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Place and date of birth: Santander, Spain – 26/11/1981

RESEARCH EXPERIENCE

- Jan 2015
present** **Postdoctoral Fellow Marie Curie CLARÍN-COFUND** (funded by FICYT (Spain) and the European Union (7th WP); ref. CLA-14-146). *Rational design of bioactive compounds based on Myelin (Multiple Sclerosis): Organic/peptide synthesis, molecular modeling, docking studies, structure-activity relationship and pharmacophore analysis.* Assoc. Prof. Theodore Tselios research group, Department of Chemistry, University of Patras. <http://www.chem.upatras.gr/faculty/tselios>
- Mar 2012
Dec 2014** **Postdoctoral Fellow JAE-doc2010** (funded by the Spanish Government). *Asymmetric synthesis of enantiopure compounds using sulphur-based auxiliaries.* Prof. Roberto Fernández de la Pradilla and Dr Alma Viso research group, IQOG-CSIC, Spanish National Research Council. <http://www.iqog.csic.es/iqog/es/sepco/sas>
- Jun 2010
Mar 2012** **Postdoctoral Fellow Marie Curie FP7-PEOPLE-2009-IEF** (ref. PIEF-GA-2009-253604). *Synthetic methodology development and asymmetric organocatalysis. (isothiourreas, amidines); Stereoselective synthesis of chiral building blocks.* Prof. Andrew D. Smith research group, School of Chemistry and Centre for Biomolecular Sciences, University of St Andrews (UK). <http://chemistry.st-andrews.ac.uk/staff/ads/group/index.html>
- Sep 2009
Mar 2010** **Postdoctoral Research Assistant** (funded by Cancer Research UK). *Development of inhibitors to target challenging proteins; Design, docking studies, synthesis and structure-activity relationship.* Prof. Steve G. Davies and Dr Angela Russell research group, Chemistry Research Laboratory, University of Oxford (UK). <http://research.chem.ox.ac.uk/angela-russell.aspx>
- May 2009
Jul 2009** **Visiting researcher** in Prof. Steve G. Davies Group. Chemistry Research Laboratory, University of Oxford (UK).
- Sep 2004
May 2009** **PhD in Organic Chemistry (Cum Laude); Scope and synthetic applications of samarium and lithium organometallics.** Prof. José M. Concellón Gracia and Prof. Humberto Rodríguez-Solla research group. Organic and Inorganic Chemistry Department. University of Oviedo (Spain). <http://grupos.uniovi.es/web/gso/presentacion>
- Jul 2008
Sep 2008** **Visiting researcher** in Prof. Georgos Kokotos Group. Organic Chemistry Department, University of Athens (Greece).
- Jul 2007
Sep 2007** **Visiting researcher** in Prof. Andrew D. Smith Group. School of Chemistry and Centre for Biomolecular Sciences, University of St Andrews (UK).

- Jul 2006** **Visiting researcher** in Prof. Varinder K. Aggarwal Group. Organic Chemistry Department,
Sep 2006 University of Bristol (UK).
- Sep 2006** **Master Degree in Organometallic Chemistry (outstanding qualification)**. Organic and
Inorganic Chemistry Department, University of Oviedo (Spain).
- Sep 2004** **Bachelor in Chemistry**, University of Oviedo (Spain).

GRANTS AND AWARDS

- 2014** **Postdoctoral Fellowship Marie Curie CLARÍN-COFUND 2014-2016** (Outgoing Grant, ref. ACA14-24) awarded by FICYT (Fundación para el Fomento en Asturias de la Investigación Científica Aplicada y la Tecnología, Spain).
- 2012** **Postdoctoral Fellowship JAE-doc2010** (ref. JAEDOC100) awarded by the Spanish Government.
- 2010** **Annual prize for outstanding PhD thesis** awarded by the University of Oviedo (Spain).
- 2010** **Postdoctoral Marie Curie Intra-European Fellowship FP7-PEOPLE-2009-IEF** (ref. PIEF-GA-2009-253604) awarded by the European Commission.
- 2005** **Predoctoral Fellowship FPI** (ref. BES-2005-9084) awarded by the Spanish Government.
- 2004** **Graduate Internship Scholarship** awarded by the University of Oviedo (Spain) for a 3-month internship in ASTURPHARMA S.A. (Asturias, Spain); Pharmaceutical company authorized by the U.S. Food and Drugs Administration. Work experience in the Analytical Quality Control Laboratory.

PUBLICATIONS

1. "Sulfinyl-Mediated Stereoselective Overman Rearrangements and Diels-Alder Cycloadditions" Ignacio Colomer, Chirag Gheewala, Carmen Simal, Marina Velado, Roberto Fernández de la Pradilla and Alma Viso *J. Org. Chem.* **2016**, *00*, manuscript accepted.
2. "Cyclic peptides on a merry-go-round; towards drug design" Anthi Tapeinou, Minos-Timotheos Matsoukas, Carmen Simal and Theodore Tselios *Biopolymers* **2015**, *104* (5), 453-461.
3. "Synthesis of Enantiopure 3-Hydroxypiperidines from Sulfinyl Dienyl Amines by Diastereoselective Intramolecular Cyclization and [2,3]-Sigmatropic Rearrangement" Carmen Simal, Robert H. Bates, Mercedes Ureña, Irene Gimenez, Christina Koutsou, Lourdes Infantes, Roberto Fernández de la Pradilla and Alma Viso *J. Org. Chem.* **2015**, *80*, 7674-7692.
4. "Exploring the scope of the isothiourethane-mediated synthesis of dihydropyridinones" Pei-Pei Yeh, David S. B. Daniels, Charlene Fallan, Eoin Gould, Carmen Simal, James E. Taylor, Alexandra M. Z. Slawin and Andrew D. Smith *Org. Biomol. Chem.* **2015**, *13*, 2177-2191.
5. "Organocatalytic Michael addition–lactonisation of carboxylic acids using α,β -unsaturated trichloromethyl ketones as α,β -unsaturated ester equivalents" Louis C. Morrill, Daniel G. Stark, James E. Taylor, Siobhan R. Smith, James A. Squires, Agathe C. A. D'Hollander, Carmen Simal, Peter Shapland, Timothy J. C. O'Riordan and Andrew D. Smith *Org. Biomol. Chem.* **2014**, *12*, 9016-9027.

6. "Remote Stereocontrol in the Synthesis of Acyclic 1,4-Diols and 1,4-Aminoalcohols from 2-Sulfinyl Dienes" Roberto Fernández de la Pradilla, Marina Velado, Ignacio Colomer, Carmen Simal, Alma Viso, Heinz Gornitzka and Catherine Hemmert *Org. Lett.* **2014**, *16*, 5200-5203.
7. "Sulfoxide-Directed Enantioselective Synthesis of Functionalized Tetrahydropyridines" Roberto Fernández de la Pradilla, Carmen Simal, Robert H. Bates, Alma Viso and Lourdes Infantes *Org. Lett.* **2013**, *15*, 4936-4939.
8. "Anhydrides as α,β -Unsaturated Acyl Ammonium Precursors: Isothiourea-promoted Catalytic Asymmetric Annulation Processes" Emily R. T. Robinson, Charlene Fallan, Carmen Simal, Alexandra M. Z. Slawin and Andrew D. Smith *Chem. Sci.* **2013**, *4*, 2193-2200.
9. "Dihydropyridones: Catalytic Asymmetric Synthesis, N- to C-Sulfonyl Transfer, and Derivatizations" Carmen Simal, Tomas Lebl, Alexandra M. Z. Slawin and Andrew D. Smith *Angew. Int. Ed.* **2012**, *51*, 3653-3657 (*Synfacts* **2012**, *8*, 0558).
10. "Organocatalytic Functionalization of Carboxylic acids: Isothiourea-Catalyzed Asymmetric Intra- and Intermolecular Michael Addition-Lactonizations" Dorine Belmessieri, Louis C. Morrill, Carmen Simal, Alexandra M. Z. Slawin and Andrew D. Smith *J. Am. Chem. Soc.* **2011**, *133*, 2714-2720 (*Synfacts* **2011**, *4*, 0436).
11. "Synthesis and Synthetic Applications of Samarium Enolates of Unmasked Amides: Efficient Synthesis of 3-Aminoamides and 3-Amino-2-chloroamides" José M. Concellón, Humberto Rodríguez-Solla, Carmen Concellón, Carmen Simal and Noemí Alvarado *Synlett* **2010**, 2119-2121.
12. "Sequential Synthesis of (*E*)- α,β -Unsaturated Primary Amides with Complete Stereoselectivity" José M. Concellón, Humberto Rodríguez-Solla, Carmen Concellón, Carmen Simal and Noemí Alvarado *J. Org. Chem.* **2010**, *75*, 3451-3453.
13. "The Addition Reaction of Samarium Enolates and 2-Haloenolates Derived from Esters, and Amides to Imines. Totally Stereoselective Synthesis of Enantiopure 3,4-Diamino Esters or Amides", José M. Concellón, Humberto Rodríguez-Solla, Carmen Simal, Vicente del Amo, Santiago García-Granda and M. Rosario Díaz *Adv. Synth. Catal.* **2009**, *351*, 2991-3000.
14. "Isothiourea-Catalysed Enantioselective Carboxyl Group Transfer", Caroline Joannesse, Craig P. Johnston, Carmen Concellón, Carmen Simal, Douglas Philp and Andrew D. Smith *Angew. Chem. Int. Ed.* **2009**, *48*, 8914 - 8918 (*Synfacts* **2010**, *1*, 0109).
15. "The Use of Samarium Enolates, a Novel Alternative in the Addition Reactions to Imines. Synthesis of 3-Aminoesters, Amides and Enantiopure 3,4-Diaminoester", José M. Concellón, Humberto Rodríguez-Solla and Carmen Simal *Adv. Synth. Catal.* **2009**, *351*, 1238-1242 (*Synfacts* **2009**, *9*, 1013).
16. "Addition Reactions of Chloro- or Iodomethylithium to Imines. Synthesis of Enantiopure Aziridines and β -Chloroamines", José M. Concellón, Humberto Rodríguez-Solla, Pablo L. Bernad and Carmen Simal *J. Org. Chem.* **2009**, *74*, 2452-2459.
17. "General, Stereoselective Synthesis of (*Z*)- β,γ -Unsaturated Nitriles Promoted by Samarium Diodide", José M. Concellón, Humberto Rodríguez-Solla, Carmen Simal, David Santos and Nieves R. Paz *Org. Lett.* **2008**, *10*, 4549-4552.

18. "Addition Reactions of Iodomethylithium to Imines. A Direct and Efficient Synthesis of Aziridines and Enantiopure Amino Aziridines". José M. Concellón, Humberto Rodríguez-Solla and Carmen Simal *Org. Lett.* **2008**, *10*, 4457-4460 (*Synfacts* **2009**, *2*, 0196).
19. "Amidine catalysed O- to C-carboxyl transfer of heterocyclic carbonate derivatives", Caroline Joannesse, Carmen Simal, Carmen Concellón, Jennifer E. Thomson, Alexandra M. Z. Slawin and Andrew D. Smith *Org. Biomol. Chem.* **2008**, *6*, 2900-2907.
20. "The First Cyclopropanation Reaction of Unmasked α,β -Unsaturated Carboxylic Acids: Direct and Complete Stereospecific Synthesis of Cyclopropanecarboxylic Acids Promoted by Sm/CHI₃". José M. Concellón, Humberto Rodríguez-Solla and Carmen Simal *Org. Lett.* **2007**, *9*, 2685-2688.
21. "A Convenient Synthesis of (Z)-Allylsilanes with Good Stereoselectivity Promoted by Samarium Diodide", José M. Concellón, Humberto Rodríguez-Solla, Carmen Simal and Cecilia Gómez *Synlett* **2007**, 75-78.
22. "Photoinduced Metalation of Nonactivated C-Cl Bonds with Samarium Diodide: Synthesis of Alkenes with High (Z)-Selectivity through β -Elimination Reactions", José M. Concellón, Humberto Rodríguez-Solla, Carmen Simal and Mónica Huerta *Org. Lett.* **2005**, *7*, 5833-5835.

CONTRIBUTION TO SCIENTIFIC MEETINGS

- | | |
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| Jul 2013 | 18th European Symposium on Organic Chemistry (ESOC 2013) , Marseille, France. Poster: P2-186. "Sulfoxide-Directed Enantioselective Synthesis of Functionalized Tetrahydropyridines" |
| Sep 2011 | Marie Curie Researchers Symposium: "SCIENCE-Passion, Mission, Responsibilities" , Warsaw, Poland. Poster: Advancement of knowledge base; K-41. "Organocatalytic Synthesis of δ -Lactams using Isothioureas" |
| Aug 2011 | 242th ACS National Meeting , Denver, USA. Poster: ORGN-582. "Organocatalytic Functionalization of Carboxylic Acids using Isothioureas" |
| Jul 2011 | XXXIII Spanish Royal Society of Chemistry Meeting (RSEQ) , Valencia, Spain. Poster: CAT.P03. "Organocatalytic Functionalization of Carboxylic Acids using Isothioureas" |
| Aug 2007 | 14th IUPAC International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis OMCOS 14 , Nara, Japan. Poster: P-106. "Stereospecific Cyclopropanation of Highly Substituted α,β -Enamides or Acids Promoted by CrCl ₂ or Sm/CHI ₃ . Stereoselective Synthesis of Cyclopropyl Amides, Ketones and Acids" |
| Sep 2005 | XXX Spanish Royal Society of Chemistry Meeting (RSEQ) , Lugo, Spain. Oral Communication: GI-QO-CO19. "Síntesis de Olefinas y Cetonas α,β -insaturadas empleando Diyoduro de Samario" |
| Aug 2005 | 230th ACS National Meeting , Washington, USA. Poster: ORGN-114. "New Applications of Transition Metal-based Single Electron Reducing Agents in Organic Synthesis: Samarium Diodide-promoted β -Elimination Reactions" |

OTHER RELEVANT DETAILS

- 2015-present** Supervision of a number of undergraduate, MSc as well as PhD students within the research group of Assoc. Prof. Theodore Tselios, at the University of Patras, Greece.
- 2012-14** Supervision of a number of undergraduate and visiting students within the research group of Prof. Roberto Fernández de la Pradilla, at the IQOG-CSIC, Spain (5 students in total).
- 2010-12** Supervision of a number of undergraduate and visiting students as well as PhD students within the research group of Prof. Andrew D. Smith, at the University of St Andrews, UK (6 students in total).
- 2009** Demonstrator in the Organic Chemistry undergraduate laboratory (2nd year, 60 h), at the University of Oviedo, Spain.

Language skills **Spanish** (native), **English** (fluent, C1) and **Greek** (intermediate level, B1)

Technical skills Strong synthetic chemistry experience and purification techniques in organic chemistry. Experience in analytical methods and further structural elucidation: Nuclear Magnetic Resonance (NMR), Gas Chromatography-Mass Spectrometry (GC-MS), Infrared Spectroscopy (IR), High-Performance Liquid Chromatography (HPLC), Polarimeter.

Computing skills Microsoft Office: practical knowledge
Scientific software: ChemOffice, MestRe-Nova, Top-Spin, iNMR
Scientific database: Scifinder, Reaxys, ISI Web of Science

REFERENCES

- Prof. Roberto Fernández de la Pradilla, IQOG-CSIC (Spain): rfradilla@iqog.csic.es
- Prof. Andrew D. Smith, University of St Andrews (UK): ads10@st-andrews.ac.uk
- Prof. Humberto Rodríguez-Solla, University of Oviedo (Spain): hrosolla@uniovi.es