last 10 years*)

1. Project: Strategies for 3d-metal-catalyzed C-H activation. Synthetic applications and Machine Learning approaches for chemical reactivity and biological activity (SYML)
Principal Investigator: Esther Lete, Nuria Sotomayor *Code*: PID2022-137365NB-I00
Funding entity: MINECO (Call 2019, State Plan for R+D+i Projetcs-PGC B Type)
Start-End date: 01/09/2023-31/08/2026

2. 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

3. Project: Grants for Consolidated Research Groups of Universities of the Basque Country
Principal Investigator: Esther Lete, José Luis Vicario *Code: IT1558-22*
Funding entity: Basque Government (Call 2021)
Start-End date: 01/01/2022-31/12/2025

4. 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: CTQ2016-74881-P*
Funding entity: MINECO (Call 2015, State Plan for R+D+i Projetcs)
Start-End date: 30/12/2016-29/12/2019

5. 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

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

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

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

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

ELKARTEK program *(Basque Government, Industry Department)*

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 Prevention (AIMOFGIF) *Code: KK-2022/00032*
Partners: UPV/EHU, BCmaterials, Instituto Biodonostia, Instituto de Investigación Sanitaria Biocruces Bizkaia, TECNALIA
Start-End date:01/01/2022- 31/12/2023
Principal Investigator: O. Castillo (Subproject PI Humberto González Díaz)

2. Project: Integrated platform for the discovery of candidates for calmodulinopathies (CardiCaM)
Partners: UPV/EHU, Instituto Biofisika CSIC-UPV/EHU, Donostia International Physics Center (DIPC), GAIKER, TEKNIKER *Code: KK-2020/00110*
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 Petro-chemistry with PTML models (CHAIN) *Code: KK-2019/00037*
Partners: UPV/EHU (Departments of Physical Chemistry and Organic Chemistry II), Petronor
Start-End date:01/01/2019- 31/12/2020
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
Start-End date:01/01/2017- 30/06/2018
Principal Investigator: Javier Meana (Subproject PI Esther Lete)

GAITEK Program (*(Basque Government, Industry Department)*
5. *Contract/project*: Definition of laboratory techniques and processes for virtualization/ Virtualization methods for laboratory techniques and processes. Rrequirements analysis and scenarios.
Code: Gaitek 2011 (OTRI 2011 0627), Gaitek 2012 (OTRI 2012.0055)
Partners: UPV/EHU, Identity Buildings SL company, Virtualware, S.A company
Start-End date: 01/10/2011-31/12/2013 *Total amount (euros)*: 19,148
*Principal Investigato*r: Nuria Sotomayor

C.5. Supervision of PhD Thesis, master/bachelor's degree projects:
23 PhDs supervised (7 since 2013), 7 obtained International Mention and 4 Extraodinary Doctoral awards. It should be noted that 9 of them achieved positions at Universities or Research Institutes in Spain or outside, 7 achieved scientific/technical positions at Pharma/Chemistry Industry, 1 achieved high-level technician NMR position at UPV/EHU. About 10 postdoc supervised. Most of them (>70%) hold research-oriented positions.
Member of over 50 PhD evaluation committees. Over 40 master projects and over 10 bachelor's degree projects supervised.

C.6. Responsabilities in Training Programs (last 10 years)
1. *Project/Program*: Glyco-Nanoparticles for Applications in Advanced Nanomedicine (NanoCarb) (https://www.nanocarb.eu/network/partner-organisations/).
Funding entity: European Union's Horizon 2020 research and innovation programme under the MSC grant agreement No 814236 (8 Beneficiaries, 9 Partners Organizations
Coordinator: Marco Monopoli, RSC (Ireland) *Start-End date*: 01/10/2018-30/09/2020
Team Leader of the UPV/EHU training program (Partner organization): Esther Lete Expósito
2. *Project/Program*: Interuniversity Doctoral Program in Synthetic and Industrial Chemistry
Quality (ref. MCD2007-00026,) and Excellence mentions (ref. MEE2011-0092)
Entities: UPV/EHU, UPNA
Coordinator: Esther Lete Expósito *Start-End date:* 01/10/2007-present

C.7. Others
1. Scientific committees: International Scientific committee (permanent) of conference series: Heterocycles in Bioorganic Chemistry (2019-present); MOL2NET: International Conference on Multidisciplinary Sciences, since 20015; RSEQ annual meeting (2018-19).
2. Coordinator of ERASMUS+ University of Rostock, Germany.
3. Referee of scientific journals [J. Org. Chem., Org. Lett., JACS (ACS), Eur. J. Org. Chem., Adv. Synth. Catal. (Wiley), Chem. Commun., RSCAdv (RSC)]
4. Evaluator of research projects: ANEP, ANR (France), ACS Research Petroleum Fund (USA), Panel Member the Basic Chemistry Program of the State Plan for R+D+i (2017).
5. Memberships of scientific societies: RSEQ, SEQT, ACS