

Part A. PERSONAL INFORMATION

Enrique Gómez Bengoa
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Researcher ID: F-8371-2015
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A.1. Current position

Name of the University: University of the Basque Country (UPV-EHU)
Department: Organic Chemistry I
Address: Manuel de Lardizabal 3, 20018 San Sebastián, Spain
Office Phone: (+34) 943015305
e-mail: enrige.gomez@ehu.eus
Current Position: Profesor Agregado (October 17, 2008)
UNESCO Code: 2306
Key words: Computational Chemistry, Organocatalysis, Organometallics

A.2. Education

PhD: Universidad Autónoma de Madrid 1994

A.3. JCR articles, h Index, thesis supervised (04.02.2022)

- 112 peer-reviewed contributions in major international journals
- 90 articles in journals of the first quartile
- 3350 times cited (excluding self citations)
- Average citation per item: 33.2
- H-index = 35 (Web of Science).
- 4 Sexenios (Last one recognized in 2019)
- 6 PhD Thesis, 2 Master Thesis, 16 Bachelor Theses directed
- 13 Undergraduate Students supervised during Internships at Sanofi-Aventis Frankfurt (4) and Bayer CropScience GmbH Deutschland (9).

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

Enrique Gomez Bengoa (Vitoria-Gasteiz, 1966), graduated at the Autonomous University of Madrid in 1989. He obtained his PhD in Chemistry in 1994 at the same University under the direction of Prof. Antonio M. Echavarren. Later, he conducted two post-doctoral stays, the first one (1995) at the University of Gottingen (Germany) under the supervision of Prof. Ullrich Groth and the second (years 1996 and 1997) in the Department Chemistry at Boston College (Massachusetts) under the supervision of Prof. Amir Hoveyda. During these formative years, he worked in the field of organometallic chemistry and its application to organic synthesis. In 1998 he joined the Department of Organic Chemistry I at the University of the Basque Country (UPV-EHU) and since 2008 occupies a place of Associate Professor (Profesor Agregado). In mid-2005, he entered the field of Theoretical and Computational Chemistry, and he is dedicated since then to the elucidation of mechanisms of both organometallic and organocatalytic reactions by computer calculations, in collaboration with various European groups of experimental chemistry. Specifically, the group currently maintains about 25 active collaborations, from which about 70 experimental / theoretical publications have appeared in the last ten years.

He has participated in two European H2020 ITN Networks: ECHONET (2013-2016) and CATMEC (2017-2020).

In 2017, he was Invited Professor in the University of Zürich for two months.

Part C. RELEVANT MERITS

C.1. Publications

Selected publications for the period 2016-2022 (22 shown, out of total of 60 in the period)

- "Conformational Flexibility as a Tool for Enabling Site Selective Fuctionalization of Unactivated sp^3 C-O Bonds in Cyclic Acetals" Romano, Ciro; Talavera, Laura; Gómez-Bengoa, Enrique; Martín, Rubén. *J. Am. Chem. Soc.* **2022**, *144*, 11558-11563.
- "Synthesis of Cyclometalated Gold(III) Complexes via Catalytic Rhodium to Gold(III) Transmetalation" Martín, Jaime; Gómez-Bengoa, Enrique; Genoux, Alexandre; Nevado, Cristina. *Angew. Chem. Int. Ed.* **2022**, e202116755
- "Stereoselective Alkylation of Chiral Titanium(IV) Enolates with *tert*-Butyl Peresters". Pérez-Palau, Marina; Sanosa, Nil; Romea, Pedro; Urpí, Félix; López, Rosa; Gómez-Bengoa, Enrique; Font-Bardia, Mercè. *Org. Lett.* **2021**, *23*, 8852-8856
- "Au(I)-Catalyzed Hydroalkynylation of haloalkynes" García-Fernández, Pedro D.; Iglesia-Sigüenza, Javier; Rivero-Jerez, Paula S.; Díez, Elena; Gómez-Bengoa, Enrique; Fernández, Rosario; Lassaletta, José M. *J. Am. Chem. Soc.* **2020**, *142*, 16082-16089
- "An umpolung strategy to react catalytic enols with nucleophiles" Sanz-Marco, Amparo; Martínez-Erro, Samuel; Pauze, Martin; Gómez-Bengoa, Enrique; Martín-Matute, Belén. *Nature Commun.* **2019**, *10*, 5244-5252
- "Base-Catalyzed [1,*n*]-Proton Shifts in Conjugated Polienyl Alcohols and Ethers". Molleti, N., Martínez-Erro, S.; Carretero-Cerdán, A.; Sanz-Marco, A.; Gómez-Bengoa, E.; Martín-Matute, B. *ACS Catalysis*, **2019**, *9*, 9134-9139.
- "Brønsted Base Catalyzed One-Pot Synthesis of Stereodefined Six-Member Carbocycles Featuring Transient Trienolates and a Key Intramolecular 1,6-Addition" Olaizola, O.; Iriarte, I.; Zanella, G.; Gómez-Bengoa, E.; Ganboa, I.; Oiarbide, M.; Palomo, C. *Angew. Chem. Int. Ed.* **2019**, *58*, 14250-14254
- "Oxidant Speciation and Anionic Ligand Effects in the Gold-catalyzed Oxidative Coupling of Arenes and Alkynes" Hofer, M.; de Haro, T.; Gómez-Bengoa, E.; Genoux, A.; Nevado, C. *Chem. Sci.* **2019**, *10*, 8411-8420
- "Branched Ketone Dienolates: Base-Catalyzed Generation and Regio- and Enantioselective Addition Reactions" Urruzuno, I.; Mugica, O.; Zanella, G.; Vera, S.; Gómez-Bengoa, E.; Oiarbide, M.; Palomo, C. *Chem. Eur. J.* **2019**, *25*, 9701-9709
- "Dynamic Kinetic Asymmetric Heck Reaction for the Simultaneous Generation of Central and Axial Chirality" Carmona, J. A.; Hornillos, V.; Ramírez-López, P.; Ros, A.; Iglesias-Sigüenza, J.; Gómez-Bengoa, E.; Fernández, R.; Lassaletta, J. M. *J. Am. Chem. Soc.* **2018**, *140*, 11067-11075
- "Intermediacy of Ni-Ni Species in sp^2 C-O Bond Cleavage of Aryl Esters: Relevance in Catalytic C-Si Bond Formation" Somerville, R. J.; Halle, L. V. A.; Gómez-Bengoa, E.; Burés, J.; Martín, R. *J. Am. Chem. Soc.* **2018**, *140*, 8771-8780
- "Synthetic and Mechanistic Investigation of an Oxime Ether Electrocyclization Approach to Heteroaromatic Boronic Acid Derivatives" Mora-Radó, H.; Sotorríos, L.; Ball-Jones, M. P.; Bialy, L.; Czechtizky, W.; Méndez, M.; Gómez-Bengoa, E.; Harrity, J. P. A. *Chemistry, A European Journal* **2018**, *24*, 9530-9534

- "Baldwin-type Rules for Metal Controlled Intramolecular Migratory Insertions. A Computational Study of Ni, Pd and Pt case" Fiser, B.; Cuerva, J. M.; Gómez-Bengoa, E. *Organometallics* **2018**, 37, 390-395
- "Mild Base- and Additive-free Ir-Catalyzed ortho-Iodination of Benzoic Acids: Scope and Mechanistic Investigations" Erbing, E.; Sanz-Marco, A.; Vázquez-Romero, A.; Malmberg, J.; Johansson, M. J.; Gómez-Bengoa, E.; Martín-Matute, B. *ACS Catalysis* **2018**, 8, 920-925
- "The First Gold(III)-Formate: Evidence for β -Hydride Elimination" Kumar, R.; Krieger, J.-P.; Gómez-Bengoa, E.; Fox, T.; Linden, A.; Nevado, C. *Angew. Chem. Int. Ed.* **2017**, 56, 12862-12865
- "Pd-Catalyzed Hydroamination of Alkoxyallenes with Azole Heterocycles: Examples and Mechanistic Proposal" Bernar, I.; Fiser, B.; Blanco-Ania, D.; Gómez-Bengoa, E.; Rutjes, F. *Org. Lett.* **2017**, 19, 4211-4214
- "Selective C(sp²)-H Halogenation of "Click" 4-Aryl-1,2,3-Triazoles" Goitia, A.; Gómez-Bengoa, E.; Correa, A. *Org. Lett.* **2017**, 19, 962-965.
- "Expeditionary Stereoselective Synthesis of Elaborated Ketones via Remote Csp³-H Functionalization" Shu, W.; Llorente, A.; Gómez-Bengoa, E.; Nevado, C. *Nature Commun.* **2017**, 8, 13832
- "Versatile Synthesis and Enlargement of Functionalized Distorted Heptagon-Containing Nanographenes" Marquez, I. R.; Fuentes, N.; Cruz, C. M.; Puente-Muñoz, V.; Sotorrios, L.; Marcos, M. L.; Choquesillo-Lazarte, D.; Biel, B.; Crovetto, L.; Gómez-Bengoa, E.; González, M. T.; Martín, R.; Cuerva, J. M.; Campaña, A. G. *Chem. Sci.* **2017**, 8, 1068-1074
- "Efficient Construction of Cyclopenta[b]indol-1-ones by a Tandem Gold(I)-Catalyzed Rearrangement/Nazarov Reaction and Application to the Synthesis of Bruceolline H" Scarpi, D.; Petrovic, M.; Fiser, B.; Gómez-Bengoa, E.; Occhiato, E. *Org. Lett.* **2016**, 18, 3922-3925
- "A Modular Class of Fluorescent Difluoroboranes: Synthesis, Structure, Optical Properties, Theoretical Calculations and Applications for Biological Imaging" Bachollet, S. P. J. T.; Volz, D.; Fiser, B.; Münch, S.; Röncke, F.; Carrillo, J.; Adams, H.; Schepers, U.; Gómez-Bengoa, E.; Bräse, S.; Harrity, J. P. A. *Chem. Eur. J.* **2016**, 22, 12430-12438
- "A Dynamic Kinetic C-P Cross-Coupling for the Asymmetric Synthesis of Axially Chiral P,N Ligands" Ramírez-López, P.; Ros, A.; Estepa, B.; Fernández, R.; Fiser, B.; Gómez-Bengoa, E.; Lassaletta, J. M. *ACS Catalysis* **2016**, 6, 3955-3964

C.2. IP in Research projects and grants (since 2016)

1. **AiRPaDD, Industrial Doctorate Network**, in collaboration with the companies AstraZeneca (Göteborg) and Sanofi-Aventis (Frankfurt) and one academic partner, Prof. Harrity (Univ. Sheffield).
From 2023-2027.

Coordinator of the Network: Enrique Gómez Bengoa
European Commission
245.000 € (UPV-EHU)

2. *“Estudios Computacionales y Experimentales sobre Activación C-H Catalizada por paladio” Sinergia Experimental y Teórica para el desarrollo de nuevos métodos sintéticos*”

From 01-01-2020 to 31-5-2024

Principal Researcher UPV-EHU: Enrique Gómez-Bengoa

MINECO PID2019-110008GB-I00

54.500 €

3. *“Movilidad de Investigadores. Suiza”*

UPV/EHU: MOV16/29

From 07-01-2017 to 6-03-2017

Invited Professor University of Zürich: Enrique Gómez-Bengoa

2.300,00 €

4. *“Catalytic Methods for Sustainable Synthesis. A Merged Experimental and Computational Approach (CATMEC)”*

European comisión: H2020-MSCA-ITN14/06. 721223

From 01-01-2017 to 31-12-2020

Principal Researcher UPV-EHU: Enrique Gómez-Bengoa

Coordinator: J. Harrity (University of Sheffield)

495.745,92 € (UPV/EHU)

5. *“Sinergia Experimental y Teórica para el desarrollo de nuevos métodos sintéticos”*

MINECO G16-P38

From 01-01-2017 to 31-12-2019

Principal Researcher UPV-EHU: Enrique Gómez-Bengoa

CTQ2016-78083-P

32.397,75 €

6. *“Expanding Capabilities in Heterocyclic Organic Synthesis (ECHONET)”*

European commission: 7PM-People-ITN12/06. 316379

From 01-01-2013 to 31-12-2016

Principal Researcher UPV-EHU: Enrique Gómez-Bengoa

Coordinator: J. Harrity (University of Sheffield)

226.681,62 € (UPV/EHU)