

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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I am a highly motivated **organic/computational chemist** with a particular interest in the synthesis and biosynthesis of natural products. With an interdisciplinary PhD in organic and computational chemistry and a MSc in Catalysis, I have valuable experience in designing, modelling and understanding organocatalytic and metal mediated catalytic transformations. In addition, I gained solid knowledge of organic synthesis through working on the synthesis of compounds with biological activity while holding a postdoctoral position at the Institute of Transformative Bio-Molecules (ITbM, Japan). **Within the multidisciplinary Goss group**, my current research focuses on the development of mild and aqueous methodologies in the context of new natural product analogue generation.

Awards

July 2011 Poster Prize *XXXIII Reunión Bienal de la Real Sociedad Española de Química, Valencia, Spain*

Employment record

Post Doctoral Research Fellow, School of Chemistry, University of St Andrews, Dr Rebecca Goss group
August 2014 -present

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 groups
September 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:** synthetic organic/organometallic chemistry, homogeneous catalysis, organic synthesis, inert-atmosphere chemical manipulation (Schlenk line and dry box), flash and gas chromatography
- **Chemical characterization:** NMR, MS, UV, IR, XPS
- **Computational Chemistry:** profound knowledge of molecular modeling including applications to real systems (eg. solvent effects), DFT methods, software (ADF, Gaussian, Schrödinger)
- **Knowledge in IT skills:** such as MS Office, ChemOffice, Mestrenova and Scifinder

Research Presentations

Oral communications

Congres: Nobel Campus, *Chemistry for life* **Place:** Port Aventura, Spain **Year:** 2012

Authors: Cristina Pubill-Ulldemolins, Carles Bo, Elena Fernández **Title:** Unravelling the mechanism of metal-free catalytic β -borations

Selected candidate for an Interview in a National newspaper *La Vanguardia*, June 2012

Congres: ICIQ Young seminar **Place:** ICIQ, Tarragona, Spain **Year:** 2011

Authors: Cristina Pubill-Ulldemolins, Carles Bo, Elena Fernández **Title:** Unravelling the mechanism of unprecedented metal-free catalytic borations

Congres: Euroboron V **Place:** Edinburgh, United Kingdom **Year:** 2010

Authors: Cristina Pubill-Ulldemolins, Carles Bo, Jose A. Mata, Elena Fernández **Title:** Catalytic diboration of endocyclic alkenes: mechanistic insights (*Flash-poster presentation*)

Congres: Sisena trobada de Joves Investigadors dels Països Catalans **Place:** Valencia, Spain **Year:** 2010

Authors: **Title:** Influència dels lligands carbens N-heterocíclics en l'adició catalítica de borans a olefines cícliques

Posters

Congres: 18th International Symposium in Homogeneous Catalysis **Place:** Toulouse, France **Year:** 2012

Authors: Cristina Pubill-Ulldemolins, Amadeu Bonet, Henrik Gulyás, Elena Fernández, Carles Bo **Title:** On the Mechanism of PR_3 -Assisted Organocatalytic β -Borationreaction: Origin of the enantioinduction

Congres: IME Boron XIV conference **Place:** Niagara Falls, Canada **Year:** 2011

Authors: Cristina Pubill-Ulldemolins, Amadeu Bonet, Carles Bo, Henrik Gulyás, Elena Fernández **Title:** Transition metal-free β -boration: the role of the base

Congres: 2nd China-Spain Bilateral Symposium on Catalysis **Place:** Tarragona, Spain **Year:** 2010

Authors: Cristina Pubill-Ulldemolins, J. A. Mata, Carles Bo, Elena Fernández **Title:** Metal catalyzed diboration of endocyclic alkenes: experimental and theoretical approach

Congres: 17th International Symposium on Homogeneous Catalysis **Place:** Poznan, Poland **Year:** 2010

Authors: Cristina Pubill-Ulldemolins, Carles Bo, Jose A. Mata, Elena Fernández **Title:** Catalytic diboration of endocyclic alkenes: mechanistic insights

Congres: XXVII Reunión el Grupo especializado en Química Organometálica **Place:** Huelva, Spain **Year:** 2010

Authors: Cristina Pubill-Ulldemolins, Carles Bo, Jose A. Mata, Elena Fernández **Title:** Diboración catalítica de alquenos endocíclicos: estudio mecanístico

Congres: Organometallic Chemistry directed towards Organic Synthesis (OMCOS) **Place:** Glasgow, United Kingdom **Year:** 2009

Authors: Cristina Pubill-Ulldemolins, Macarena Poyatos, Carles Bo, Elena Fernández **Title:** Catalytic Borylation of vinylic C-H bonds as a matter of regioselectivity

Funding Awarded

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

- Trained and supervised undergraduate students involving detailed research plans, experiment set-up and follow-up of their research progress (postdoctoral period)
- Trained and supervised the computational work of a first year master student (PhD period).
- Participated in the writing of papers and successful grant proposals (postdoctoral and PhD period).

Publications

1. 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
2. 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
3. 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
4. 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
5. 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
6. 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
 7. 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)
 8. 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
 9. 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 ;
 10. 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, EikeHübner, Frank W. Heinemann, Marion Wolf, Nicolai Burzlaff, *Eur. J. Inorg. Chem.*, **2010**, 19, 2962