

## Researcher Profile

**Conferences:** 12 oral / 4 poster presentations

**PhD research stays:** 2

**Teaching experience:** 147 h

**Courses:** 10

**Research projects:** 8

**Postdoc international awards:** 3

**Publication highlights:** 1 *Science*, 1 *Nature*, 1 *Nature Catal.*, 2 *J. Am. Chem. Soc.*, 2 *Angew. Chem. Int. Ed.*

**Major fields of expertise:** ◦ *Computational and Experimental Organic Chemistry* ◦ *Machine Learning*

**Minor fields of expertise:** ◦ *Machine Learning* ◦ *Medicinal Chemistry* ◦ *Chemical Graphic Design*

**Relevant software:** ◦ *Gaussian* ◦ *ORCA* ◦ *COSMO-RS (TURBOMOLE)* ◦ *Spartan* ◦ *PyMol* ◦ *Photoshop*

**Languages:** ◦ *Spanish (fluent)* ◦ *English (fluent)* ◦ *Catalan (fluent)*

**Computer languages:** ◦ *Python (advanced)* ◦ *R (advanced)* ◦ *Java (intermediate)*

**Articles:** 32

**Book chapters:** 1

**Patents:** 1

**Journal covers:** 5

**h-index:** 14 (*Web of Science*)

**Total citations:** 494

## Education and Work Experience

**04.2022-Present** *Juan de la Cierva Fellowship*. ISQCH (CSIC)-University of Zaragoza, Zaragoza, Spain. Host group: María Concepción Gimeno Floría's group.

**03.2018-03.2022** *Postdoctoral Fellowship*. Postdoctoral Research Associate with Dr. Robert S. Paton. Colorado State University, Fort Collins (CO), United States.

**08.2014-12.2017** *Doctoral Thesis "Synthesis of Squaramides and their Application in Organocatalysis: Computational and Experimental Studies"*. ISQCH (CSIC)-University of Zaragoza, Zaragoza, Spain. PhD Directors: Dr. Raquel P. Herrera and Dr. Eugenia Marqués López.

**09.2013-07.2014** *M.S. in Chemical Research*. University of Zaragoza, Zaragoza, Spain. Master Directors: Dr. Raquel P. Herrera and Dr. Eugenia Marqués López.

**09.2007-06.2013** *B.S. in Chemistry*. University of Alicante, Alicante, Spain.

## Relevant publications (Researcher ID: AFQ-0674-2022, ORCID: 0000-0002-0769-7168)

- Zhang, X.; Nottingham, K. G.; Patel, C.; Alegre-Requena, J. V.; Levy, J. N.; Paton, R. S.; McNally, A. Phosphorus-Mediated sp<sup>2</sup>-sp<sup>3</sup> Couplings for C-H Fluoroalkylation of Azines. *Nature* **2021**, *594*, 217-222.
- Ye, Y.; Du, L.; Zhang, X.; Newmister, S.; McCauley, M.; Alegre-Requena, J. V.; Zhang, W.; Mu, S.; Minami, A.; Fraley, A.; Adrover-Castellano, M.; Carney, N.; Shende, V.; Qi, F.; Oikawa, H.; Kato, H.; Tsukamoto, S.; Paton, R. S.; Williams, R.; Li, S.; Sherman, D. Fungal-Derived Brevianamide Assembly by a Stereoselective Semi-Pinacolase. *Nature Catal.* **2020**, *3*, 497-506.
- Hilton, M. C.; Zhang, X.; Boyle, B. T.; Alegre-Requena, J. V.; Paton, R. S.; McNally, A. Heterobiaryl Synthesis by Contractive C-C Coupling via P(V) Intermediates. *Science* **2018**, *362*, 799-804.
- Modak, A.; Alegre-Requena, J. V.; de Lescure, L.; Rynders, K. J.; Paton, R. S.; Race, N. J. Homologation of Electron-Rich Benzyl Bromide Derivatives via Diazo C-C Bond Insertion. *J. Am. Chem. Soc.* **2022**, *144*, 86-92.
- Levy, J. N.; Alegre-Requena, J. V.; Liu, R.; Paton, R. S.; McNally, A. Selective Halogenation of Pyridines Using Designed Phosphine Reagents. *J. Am. Chem. Soc.* **2020**, *142*, 11295-11305.

- Popescu, M. V.; Mekereeya, A.; Alegre-Requena, J. V.; Paton, R. S.; Smith, M. D. Visible-Light-Mediated Heterocycle Functionalization via Geometrically Interrupted [2+2] Cycloaddition. *Angew. Chem. Int. Ed.* **2020**, *59*, 23020-23024.
- Koniarczyk, J. L.; Greenwood, J. W.; Alegre-Requena, J. V.; Paton, R. S.; McNally, A. A Pyridine-Pyridine Cross-Coupling Reaction via Dearomatized Radical Intermediates. *Angew. Chem. Int. Ed.* **2019**, *58*, 14882-14886.
- Alegre-Requena, J. V.; Marqués-López, E.; Herrera, R. P. "Push-Pull  $\pi+\pi^-$ " (PP $\pi\pi$ ) Systems in Catalysis. *ACS Catal.* **2017**, *7*, 6430-6439.

#### Patents

- Alegre-Requena, J. V.; Marqués-López, E.; Herrera, R. P. One-Pot Synthesis of Squaramides. Eur. Pat. Appl. 14382260, 2014; WO2016005407 A1 (PCT), 2016.

#### Oral presentations (most relevant shown)

- Alegre-Requena, J. V.; Paton, R. S. Mechanism, Selectivity and Orbital Symmetry of CF<sub>3</sub>-Py Ligand Couplings at Pentacoordinated Phosphorous. **258<sup>th</sup> ACS National Meeting & Exposition**. San Diego, CA, United States, August 2019.
- Alegre-Requena, J. V.; Paton, R. S. Computational Mechanistic Study of a P<sub>4</sub>-Catalyzed anti-Markovnikov Alcohol Addition to Styrene Derivatives. **257<sup>th</sup> ACS National Meeting & Exposition**. Orlando, FL, United States, April 2019.
- Alegre-Requena, J. V.; Paton, R. S. Ligand Coupling at Phosphorus: Mechanism, Selectivity and Orbital Symmetry. **256<sup>th</sup> ACS National Meeting & Exposition**. Boston, MA, United States, August 2018.
- Alegre-Requena, J. V.; Marqués-López, E.; Herrera, R. P. "Push-pull"  $\pi+\pi^-$  (PP $\pi\pi$ ) Systems: A New Type of Interaction System in Catalysis. **XIV Young Researchers Symposium of the Spanish Royal Society of Chemistry-Sigma Aldrich**. Badajoz, Spain, November 2017.
- Alegre-Requena, J. V.; Marqués-López, E.; Herrera, R. P. Squaramides, Key Structures in Diverse Fields of Chemistry. **V G-9 Doctoral Conference**. Palma de Mallorca, Spain, February 2017.
- Alegre-Requena, J. V.; Marqués-López, E.; Herrera, R. P. Studying Computationally Anion- $\pi$  Interactions for the First Time in Asymmetric Catalysis: Squaramide-Catalyzed Henry Reactions. **8<sup>th</sup> European Symposium on Computing  $\pi$ -Conjugated Compounds**. Malaga, Spain, January 2017.
- Alegre-Requena, J. V.; Marqués-López, E.; Herrera, R. P. Expanding the Boundaries of Asymmetric Squaramide Organocatalysis: Henry Reactions Driven by Anion- $\pi$  Interactions. **XIII Young Researchers Symposium of the Spanish Royal Society of Chemistry-Sigma Aldrich**. Logroño, Spain, November 2016.
- Alegre-Requena, J. V.; Marqués-López, E.; Herrera, R. P. One-pot Synthesis of Unsymmetrical Squaramides and their Application in Organocatalytic Henry Reactions. **XII Young Researchers Symposium of the Spanish Royal Society of Chemistry-Sigma Aldrich**. Barcelona, Spain, November 2015.

#### Awards

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|----------------|--|
| <b>04.2019</b> | <i>Winner of the 2019 Catalysts Travel Award granted by the Catalysts journal of MDPI.</i>                                   |
| <b>04.2019</b> | <i>Winner of the 2019 Wiley Computers in Chemistry Outstanding Postdoc Award granted by the ACS COMP Division.</i>           |
| <b>04.2019</b> | <i>Winner of the 2019 Molecules Travel Award granted by the Molecules journal of MDPI.</i>                                   |
| <b>04.2019</b> | <i>Extraordinary PhD Award (ranked first among all the PhD students from Science of the University of Zaragoza).</i>         |
| <b>06.2018</b> | <i>Finalist in the X SusChem PREDOC-MESTRELAB Award granted by the Young Researchers Spanish Royal Society of Chemistry.</i> |

### PhD Research Stays

- 08.2015-10.2015** *Gelation Ability of Squaramides and Other Gelators*. University of Regensburg, Regensburg, Germany. Supervisor: Dr. David Díaz Díaz.
- 09.2014-12.2014** *Biological Properties of Different Squaramides and  $\alpha$ -Hydroxyphosphonates*. Institute of Advanced Chemistry of Catalonia, Barcelona, Spain. Supervisor: Dr. Gemma Triola Guillem.

### Teaching Experience

- 01.2019-05.2019** *Organic Molecular Structure Determination (27 h)*. Chemistry graduate program, Colorado State University, Fort Collins, CO, United States.
- 05.2017** *Chemistry and Optical Materials (32 h)*. B.S. in Optics and Optometry, 1<sup>st</sup> year, University of Zaragoza, Zaragoza, Spain.
- 02.2017-03.2017** *Chemistry Laboratory (28 h)*. B.S. in Chemistry, 2<sup>nd</sup> year, University of Zaragoza, Zaragoza, Spain.
- 03.2016-04.2016** *Introduction to Chemistry Laboratory (44 h)*. B.S. in Chemistry, 1<sup>st</sup> year, University of Zaragoza, Zaragoza, Spain.
- 03.2016** *General Chemistry (16 h)*. B.S. in Biotechnology, 1<sup>st</sup> year, University of Zaragoza, Zaragoza, Spain.

### Research Projects

- 07.2020-07.2022** *Mechanistic Studies on Organic Synthesis and Catalysis (XNAS allocation CHE200033)*. XSEDE allocation for:  
07/01/2020 – 06/30/2021: 442,542 SUs and 1,000 GB, 9,602.90 USD  
07/01/2021 – 06/30/2022: 1,033,814 SUs and 1,000 GB, 7,608.52 USD  
In total 1,476,356 SUs and 2,000 GB, 17,211.42 USD.  
Principal Investigator: Dr. Juan V. Alegre Requena.
- 12.2019-12.2020** *Photocatalyzed Spirocyclizations and Base-Promoted Anti-Markovnikov Alcohol Additions (XNAS allocation CHE190111)*. XSEDE allocation for:  
12/01/2019 – 11/30/2020: 100,000 SUs and 1,500 GB, 3,966.50 USD  
Principal Investigator: Dr. Juan V. Alegre Requena.
- 10.2018-03.2022** *Theory of New Organic Reactions (XNAS allocation CHE180056)*. XSEDE allocation for:  
10/01/2018 – 09/30/2019: 698,000 SUs and 1,000 GB, 13,521.39 USD  
04/01/2020 – 03/31/2021: 1,861,500 SUs and 1,000 GB, 35,405.09 USD  
04/01/2021 – 03/31/2022: 3,163,174 SUs and 1,000 GB, 26,054.02 USD  
In total 5,722,674 SUs and 3,000 GB, 74,980.50 USD.  
Principal Investigator: Dr. Robert S. Paton. Project manager: Dr. Juan V. Alegre Requena.
- 01.2018-12.2020** *New Challenges in Organocatalysis and Studies on Biological and Gelling Properties*. Project CTQ2017-88091-P from the Ministry of Economic Affairs and Digital Transformation of Spain (54,450.00 EUR).  
Principal Investigator: Dr. Raquel P. Herrera.
- 01.2018-12.2018** *Henry Reactions from Alcohols through in situ Oxidations*. Project JIUZ-2017-CIE-05 of the University of Zaragoza (2,000.00 EUR).  
Principal Investigator: Dr. María Eugenia Marqués López.
- 01.2017-12.2019** *Gold and Silver Chemistry*. Project E07\_17R from the Government of Aragon (41,770.00 EUR).  
Principal Investigator: Dr. M. Concepción Gimeno.
- 01.2015-12.2016** *Asymmetric Organocatalysis*. Project E104 from the Government of Aragon (3,364.00 EUR).  
Principal Investigator: Dr. Raquel P. Herrera.
- 01.2015-12.2015** *Squaramides: Study of their Synthesis and Applications*. Project JIUZ-2014-CIE-07 of the University of Zaragoza (2,100.00 EUR).  
Principal Investigator: Dr. María Eugenia Marqués López.