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Obtained her B. Sc. Degree in Chemistry, and her Ph.D. Degree (1993) at the UPV/EHU on the synthesis of isoquinoline alkaloids under the supervision of Prof. Lete and Domínguez. After post-doctoral research at the University of Waterloo (Canada) with Prof. Victor Snieckus (1994-1995), on directed *ortho*-metalation and cross-coupling reactions, she returned to the Dept. of Organic Chemistry II of the UPV/EHU in Bilbao (1995), contributing to the development of new research lines within the group led by Prof. E. Lete. Then, she was promoted to Senior Lecturer (Prof. Titular) in 1998, and to Full Professor (CU) in 2010. Together with Prof. E. Lete, she is now leading the group "Organometallics 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" led by Prof. E. Lete and Prof. J. L. Vicario. 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 alkenylation of (hetero)arenes. 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 hydroarylation, allylation and aminocarbonylation 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 biologically relevant heterocyclic systems, 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 (9 national projects since 1996), and she is co-Principal Investigator of the three last projects (CTQ2016, PID-2019, PID-2022) (See section C3). She has also participated in contracts with chemical companies (MAXAM SA, Petronor), and with multidisciplinary partners (Virtualware, HiB), being PI of two of these contracts (see section C4). More recently, she has also been involved in multidisciplinary projects with companies and technology centers financed by the ELKARTEK program of the Department of Industry of the Basque Government. These are oriented projects mainly in the area of drug discovery, and more recently for the development of novel electrolytes for lithium batteries. Some of the topics include neuropsychiatric diseases, calmodulinopathies, or development of MOF drug release systems for gastrointestinal cancer. These projects have involved the collaboration with different partners from UPV/EHU, Instituto Biofisika CSIC-UPV/EHU, BCmaterials, Instituto Biodonostia, Instituto Biocruces, TECNALIA, Donostia International Physics Center (DIPC), GAIKER, TEKNIKER or EnergiGUNE (see section C4).

As a result, she has authored over 100 publications in indexed journals, book chapters and reviews, and >95 communications to conferences. Training of researchers has also been a constant. She has supervised 19 PhD thesis (5 International Mention, 2 Extraordinary Doctoral

awards). The doctors formed under her supervision achieved positions at Universities or Research Institutes in Spain [CIDETEC, UPV/EHU, ISCH (U. Zaragoza, CSIC)], or outside (Salahaddin Univ., Iraq), or have achieved scientific positions at Pharma/Chemistry Industry [Syncom BV, (Groningen, NL), TH Company, Lucart, (Bizkaia), Pharmamar, (Madrid), Praxis Pharmaceutical, I+Med (Álava), TEVA PHARMA, (Zaragoza)], while others went to secondary education and technical works. She has also supervised >60 Master/BSc students.

She has taken part in evaluation panels for research activities in a national level [ANECA panel for the evaluation of Research (Sexenios) 2022, 2023; AEI, evaluation of Ramon y Cajal program, 2024] and also internationally [External reviewer for ANR (France, 2012) and FWO (Belgium, 2017)]. She also regularly acts as reviewer for scientific journals (ACS, RSC, Wiley, Thieme, Elsevier).

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

### Publication List (December 2025)

104. Baltasar-Marchueta, M.; López, N.; Alicante, S.; Barbolla, I.; Garcia Ibarluzea, M.; Ramis, R.; Salomón, A. M.; Muguruza-Montero, A.; Nuñez Viadero, E.; Leonardo, A.; Arrasate, S.; Sotomayor, N.; Montemore, M. M.; Villarroel, A.; Bergara, A.; Lete, E.; González-Díaz, H. Machine Learning Approach for Predicting Drug-Like Molecules Targeting Calmodulin Pathway Proteins, *J. Chem. Inf. Model.* **2025**, *61*, 11892.

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Theoretical Enantioselectivity Optimization. Online Tool for Selection and Design of Chiral Catalysts and Products. *J. Cheminformatics*, **2024**, 16, 9.

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