

Cristina Pubill Ulldemolins

Date of Birth: 27th September 1985. **Nationality:** Spanish

School of Chemistry, Biomedical Sciences Research Complex, University of St Andrews, Fife, KY169ST

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As a highly motivated **organic/computational chemist**, I am particularly interested in the synthesis/biosynthesis, synthetic modification and computational modelling of biomolecules. During an interdisciplinary PhD in organic and computational chemistry and MSc in Catalysis, I obtained solid experience in designing, modelling and understanding organocatalytic and metal-mediated catalytic transformations. As a Postdoctoral Fellow at the ITbM, Canada and Japan, I acquired further expertise in organic synthesis by working on the preparation of bio-active compounds. **Within the multidisciplinary Goss group** at St Andrews, my research focuses on developing mild-aqueous methods for new-to-nature bio-metabolite functionalization while learning about reprogramming biosynthesis. Recently, I was awarded with an EPSRC-IAA Fellowship to start to make progress on my independent research project on the modulation of bioactive peptides through an iterative experimental and computational approach.

Awards

- June 2017 Selected as a talented young scientist/participating candidate by the European Commission for the “67th Lindau Nobel Laureate Meeting, dedicated to Chemistry” and “The Baden-Württemberg Post Conference Programme for Young Scientists” in Baden-Württemberg, Germany
- July 2011 Poster Prize *XXXIII Reunión Bienal de la Real Sociedad Española de Química, Valencia, Spain*

Employment record

EPSRC-IAA 17-18 Research Fellow, School of Chemistry, University of St Andrews, Professor Rebecca J. M. Goss group

May 2018 – present

Postdoctoral Research Fellow, School of Chemistry, University of St Andrews, Professor Rebecca J. M. Goss group

May 2017 – April 2018

Marie Skłodowska-Curie Individual Fellowship (IF), School of Chemistry, University of St Andrews, Dr Rebecca J. M. Goss group

May 2015 – April 2017

Post Doctoral Research Fellow, School of Chemistry, University of St Andrews, Dr Rebecca J. M. Goss group

August 2014 – April 2015

Post Doctoral Research Fellow, Institute of Transformative Bio-Molecules (WPI-ITbM), Nagoya University, Dr Cathleen Crudden group

May 2013 - March 2014

Post Doctoral Research Fellow, Department of Physical and Inorganic Chemistry, Universitat Rovira i Virgili (URV), Prof. Elena Fernández group

January 2013 - April 2013

Education

Interdisciplinary PhD in Organic and Computational Chemistry, URV and Institut Català d'Investigació Química (ICIQ) Prof. Elena Fernández and Prof. Carles Bo groupsSeptember 2008–December 2012 (Awarded December 2012, Excellent *suma cum laude*)

- Successfully designed, developed, applied and fully understood novel organocatalytic and metal mediated catalytic methodologies in the synthesis of organoboron compounds.
- Performed research in international laboratories:
 - Queen's University, **Dr Cathleen Crudden group**, Ontario, **Canada**
May to October 2011
 - Durham University **Prof. Todd Marder group**, **United Kingdom**
July to September 2009

MSc. in Catalysis, Universitat Rovira i Virgili, Spain

2008-2009 (Awarded June 2009)

BSc. in Chemistry, Universitat Rovira i Virgili, Spain

2003-2008 (Awarded April 2008)

- **Erasmus Exchange Program**, Friedrich-Alexander University, Erlangen, **Germany**
October 2007 to July 2008

Highlighted Skills and Knowledge

- **Laboratory:** extensive experience in methodology development and optimization of new catalytic reaction conditions, especially organometallic reactions; synthetic organic/inorganic chemistry, homogeneous catalysis, multi-step organic synthesis, inert-atmosphere chemical manipulation (Schlenk line and dry box), flash and gas chromatography
- **Purification and characterization techniques:** extensive experience with up-to-date purification automated and manual chromatographic techniques and modern characterization techniques (NMR, IR, UV-Vis, MS) of new molecules/compounds
- **Synthetic biology:** competent in reprogramming biosynthesis and protein purification
- **Computational chemistry:** profound knowledge of molecular modelling especially in performing relevant DFT calculations including applications to understand and inform real systems; Proficient in mechanism determination of organic and inorganic reactions
- **Management skills:** broad project management experience, great leadership, excellent interpersonal and communication skills; self-driven, highly communicative
- **Languages:** excellent written and oral English, Spanish and Catalan, competent level of German
- International research experience: performed research in **Germany, United Kingdom, Spain, Canada and Japan**

Research Presentations**Oral communications (5)**

Selective functionalisation and diversification of halogenated compounds through mild aqueous cross-coupling methodologies: from organic molecules to natural products; Cristina Pubill-Ulldemolins, Michael J. Corr, Sunil V. Sharma, Enrico Marelli, Rebecca J. M. Goss; 253rd ACS National Meeting & Exposition – Advanced Materials, Technologies, Systems & Processes, San Francisco, USA, April 2017

Unravelling the mechanism of metal-free catalytic β -borations; Cristina Pubill-Ulldemolins, Carles Bo, Elena Fernández; Nobel Campus, *Chemistry for life*, Port Aventura, Spain, July 2012
Selected candidate for an Interview in a National newspaper La Vanguardia, June 2012

Unravelling the mechanism of unprecedented metal-free catalytic borations; Cristina Pubill-Ulldemolins, Carles Bo, Elena Fernández, ICIQ Young seminar, ICIQ, Tarragona, Spain, December 2011

Catalytic diboration of endocyclic alkenes: mechanistic insights (*flash-poster presentation*); Cristina Pubill-Ulldemolins, Carles Bo, Jose A. Mata, Elena Fernández, Euroboron V, Edinburgh, United Kingdom, September 2010

Influència dels lligands carbens N-heterocíclics en l'adició catalítica de borans a olefines cíclicues; Cristina Pubill-Ulldemolins, Carles Bo, Jose A. Mata, Elena Fernández, Sisena trobada de Joves Investigadors dels Països Catalans, València, Spain, February 2010

Posters (*most recent ones out of 10*)

Expanding the GenoChemetics toolkit with new aqueous cross coupling methodologies; Cristina Pubill-Ulldemolins, Michael J. Corr, Sunil V. Sharma, Enrico Marelli, Rebecca J. M. Goss ; ECECR2 & Industry Chemistry Forum, St Andrews, UK, September 2017

Pd mediated selective functionalisation and diversification of biologically relevant halogenated molecules through mild cross-coupling methodologies in water; Cristina Pubill-Ulldemolins, Sunil V. Sharma, Enrico Marelli, Michael J. Corr, Rebecca J. M. Goss ; 253rd ACS National Meeting & Exposition – Advanced Materials, Technologies, Systems & Processes, **San Francisco**, USA, April 2017

On the Mechanism of PR₃-Assisted Organocatalytic β -Boration reaction: Origin of the enantioinduction; Cristina Pubill-Ulldemolins, Amadeu Bonet, Henrik Gulyás, Elena Fernández, Carles Bo, 18th International Symposium in Homogeneous Catalysis, Toulouse, France, July 2012 ; Also presented in the Nobel Campus, Chemistry for life, Port Aventura, Spain, July 2012

Transition metal-free β -boration: the role of the base; Cristina Pubill-Ulldemolins, Amadeu Bonet, Carles Bo, Henrik Gulyás, Elena Fernández, IME Boron XIV conference, Niagara Falls, Canada, September 2011

Funding Awarded

2018	Martí i Franquès Fellowship - Attracting the best scientific talent to Southern Catalonia ~€30K
2018	EPSRC-IAA 2017-18, £18K
2015-2017	Marie Skłodowska-Curie Individual Fellowship (IF) ~£127K
2011	BE 2010 Fellowship: mobility grant for stays outside Catalonia, AGAUR, Spain
2008-2009	Mobility Fellowship for students of an official MSc, URV, Spain
2008-2012	ICIQ fellowship Project, ICIQ, Spain
2008-2009	Fellowship “Iniciació a la recerca”, URV, Spain
2007-2008	Erasmus Exchange Program Fellowship, European Commission

Administrative Experience/ Teaching

Supervision of students

2015 - 2018	3 4 th year undergraduate students, St Andrews University, St Andrews, Scotland, United Kingdom
2015 - 2016	2 Undergraduate summer students, St Andrews University, St Andrews, Scotland, United Kingdom
2013	2 Undergraduate summer students, Queen's University, Kingston, Ontario, Canada.

2011 – 2011 1 Master Student, Institut Català d'Investigació Química (ICIQ) and University Rovira i Virgili (URV), Tarragona, Catalonia, Spain.

Teaching experience

- 2014 – 2017 Organized, managed and taught biocatalysis and Pd mediated Catalysis lectures and conducted the annual practical training program at CRITICAT PhD student rotation at University of St Andrews (Scotland, UK)
- 2014 – 2017 Prepared workshops/handouts, taught and conducted tutorials on Organometallic chemistry/ catalysis/ bioorthogonal reactions /Nanoparticles in medicine University of St Andrews (Scotland, UK)
- 2013 Prepared workshops/handouts, taught and conducted tutorials on Organic synthesis with a special focus on total synthesis of natural Products Queens University, Kingston, Canada (funded by the ITbM)

Administrative experience

- ***External reviewer*** for the “International Doctorate” distinction of two doctoral thesis titled: "Catalytic access to (poly)borylated compounds by coupling unsaturated substrates and diboron or methylidiboron reagents" by the doctoral student Núria Miralles Prat, Universitat Rovira i Virgili, Tarragona, Spain, February **2018**
“Selective polyfunctional synthesis through organoboron compounds” by Dr Enrico La Cascia (Prof. Elena Fernández and Prof. Andrew Whiting groups), Universitat Rovira i Virgili, Tarragona, Spain, November **2016**
- Participation as a chair of the first session in the Mini Postdoctoral Symposium, University of St Andrews, UK, March **2016**
- Organising team member of the 1st Chemistry postdoc’s academic career event, University of St Andrews, UK, November **2016**
- ***External examiner*** of the doctoral thesis titled: “Theoretical and experimental understanding of the pull-push effect on the synthesis of organoboranes, sulfides and selenides- defended by Dr Xavier Sanz López; (Prof. Elena Fernández and Prof. Carles Bo groups), Universitat Rovira i Virgili, Tarragona, Spain, October **2015**

Publications

1. Developing a Bench-Scale Green Diboration Reaction toward Industrial Application; Albert Farrea, Rachel A. Briggs, **Cristina Pubill-Ulldemolins**, Amadeu Bonet, *Synthesis*, **2017**, 49(21), 4775.
I am corresponding author on this paper
2. Living GenoChemetics: Synthesis through Hyphenating Synthetic Biology and Synthetic Chemistry *in vivo*; Sunil V. Sharma, Xiaoxue Tong, **Cristina Pubill-Ulldemolins**, Christopher Cartmell, Emma J. A. Bogosyan, Emma J. Rackham, Enrico Marelli, Refaat B. Hamed, Rebecca J. M. Goss, *Nat. Commun.*, **2017**, 8(10), 229
3. Sonogashira Diversification of Unprotected Halotryptophans, Halotryptophan containing Tripeptides; and Generation of a New to Nature Bromo-natural Product and its Diversification in Water; Michael J. Corr, Sunil V. Sharma, **Cristina Pubill-Ulldemolins**, Rhea T. Bown, Pierre Poirot, Duncan R. M. Smith, Christopher Cartmell, Antoine Abou-Fayad and Rebecca J. M. Goss, *Chem. Sci.*, **2017**, 8, 2039.

4. Origins of observed reactivity and specificity in the addition of B₂Cl₄ and analogues to unsaturated compounds;
Cristina Pubill-Ulldemolins, Elena Fernández, Carles Bo, John M. Brown, *Org. Biomol. Chem.* **2015**, 13(37), 9619
5. A One-Pot Synthesis of Symmetrical and Unsymmetrical Dipeptide Ureas;
Antoine Abou Fayad, **Cristina Pubill-Ulldemolins**, Sunil V. Sharma, David Day, Rebecca J. M. Goss, *Eur. J. Org. Chem.*, **2015**, 5603
6. Metal-free borylative ring-opening of vinyl epoxides and aziridines;
Xavier Sanz, Graham M. Lee, **Cristina Pubill-Ulldemolins**, Amadeu Bonet, Henrik Gulyás, Stephen A. Westcott, Carles Bo, Elena Fernández, *Org. Biomol. Chem.*, **2013**, 11(40), 7004
I am corresponding author on this paper
7. Rhodium-NHC complexes mediate diboration versus dehydrogenative borylation of cyclic olefins: a theoretical explanation;
Cristina Pubill-Ulldemolins, Macarena Poyatos, Carles Bo, Elena Fernández, *Dalton Trans.*, **2013**, 42, 746
8. Essential role of phosphines in organocatalytic β -boration reaction;
Cristina Pubill-Ulldemolins, Amadeu Bonet, Carles Bo, Henrik Gulyás, Elena Fernández, *Org. Biomol. Chem.*, **2012**, 10, 9677
9. Nucleophilic boron strikes back;
Henrik Gulyás, Amadeu Bonet, **Cristina Pubill-Ulldemolins**, Cristina Solé, Jessica Cid, and Elena Fernández, *Pure Appl. Chem.*, **2012**, 84, 11, 2219
10. Activation of Diboron Reagents with Brønsted Bases and Alcohols: An Experimental and Theoretical Perspective of the Organocatalytic Boron Conjugate Addition Reaction;
Cristina Pubill-Ulldemolins, Amadeu Bonet, Carles Bo, Henrik Gulyás, Elena Fernández, *Chem. Eur. J.*, **2012**, 18, 1121
11. L'edat del Bor: reacció de β -boració catalítica; Boron age: catalytic β -boration;
Amadeu Bonet, Manuel Soriano, **Cristina Pubill-Ulldemolins**, Cristina Solé, Jessica Cid, Elena Fernández, *Revista de la Societat Catalana de Química*, **2011**, 10, 15
12. Transition-Metal-Free Diboration Reaction by Activation of Diborons with Simple Lewis Bases;
Amadeu Bonet, **Cristina Pubill-Ulldemolins**, Carles Bo, Henrik Gulyás, Elena Fernández, *Angew. Chem. Int. Ed.*, **2011**, 50, 7158 (VIP)
13. A new context for palladium mediated B-addition reaction: an open door to consecutive functionalization;
Cristina Pubill-Ulldemolins, Amadeu Bonet, Carles Bo, Henrik Gulyás, Elena Fernandez, *Org. Biomol. Chem.*, **2010**, 8(12), 2667
14. Perceptible Influence of Pd and Pt Heterocyclic Carbene-Pyridyl Complexes in Catalytic Diboration of Cyclic Alkenes;
Cristina Pubill-Ulldemolins, Carles Bo, Jose A. Mata, Elena Fernandez, *Chem. Asian J.*, **2010**, 5, 261 ;
15. Bis(3,5-dimethyl-4-vinylpyrazol-1-yl)acetic Acid: A new Heteroscorpionate Building Block for Copolymers that Mimic the 2-His-1-carboxylate Facial triad;
Gazi Türkoglu, **Cristina Pubill-Ulldemolins**, Rainer Müller, Eike Hübner, Frank W. Heinemann, Marion Wolf, Nicolai Burzlaff, *Eur. J. Inorg. Chem.*, **2010**, 19, 2962