# Daniel Marcos Atanes

PhD in Organic Chemistry

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## PROFILE

I am a chemist with a strong background in organometallic catalysis and ligand design, specializing in iridium-catalyzed C–H borylation driven by non-covalent interaction strategies. I recently completed my Ph.D. in Organic Chemistry at the Universidade de Santiago de Compostela under the supervision of Prof. José Luis Mascareñas, combining organic synthesis and computational tools (DFT, NCI analysis) to uncover mechanistic insights into selective C–H activation. My research includes international training at CIC bioGUNE (computational chemistry) and a Fulbright-funded stay in Prof. John F. Hartwig's lab at UC Berkeley, where I developed supramolecular ligands and explored polymer functionalization. I aim to bridge fundamental reactivity studies with applied catalysis in both academic and industrial settings.

## EDUCATION

**Ph.D. in Chemistry,** 2019 –2025
Universidade de Santiago de Compostela, Spain
Dissertation: Ligand-controlled selective C–H borylations using Iridium catalysts
**Master of Science in Organic Chemistry,** 2018 – 2019
Universidade de Santiago de Compostela, Spain
**Bachelor of Science in Chemistry,** 2014– 2018
Universidade de Santiago de Compostela, Spain

## RESEARCH EXPERIENCE

**Ph.D. Researcher,** 2019 –2025
Advisor: prof. José Luis Mascareñas— CiQUS, Universidade de Santiago de Compostela
Focused on the development of ligand-controlled Ir-catalyzed C–H borylation reactions, combining experimental methodology with mechanistic insights from computational chemistry.

- Early-stage work explored supramolecularly assisted C–H functionalization using hydrogen-bond donor motifs (urea, thiourea, squaramide).
- Discovered two new classes of selective borylation: *ortho*-borylation of aromatic amides and N-methyl borylation of aliphatic amides**,** enabled by 5-$CF_3$ modified bipyridine ligands.

- Used computational methods (DFT and NCI analysis) to rationalize reactivity and selectivity trends, bridging theory and experiment.

**Master student researcher,** 2018 –2019
Advisor: prof. José Luis Mascareñas & prof. Moisés Gulías Costa— CiQUS, Universidade de Santiago de Compostela
Focused on Rh(III)-catalyzed C–H activation strategies for the synthesis of benzoxepines and coumarins, as well as preliminary work on supramolecular control in polyaromatic functionalization.
- Developed a scalable (up to 33 mmol) method for synthesizing benzoxepines and coumarins from 2-alkenylphenols using low catalyst loadings (≤0.75 mol%).
- Applied the methodology in the total synthesis of natural products (Osthole) and bioactive targets (CYP19 inhibitor).
- Initiated proof-of-concept studies on remote C–H activation of polyaromatic systems using supramolecular interactions and Pd-catalyzed CMD models.
- Synthesized tailored ligands and substrates to probe weakly guided selectivity; preliminary products detected via HRMS and NMR.

**Undergraduate researcher,** 2017 –2018
Advisor: prof. José Luis Mascareñas & prof. Moisés Gulías Costa— CiQUS, Universidade de Santiago de Compostela
Conducted exploratory research on remote C–H activation strategies in biphenyl systems using metal catalysis.
- Investigated the use of U-shaped covalent linkers to enable remote meta-selective C–H activation and cycloadditions with allenes or alkynes.
- Designed and synthesized π-stacked biphenyl substrates to probe weak interaction-guided C–H activation.
- Demonstrated preliminary proof-of-concept for π–π interaction-driven selectivity, supporting further studies in non-covalent control of reactivity.

**Undergraduate researcher,** 2017
Advisors: prof. Dolores Pérez Meirás & prof. Diego Peña Gil— CiQUS, Universidade de Santiago de Compostela
Participated in the synthesis of strained polycyclic aromatic hydrocarbons using aryne cyclotrimerization strategies.
- Synthesized a novel starphene derivative via transition-metal-catalyzed [2+2+2] cyclotrimerization of arynes.
- Characterized complex aromatic systems using NMR, mass spectrometry, and UV–Vis spectroscopy.
- Developed independent lab skills and deepened understanding of advanced organic transformations.

## RESEARCH STAYS

**CICbioGUNE, Derio, Spain**
CiQUS Mobility Grant, 2021
Supervisor: Gonzalo Jiménez Osés

During this one-month research stay, I applied DFT and non-covalent interaction analysis to study the mechanism of ortho-selective iridium-catalyzed borylation of aromatic amides.

**University of California, Berkeley, USA**
Fullbright Visiting Researcher, 2022 – 2023
Supervisor: prof. John F. Hartwig, Henry Rapoport Chair in Organic Chemistry

As a Fulbright Fellow in the Hartwig group, I investigated supramolecular strategies for site-selective C($sp^3$)–H functionalization in aliphatic systems. I synthesized phenanthroline ligands bearing hydrogen-bonding motifs (e.g., ureas) to promote transition-state organization. In parallel, I contributed to a project on polymer upcycling, developing a copper/NHC catalytic system for the borylation of polyvinyl chloride (PVC), yielding modified materials with improved plasticizer-like properties and reduced environmental impact.

## TEACHING EXPERIENCE

**Teaching Assistant** — Universidade de Santiago de Compostela
2021–2022
Supported laboratory instruction for undergraduate courses in **Pharmaceutical Chemistry I**, **Biomolecular Organic Chemistry**, and **Fundamentals of Organic Synthesis**. Responsibilities included guiding students through experimental procedures, troubleshooting, and ensuring safety protocols.

## OUTREACH

**Member**
Sociedade Xuvenil Galega de Química (SXGQ)
Participated in organizing chemistry outreach events and workshops aimed at engaging students and the public

**Volunteer**
Bay Area Scientists in Schools (BASIS)
Volunteered in educational programs to inspire and support science learning for school students in the Bay Area

## SELECTED PUBLICATIONS

1. Marcos-Atanes, D.; Jiménez-Osés, G.; Mascareñas, J. L. "Bis-$CF_3$-bipyridine Ligands for the Iridium-Catalyzed Borylation of N-Methylamides". *ACS Catal*. **2025**, *15*, 9, 7112–7120. **DOI**: 10.1021/acscatal.5c00933.
2. Gutiérrez-González, A.; Marcos-Atanes, D.; G. Cool, L.; López, F.; Mascareñas, J. L. "Ruthenium- catalyzed intermolecular alkene-alkyne couplings in biologically relevant media". *Chem.Sci.*, **2023**, *14*, 6408-6413, **DOI**: 10.1039/D3SC01254A.
3. Marcos-Atanes, D.; Vidal, C.; Navo, C. D.; Peccati, F.; Jiménez-Osés, G.; Mascareñas, J. L. "Iridium- Catalyzed *ortho*-Selective Borylation of Aromatic Amides Enabled by 5-Trifluoromethylated Bipyridine Ligands". *Angew. Chem. Int. Ed.* **2023**, *62*, e202214510, **DOI:** 10.1002/anie.202214510.
4. Gulías, M.; Marcos-Atanes, D.; Mascareñas, J. L.; Font, M. "Practical, Large-Scale Preparation of Benzoxepines and Coumarins through Rhodium(III)-Catalyzed C–H Activation/Annulation Reactions". *Org. Process Res. Dev*. **2019**, *23*, 8, 1669–1673, **DOI**: 10.1021/acs.oprd.9b00191.
5. Marcos-Atanes, D.; Mascareñas, J. L. "Ligand effects in iridium-catalyzed borylation reactions". *Manuscript in preparation*

## TECHNICAL SKILLS

**Experimental chemistry**

Organometallic synthesis and air-sensitive techniques (Glovebox and Schlenk line)
Reaction design, optimization, and purification
Purification, analysis & structural determination techniques (HPLC, MS, NMR)

**Computational chemistry**

Mechanistic pathway modeling using DFT (Gaussian)
Use of CREST and XTB for conformer searches and NCI for non-covalent interactions

**Scientific tools**

ChemDraw, MestReNova, Scifinder
Microsoft Office Suite
Basic Python scripting for data analysis

**Communication & collaboration**

Scientific writing and publishing
Oral and poster presentations
Teamwork and interdisciplinary collaboration

## AWARDS & HONORS

- **Fulbright–Spain Predoctoral Research Fellowship,** 2022
- **FPU Predoctoral Fellowship, Spanish Ministry of Universities,** 2018
- **Accésit "Chemists for our future",** 2018

- **Collaboration Fellowship, Spanish Ministry of Education,** 2017
- **CiQUS Summer Fellowship Programme,** 2017

## PRESENTATIONS & CONFERENCES

– **Poster**

Marcos-Atanes, D.; Mascareñas, J. L.

*Selective Borylation of Aromatic and Alkyl Amides Using $CF_3$-Modified Bipyridine Ligands*.

XL Reunión Bienal de la Real Sociedad Española de Química, Bilbao, **July-2025**

– **Poster**

Marcos-Atanes, D.; Mascareñas, J. L.

*Directing C-H Borylation with CF3-Modified Bipyridine Ligands in Aromatic and Alkyl Amides*.

12th Asian-European Symposium on Metal Mediated Organic Synthesis, Bologna, **May-2025**

– **Oral Communication**

Marcos-Atanes, D.; Vidal, C.; Navo, C. D.; Peccati, F.; Jiménez-Osés, G.; Mascareñas, J. L.

*$CF_3$-Modified Bipyridine Ligands: A Gateway to Selective Borylation of Aromatic and Aliphatic Amides*.

XXIX Reunión Bienal del grupo especializado de Química Orgánica, Santa Cruz de Tenerife, **June-2024**

– **Poster**

Marcos-Atanes, D.; Vidal, C.; Navo, C. D.; Peccati, F.; Jiménez-Osés, G.; Mascareñas, J. L.

*Novel Insights into the Regioselectivity of Aromatic C-H Borylation*.

2024 #RSCPoster LinkedIn conference, Online, **March-2024**

– **Oral Communication**

Marcos-Atanes, D.; Vidal, C.; Navo, C. D.; Peccati, F.; Jiménez-Osés, G.; Mascareñas, J. L.

*Tuning Regioselectivity in Iridium-Catalyzed Aromatic Amide Borylation with $CF_3$-Modified Bipyridine Ligands*.

XIV Spanish-Italian Symposium on Organic Chemistry, Torino, **February-2024**

– **Oral Communication**

Marcos-Atanes, D.; Vidal, C.; Navo, C. D.; Peccati, F.; Jiménez-Osés, G.; Mascareñas, J. L.

*Unlocking the Potential of Ortho-Borylation with $CF_3$- substituted Bipyridine Ligands*.

3rd Japanese Spanish Symposium on Organic Synthesis, Donostia, **October-2023**

– **Poster**

Marcos-Atanes, D.; Vidal, C.; Navo, C. D.; Peccati, F.; Jiménez-Osés, G.; Mascareñas, J. L. *Exploiting Non-Covalent Interactions for Ortho-Selective Borylation of Aromatic Amides*. ACS-Fall-2023, San Francisco/Online, **August-2023**

– **Poster**

Marcos-Atanes, D.; Vidal, C.; Navo, C. D.; Peccati, F.; Jiménez-Osés, G.; Mascareñas, J. L.
*$CF_3$ Substitution in Bipyridine Ligands: A Novel Strategy for Ortho-Selective Borylation*.
23rd Tetrahedron Symposium, Gothenburg, **June-2023**

– **Oral Communication**

Marcos-Atanes, D.; Vidal, C.; Navo, C. D.; Peccati, F.; Jiménez-Osés, G.; Mascareñas, J. L.
*Enabling ortho-selective borylation of aromatic amides with $CF_3$- modified bipyridine ligands*.
XIVth International School on Organometallic Chemistry "Marcial Moreno Mañas", Alicante, **May-2023**

– **Poster**

Marcos-Atanes, D.; Vidal, C.; Mascareñas, J. L.
*Unlocking the Potential of Ortho-Borylation with $CF_3$-Bipyridine Ligands*.
2023 #RSCPoster Twitter conference, Online, **February-2023**

– **Poster**

Marcos-Atanes, D.; Vidal, C.; Mascareñas, J. L.
*Ortho-selective borylation of benzamides enabled by bipyridine ligands featuring $CF_3$ substituents*.
XXXVIII Reunión Bienal RSEQ, Granada, **June-2022**

– **Poster**

Marcos-Atanes, D.; Vidal, C.; Mascareñas, J. L.
*Ortho-selective borylation of benzamides*.
XIIIth International School on Organometallic Chemistry "Marcial Moreno Mañas", Santiago de Compostela, **June-2022**

– **Poster**

Marcos-Atanes, D.; Vidal, C.; Mascareñas, J. L.
*Ortho selective borylation of aromatic amides using 5-substituted bipyridine ligands*.
8th Latin American Symposium on Coordination and Organometallic Chemistry, Bogotá/Online, **March- 2022**

– **Poster**

Marcos-Atanes, D.; Vidal, C.; Mascareñas, J. L.
*Ortho-borylation of benzamides by Iridium catalysis*.
2022 #RSCPoster Twitter conference, Online, **March-2022**

– **Poster**

Marcos-Atanes, D.; Vidal, C.; Mascareñas, J. L.
*Iridium catalyzed ortho-borylation of benzamides using 5-substituted bipyridine ligands*.
XVII Simposio de Investigadores Jóvenes de la RSEQ, Alcalá de Henares, **November-2021**

– **Poster**

Marcos-Atanes, D.; Vidal, C.; Mascareñas, J. L.
*Orthoborylation of benzamides using tailored bipyridine ligands*.
1ª Jornada de Jóvenes Investigadores del GEQOR, Online, **June-2021**

– **Poster**

Marcos-Atanes, D.; Vidal, C.; Mascareñas, J. L.

*Orthoborylation of benzamides using tailored bipyridine ligands*.
VIII Encontro da Mocidade Investigadora, Santiago de Compostela/Online, **May-2021**

– **Poster**

Marcos-Atanes, D.; Vidal, C.; Mascareñas, J. L.
*Orthoborylation of benzamides using tailored bipyridine ligands*.
ACS Publications Symposium "The Power of Chemical Transformations", Hong-Kong/Online, **May- 2021**

## LANGUAGES

Galician (Native)
Spanish (Native)
English (C1)