

## 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

First name			
Family name			
Gender (*)		Birth date (dd/mm/yyyy)	
Social Security, Passport, ID number			
e-mail		URL Web	
Open Researcher and Contributor ID (ORCID) (*)			

(\*) Mandatory

#### A.1. Current position

Position	Full Professor		
Initial date	10/12/2020		
Institution	Universitat Rovira i Virgili (URV)		
Department/Center	Química Física e Inorgánica	Facultad de Química	
Country	Spain	Teleph. number	977558780
Key words	Organometallics, asymmetric catalysis, ligand design, combinatorial chemistry, biocatalysis, continuous flow		

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

Period	Position/Institution/Country/Interruption cause
Jan. 2007 – Dec. 2020	Associate Professor/URV/Spain
Feb. 2003 – Dec. 2006	Ramón y Cajal fellow/URV/Spain
Feb. 2002 – Dec. 2002	Researcher/Stockholm University/Sweden
Feb. 2000 – Jan. 2002	Postdoctoral fellow/Stockholm University/Sweden

#### A.3. Education

PhD, Licensed, Graduate	University/Country	Year
Doctor in Chemistry	Universitat Rovira i Virgili/Spain	1999

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

I graduated in Chemistry at the Universitat Rovira i Virgili (URV, 1995). I completed the doctoral thesis at URV under the direction of Drs. A. Ruiz and G. Net in 1999. After a post-doctoral stay of ca 3 years at Stockholm University, under the supervision of Prof. J.E. Bäckvall in the development of new protocols of combining enzymes and metal catalysts for the preparation of chiral synthons, I returned at the URV under the Program Ramon y Cajal in 2003. I became associate professor at the area of Inorganic Chemistry in 2007 and promoted to full professor in 2020.

My research activity has been mainly focused on the design and application of new highly efficient molecular, bio-hybrid and nano-catalysts for the synthesis of products with high added value and for water oxidation. The main innovations include: a) **Discovery of molecular and nano-catalysts, using a combinatorial approach** for asymmetric C-X bond forming reactions and for water oxidation. The combinatorial approach allows the synthesis and screening of a large number of catalysts at once, with less cost and generating less by-products than traditional research. This approach allowed the discovery of highly adaptative ligands, from readily available feedstocks, with the improved ability to surpass the state-of-the-

art in several challenging enantioselective reactions (e.g. asymmetric hydrogenation of minimally functionalized olefins and cyclic  $\beta$ -enamides, asymmetric allylic substitution reactions, hydroboration of 1,1-disubstituted olefins, ...); b) **Synthesis of new metal-enzyme hybrid catalysts** with a covalent interaction for catalysis. The combination of metal catalysts with the excellent recognition properties of enzymes aids to tackle unsolved synthetic problems. Special attention was paid to develop new bioconjugation strategies for anchoring the metal complex in the desired enzyme residue. The combination of metal catalysts with the excellent recognition properties of enzymes aids to tackle unsolved synthetic problems; c) Use of experimental **mechanistic studies and DFT calculations to guide ligand design**. Research in this area has moved over the years from just explaining the catalytic results to the use of DFT to *in-silico* optimize the catalyst design as well as to develop Q2MM predictive models; d) **Development of new tandem reactions** to efficiently produce more complex chiral molecules; and e) **Use of alternative green solvents** (e.g. propylene carbonate, ionic liquids,  $\text{scCO}_2$  ...) and **the development of recycling protocols** to improve the chemical sustainability of the catalytic processes.

My research activity has been collected in 151 scientific papers in indexed journals (being ca 76% in Q1 and 38% in D1) and 20 book chapters. Among them, I would like to highlight 6 Chemical Reviews. I also co-edited two books, one on artificial metalloenzymes in catalysis and the other on metal-catalysis. On January 29, 2023, my citation report in the WOS indicates 7936 citations (52.21 average per item) and a *h* index of 46. I have also presented numerous communications (more than 100 poster presentations, ca 25 oral communications and 5 invited lectures) in national and international conferences (e.g. Bienal RSEQ, GEQO, ISHC, OMCOS, ACS ...) and I have given several invited lectures in universities.

During my independent career I have participated in more than 20 research projects (including two European projects; COST D40 and CM1205). I should highlight that I have been co-PI of the last two national projects of the research group (CTQ2016 and PID2019).

Since 2000, I co-supervised 11 PhD theses (all with European/International mention, 4 of them with the URV's PhD Prize), a similar number of Master students and several undergraduated students. I am currently co-directing 3 PhD students and a Juan de la Cierva fellow.

In 2009, I participated in the evaluation of scientific projects for the "Unity Through Knowledge Fund" of the Republic of Croatia and during the last years I have been evaluator for the ANEP and AGAUR agencies.

Concerning the technical and socioeconomic impact of my work, the expertise and know-how generated in the field of asymmetric catalysis has been the basis for the establishment of a solid cooperation with more than 20 (inter)national research groups (e.g. P.G. Andersson (Stockholm U.), M. Albrecht (Bern U.), S. Woodward (Nottingham U.) ...) and with important chemical/pharmaceutical companies (e.g. Johnson Matthey, Astra Zeneca, Bayer ...).

I received the following awards and honors: (1) recognition of outstanding research career in the I3 program (2005), (2) distinction for promoting research activities in the URV (PGIR award with funding from URV, MEDU and DIUE, 2008), (3) ICREA Academia prize (2010), and (4) recognition of quality research URV (2011).

Finally, I would like to highlight that I have hold numerous administrative positions within the URV, among them I want to highlight being Head of the Department of Physical and Inorganic Chemistry (2017-today).

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

### **C.1. Publications** (*last ten years*)

1. J. J. Verendel, O. Pàmies, M. Diéguez,\* P. G. Andersson\* "Asymmetric Hydrogenation of Olefins using Chiral Crabtree-type Catalysts – Scope and Limitations" *Chem. Rev.* **2014**, *114*, 2130–2169. Highly Cited Paper.

2. R. Bellini, M. Magre, M. Biosca, P.-O. Norrby,\* O. Pàmies,\* M. Diéguez,\* C. Moberg\* "Conformational Preferences of a Tropos Biphenyl Phosphinooxazoline - A Ligand with Wide Substrate Scope" *ACS Catal.* **2016**, 6, 1701–1712.
3. M. Magre, O. Pàmies, M. Diéguez,\* "PHOX-Based Phosphite-Oxazoline Ligands for the Enantioselective Ir-Catalyzed Hydrogenation of Cyclic  $\beta$ -Enamides" *ACS Catal.* **2016**, 6, 5186–5190.
4. M. Biosca, J. Margalef, X. Caldentey, M. Besora, C. Rodríguez-Esrich, J. Saltó, X. C. Cambeiro, F. Maseras,\* O. Pàmies,\* M. Diéguez,\* M. A. Pericàs\* "Computationally Guided Design of a Readily Assembled Phosphite-Thioether Ligand for a Broad Range of Pd-Catalyzed Asymmetric Allylic Substitutions" *ACS Catal.* **2018**, 8, 3587–3601.
5. M. Biosca, M. Magre, O. Pàmies,\* M. Diéguez\* "Asymmetric Hydrogenation of Disubstituted, Trisubstituted, and Tetrasubstituted Minimally Functionalized Olefins and Cyclic  $\beta$ -Enamides with Easily Accessible Ir-P,Oxazoline Catalysts" *ACS Catal.* **2018**, 8, 10316–10320.
6. M. Biosca, J. Saltó, M. Magre, P.-O. Norrby,\* O. Pàmies, M. Diéguez\* "An Improved Class of Phosphite-Oxazoline Ligands for Pd-Catalyzed Allylic Substitution Reactions" *ACS Catal.* **2019**, 9, 6033–6048.
7. J. Margalef,\* M. Biosca, P. de la Cruz Sánchez, J. Faiges, O. Pàmies, M. Diéguez\* "Evolution in heterodonor P-N, P-S and P-O chiral ligands for preparing efficient catalysts for asymmetric catalysis. From design to applications" *Coord. Chem. Rev.* **2021**, 446, 214120.
8. M. Diéguez, O. Pàmies, C. Moberg\* "Self-Adaptable Tropos Catalysts" *Acc. Chem. Res.* **2021**, 54, 3252–3263.
9. J. Wahlers, J. Margalef, E. Hansen, A. Bayesteh, P. Helquist, M. Diéguez, O. Pàmies, O. Weist,\* P.-O. Norrby\* "Proofreading experimentally assigned stereochemistry through Q2MM predictions in Pd-catalyzed allylic aminations" *Nature Commun.* **2021**, 12, 6719.
10. O. Pàmies, J. Margalef, S. Canellas, J. James, E. Judge, P. J. Guiry, C. Moberg, J.-E. Bäckvall, A. Pfaltz, M. A. Pericàs, M. Diéguez\* "Recent advances in enantioselective Pd-catalyzed allylic substitution - from design to applications" *Chem. Rev.* **2021**, 121, 4373–4505. Highly Cited Paper.

**C.2. Congress**, indicating the modality of their participation (invited conference, oral presentation, poster) (*last ten years*)

1. 250<sup>th</sup> American Chemical Society National Meeting; Boston (USA), August 2015. Oral communication.
2. ECIRM2018 - European Colloquium on Inorganic Reaction Mechanisms; Barcelona (Spain), July 2018. Oral communication.
3. 256<sup>th</sup> American Chemical Society National Meeting; Boston (USA), August 2018. Oral communication.
4. World Congress on Chemistry; Dubai (UAE), April 2019. Invited lecture.
5. XXXVII Reunión Bienal de la Real Sociedad Española de Química; Donostia-San Sebastián (Spain), May 2019. Oral communication.
6. IV International Conference on Catalysis and Chemical Engineering; Los Angeles (USA), February 2020. Invited lecture.
7. XXXVIII Reunión Bienal Real Sociedad Española de Química; Granada (Spain), June 2022. Oral communication.
8. XXII International Symposium on Homogeneous Catalysis; Lisboa (Portugal), July 2022. Oral communication.
9. 44<sup>th</sup> International Conference on Coordination Chemistry; Rimini (Italy), August 2022. Oral communication.



10. XL GEQO Conference - Organometallic Chemistry Group; Barcelona (Spain), September 2022. Oral communication.

**C.3. Research projects**, indicating your personal contribution. (*last ten years*)

1. Innovation in Catalysis (2021SGR00163). DURSI-AGAUR. Duration: 2022-24. PI: Montserrat Diéguez Fernández. Amount: 60.000,00 €. Type of participation: Member of the research team.

2. TAILORCAT - Tailor-made molecular catalysts and hybrid bio-catalysts for asymmetric C-X bond formation and water oxidation (PID2019-104904GB-I00). Duration: 2020-2023. Ministerio de Ciencia e Innovación. PI: Montserrat Diéguez Fernández and Oscar Pàmies Ollé. Amount: 114.950,00 €. Type of participation: Principal investigator.

3. Organometallic and homogeneous catalysis (2017SGR1472). DURSI-AGAUR. Duration: 2018-20. PI: Montserrat Diéguez Fernández. Amount: 65.896,00 € + 43.449,72 € additional from URV. Type of participation: Member of the research team.

4. OPTIMCAT- Tailor-made catalysts for chiral processes and generation of clean energy (CTQ2016-74878-P). Duration: 2016-2019. Ministerio de Economía, Industria y Competitividad. PI: Montserrat Diéguez Fernández and Oscar Pàmies Ollé. Amount: 90.750,00 € + FPI grant. Type of participation: Principal investigator.

5. Organometallic and homogeneous catalysis (2014 SGR 670). DURSI-AGAUR. Duration: 2014-2016. Principal researchers: Carmen Claver Cabrero and Montserrat Diéguez Fernández. Amount: 48.000,00 € + 30.712,33 € additional from URV. Type of participation: Member of the research team.

6. INNOVACAT-Innovative approaches to sustainable and cost-effective discovery of chiral catalysts for fine chemistry (CTQ2013-40568P). Duration: 2014-2016. Ministerio de Economía y Competitividad. Principal researcher: Montserrat Diéguez Fernández. Amount: 85.910,00 €. Type of participation: Member of the research team.

7. CARISMA-Catalytic Routines for Small Molecule Activation (CM1205). COST- European Cooperation in Science and Technology. Duration: 2013-2017. Principal researcher: Montserrat Diéguez Fernández. Amount: 540.000,00 €. Type of participation: Member of the research team.

**C.4. Contracts, technological or transfer merits**

Contract Research Agreement with Bayer AG (Germany). Contract number: T22419S. Date: 04/11/2022 – 31/01/2024. PI: M. Diéguez. 16.000 €.