



UNIVERSITY OF PATRAS, GREECE
DEPARTMENT OF CHEMISTRY

Assis. Prof. Carmen Simal Fernández

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ΠΑΝΕΠΙΣΤΗΜΙΟ
 ΠΑΤΡΩΝ
 UNIVERSITY OF PATRAS

CURRENT POSITION

06/2023 - present

Assistant Professor (Organic Chemistry). Division A - Organic Chemistry, Biochemistry and Natural Products, Department of Chemistry, University of Patras, Greece.
<http://www.chem.upatras.gr/faculty/simal>

Organic & Medicinal Chemistry. Research focused on the design, synthesis, and evaluation of pharmacologically relevant compounds. Stereoselective transformations of natural-based scaffolds and the development of bioactive molecules, particularly flavonoid derivatives, organometallic hybrids, and targeted drug conjugates. Special interest in targeted drug delivery systems, including small molecule–drug conjugates (SMDCs) and peptide–drug conjugates (PDCs), aimed at improving treatments for cancer, autoimmune diseases, and antimicrobial resistance.

PREVIOUS POSITIONS

2022 - 2023

Postdoctoral Researcher (EPAnEK / T2EAK-01924)

Laboratory of Pharmacognosy and Chemistry of Natural Products (LPCNP)/Department of Pharmacy, University of Patras, Greece.

[Laboratory of Pharmacognosy and Chemistry of Natural Products](#)

Development of new, improved strawberry cultivars in terms of aroma and flavor using chemical and genetic markers.

- Analysis optimization of volatile and non-volatile compounds of a wide range of strawberry genotypes by chromatographic techniques.

2020 - 2022

Postdoctoral Researcher (EPAnEK / T1EDK-01082)

Nanotechnology and Advanced Materials Laboratory (NAML)/Electrical and Computer Engineering Department, University of Peloponnese, Greece. <http://naml.ece.uop.gr/>

Low cost carbon-electrode based perovskite solar cells. Preparation and characterization of mixed-cation and mixed-anion perovskite structures for ambient mesoscopic C-PSCs.

- Defect passivation strategies for an enhanced efficiency and long-term stability of photovoltaic devices. Additives engineering (organic small-molecules) in perovskite precursor solution and post-deposition treatments to improve film crystallinity and suppress recombination loss.

2015 - 2017

Marie Curie-CLARIN-COFUND Postdoctoral Fellow

Department of Chemistry, University of Patras, Greece.

<http://www.chem.upatras.gr/faculty/tselios>

Rational design of bioactive compounds based on myelin basic proteins (MBP) for immunotherapy of multiple sclerosis. Molecular modelling and synthesis of peptide and non-peptide mimetics. T-cell receptor binding affinity studies.

- Synthesis and characterization of small organic molecules (pyrrole-based) and altered peptides derived from immunodominant epitope MBP₈₅₋₉₉ for tailoring immune responses.

2012 - 2015	IAE-DOC Postdoctoral Fellow Institute of General Organic Chemistry-Spanish National Research Council (IQOG-CSIC), Spain. https://www.iqog.csic.es/grupo/grupo-de-sintesis-asimetrica-con-azufre-y-boro/ <i>Asymmetric synthesis of enantiopure compounds using chiral sulphur-based auxiliaries to give access to products with medical or catalysis interest.</i> • Preparation of chiral vinyl and dienyl sulfoxides directed to the highly regio-, diastereo-, and enantioselective synthesis of <i>N</i>-heterocycles and other acyclic systems.
2010 - 2012	Marie Curie Postdoctoral Fellow [Intra-European Fellowship (IEF)] School of Chemistry and Centre for Biomolecular Sciences, University of St Andrews, United Kingdom. https://ads-group.squarespace.com/ <i>Design and synthesis of chiral isothioureas/amidines as asymmetric organocatalysts and their use as state-of-the-art Lewis bases.</i> • Catalytic enantioselective synthesis of carbo- and heterocyclic compounds promoted by isothiuronium/amidinium enolates
2009 - 2010	Postdoctoral Researcher (Cancer Research UK) Chemistry Research Laboratory (CRL), University of Oxford, United Kingdom. https://russellchem.web.ox.ac.uk/ <i>Identification of molecular targets for the treatment of prostate cancer.</i> • Development and synthesis of new potential-motif inhibitors to target PIM1-kinases. SAR studies of hit-near-neighbours. • Periodic group meetings with Chemistry Advisory Panel (Docking studies - <i>InhibOx</i>) and with the funding partnership (Cancer Research UK).

EDUCATION	
2017 - 2018	MSc in Teacher Training for Compulsory Secondary Education and Baccalaureate, Vocational Training and Language Teaching. International University La Rioja (Spain); <i>"Visual thinking in carbon chemistry"</i>
2004 - 2009	PhD in Chemistry (Organic Chemistry). Organic and Inorganic Chemistry Department, Faculty of Chemistry, University of Oviedo (Spain); <i>"Synthetic Applications of Functionalized Lithium and Samarium Organometallic Derivatives: Synthesis of (Z)-Alkenes, Cyclopropanecarboxylic Acids, Aziridines and β-Aminoesters or -amides"</i> (Cum Laude and PhD Distinction Award). Institutional Repository of the University of Oviedo
2004 - 2006	MSc in Organometallic Chemistry. Organic and Inorganic Chemistry Department, Faculty of Chemistry, University of Oviedo (Spain); <i>"Stereoselective Synthesis of (Z)-Alkenes using Samarium Diiodide"</i>
1999 - 2004	BSc in Chemistry. Faculty of Chemistry, University of Oviedo (Spain)

PUBLICATIONS

- (32)** “Visible-light Photocatalysis for Sustainable Chromene Synthesis and Functionalization”, P. Pérez-Ramos, G. Biniari, R. G. Soengas, H. Rodríguez-Solla, *C. Simal** *Chem. Eur. J.* **2025**, e202500283. <https://doi.org/10.1002/chem.202500283>
- (31)** “Rational Design, Synthesis and Binding Affinity Studies of Anthraquinone Derivatives Conjugated to Gonadotropin-Releasing Hormone (GnRH) Analogues towards Selective Immunosuppression of Hormone-Dependent Cancer”, G. Biniari, C. Markatos, A. Nteli, H. Tzoupis, *C. Simal*, A. Vlamis-Gardikas, V. Karageorgos, I. Pirmettis, P. Petrou, M. Venihaki, G. Liapakis, T. Tselios *Int. J. Mol. Sci.* **2023**, 24(20), 15232. (IF₂₀₂₃ = 6.208). <https://doi.org/10.3390/ijms242015232>
- (30)** “Monitoring of Volatile Organic Compounds in Strawberry Genotypes over the Harvest Period” K. Passa, *C. Simal*, E. Tsormpatzidis, V. Papasotiropoulos, F.N. Lamari *Plants* **2023**, 12(9), 1881. (IF₂₀₂₃ = 4.658). <https://doi.org/10.3390/plants12091881>
- (29)** “Exploring the Effect of Ammonium Iodide Salts employed in Multication Perovskite Solar Cells with a Carbon electrode” M. Bidikoudi, *C. Simal*, V. Dracopoulos, E. Stathatos *Molecules* **2021**, 26, 5737. (IF₂₀₂₀ = 4.411). <https://doi.org/10.3390/molecules26195737>
- (28)** “Exploring the Effect of Lewis-Base Additives on the Performance and Stability of Mesoscopic Carbon-Electrode Perovskite Solar Cells” M. Bidikoudi, *C. Simal*, E. Stathatos *ACS Appl. Energy Mater.* **2021**, 4, 8810-8823. (IF₂₀₂₀ = 5.76). <https://doi.org/10.1021/acsaem.1c00920>
- (27)** “Low-Toxicity Perovskite Applications in Carbon Electrode Perovskite Solar Cells—A Review” M. Bidikoudi, *C. Simal*, E. Stathatos *Electronics* **2021**, 10(10), 1145. (IF₂₀₂₀ = 2.397). <https://doi.org/10.3390/electronics10101145>
- (26)** “Design, Synthesis and evaluation of an anthraquinone derivative conjugated to myelin basic protein immunodominant (MBP 85-99) epitope: Towards selective immunosuppression” A. Tapeinou, E. Giannopoulou, *C. Simal*, B.E. Hansen, H. Kalofonos, V. Apostolopoulos, A. Vlamis-Gardikas, T. Tselios *Eur. J. Med. Chem.* **2018**, 143, 621-631. (IF₂₀₁₈ = 4.816). <https://doi.org/10.1016/j.ejmech.2017.11.063>
- (25)** “Biologically relevant conformational features of linear and cyclic proteolipid protein (PLP) peptide analogues obtained by high-resolution nuclear magnetic resonance and molecular dynamics” G.G. Kordopati, H. Tzoupis, A.N. Troganis, G.M. Tsivgoulis, S.G. Grdadolnik, *C. Simal*, T. Tselios *J. Comput. Aided Mol. Des.* **2017**, 31, 841-854. (IF₂₀₁₇ = 2.356). <https://doi.org/10.1007/s10822-017-0045-2>
- (24)** “Design and Synthesis of Non-Peptide Mimetics Mapping the Immunodominant Myelin Basic Protein (MBP83-96) Epitope to Function as T-Cell Receptor Antagonists” M.P. Yannakakis, *C. Simal*, H. Tzoupis, M. Rodi, N. Dargahi, M. Prakash, A. Mouzaki, J.A. Platts, V. Apostolopoulos, T. Tselios *Int. J. Mol. Sci.* **2017**, 18(6), 1215. (IF₂₀₁₆ = 3.687). <https://doi.org/10.3390/ijms18061215>
- (23)** “Molecular dynamics at the receptor level of immunodominant myelin oligodendrocyte glycoprotein 35–55 epitope implicated in multiple sclerosis” M.P. Yannakakis, H. Tzoupis, E. Michailidou, E. Mantzourani, *C. Simal*, T. Tselios *J. Mol. Graph. Model.* **2016**, 68, 78-86. (IF₂₀₁₉ = 2.079). <https://doi.org/10.1016/j.jmgm.2016.06.005>
- (22)** “Sulfinyl-Mediated Stereoselective Overman Rearrangements and Diels-Alder Cycloadditions” I. Colomer, C. Gheewala, *C. Simal*, M. Velado, R. Fernández de la Pradilla, A. Viso *J. Org. Chem.* **2016**, 81, 4081-4097. (IF₂₀₁₆ = 4.785). <https://doi.org/10.1021/acs.joc.6b00365>
- (21)** “Cyclic peptides on a merry-go-round; towards drug design” A. Tapeinou, M.T. Matsoukas, *C. Simal*, T. Tselios *Biopolymers (Pept Sci)* **2015**, 104(5), 453-461. (IF₂₀₁₉ = 1.865). <https://doi.org/10.1002/bip.22669>

- (20)** "Synthesis of Enantiopure 3-Hydroxypiperidines from Sulfinyl Dienyl Amines by Diastereoselective Intramolecular Cyclization and [2,3]-Sigmatropic Rearrangement" C. Simal, R.H. Bates, M. Ureña, I. Giménez, C. Koutsou, L. Infantes, R. Fernández de la Pradilla, A. Viso *J. Org. Chem.* **2015**, *80*, 7674-7692. (IF₂₀₁₅ = 5.076). <https://doi.org/10.1021/acs.joc.5b01307>
- (19)** "Exploring the scope of the isothioureia-mediate synthesis of dihydropyridinones" P. Yeh, D.S.B. Daniels, C. Fallan, E. Gould, C. Simal, J.E. Taylor, A.M.Z. Slawin, A.D. Smith *Org. Biomol. Chem.* **2015**, *13*, 2177-2191 (*Synfacts* **2015**, *11*, 0250). (IF₂₀₁₅ = 3.753). <https://doi.org/10.1039/c4ob02408g>
- (18)** "Organocatalytic Michael addition–lactonisation of carboxylic acids using α,β -unsaturated trichloromethyl ketones as α,β -unsaturated ester equivalents" L.C. Morrill, D.G. Stark, J.E. Taylor, S.R. Smith, J.A. Squires, A.C.A. D'Hollander, C. Simal, P. Shapland, T.J.C. O'Riordan, A.D. Smith *Org. Biomol. Chem.* **2014**, *12*, 9016-9027 (*Synfacts* **2015**, *11*, 0315). (IF₂₀₁₄ = 3.821). <https://doi.org/10.1039/c4ob01788a>
- (17)** "Remote Stereocontrol in the Synthesis of Acyclic 1,4-Diols and 1,4-Aminoalcohols from 2-Sulfinyl Dienes" R. Fernández de la Pradilla, M. Velado, I. Colomer, C. Simal, A. Viso, H. Gornitzka, C. Hemmert *Org. Lett.* **2014**, *16*, 5200-5203. (IF₂₀₁₄ = 6.324). <https://doi.org/10.1021/ol502592y>
- (16)** "Sulfoxide-Directed Enantioselective Synthesis of Functionalized Tetrahydropyridines" R. Fernández de la Pradilla, C. Simal, R.H. Bates, A. Viso, L. Infantes *Org. Lett.* **2013**, *15*, 4936-4939. (IF₂₀₁₃ = 6.142). <https://doi.org/10.1021/ol402141d>
- (15)** "Anhydrides as α,β -Unsaturated Acyl Ammonium Precursors: Isothioureia-promoted Catalytic Asymmetric Annulation Processes" E.R.T. Robinson, C. Fallan, C. Simal, A.M.Z. Slawin, A.D. Smith *Chem. Sci.* **2013**, *4*, 2193-2200. (IF₂₀₁₃ = 7.525). <https://doi.org/10.1039/C3SC50199J>
- (14)** "Dihydropyridones: Catalytic Asymmetric Synthesis, *N*- to C-Sulfonyl Transfer, and Derivatizations" C. Simal, T. Lebl, A.M.Z. Slawin, A.D. Smith *Angew. Int. Ed.* **2012**, *51*, 3653-3657 (*Synfacts* **2012**, *8*, 0558). (IF₂₀₁₂ = 13.455). <https://doi.org/10.1002/anie.201109061>
- (13)** "Organocatalytic Functionalization of Carboxylic acids: Isothioureia-Catalyzed Asymmetric Intra- and Intermolecular Michael Addition-Lactonizations" D. Belmessieri, L.C. Morrill, C. Simal, A.M.Z. Slawin, A.D. Smith *J. Am. Chem. Soc.* **2011**, *133*, 2714-2720 (*Synfacts* **2011**, *4*, 0436). (IF₂₀₁₁ = 9.907). <https://doi.org/10.1021/ja109975c>
- (12)** "Synthesis and Synthetic Applications of Samarium Enolates of Unmasked Amides: Efficient Synthesis of 3-Aminoamides and 3-Amino-2-chloroamides" J.M. Concellón, H. Rodríguez-Solla, C. Concellón, C. Simal, Noemí Alvaredo *Synlett* **2010**, *14*, 2119-2121. (IF₂₀₁₀ = 2.447). <https://doi.org/10.1055/s-0030-1258535>
- (11)** "Sequential Synthesis of (*E*)- α,β -Unsaturated Primary Amides with Complete Stereoselectivity" J.M. Concellón, H. Rodríguez-Solla, C. Concellón, C. Simal, N. Alvaredo *J. Org. Chem.* **2010**, *75*, 3451-3453. (IF₂₀₁₀ = 4.002). <https://doi.org/10.1021/jo100320j>
- (10)** "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" J.M. Concellón, H. Rodríguez-Solla, C. Simal, V. del Amo, S. García-Granda, M.R. Díaz *Adv. Synth. Catal.* **2009**, *351*, 2991-3000. (IF₂₀₀₉ = 5.187). <https://doi.org/10.1002/adsc.200900534>
- (9)** "Isothioureia-Catalysed Enantioselective Carboxyl Group Transfer" C. Joannesse, C.P. Johnston, C. Concellón, C. Simal, D. Philp, A.D. Smith *Angew. Chem. Int. Ed.* **2009**, *48*, 8914-8918 (*Synfacts* **2010**, *1*, 0109). (IF₂₀₀₉ = 11.829). <https://doi.org/10.1002/anie.200904333>
- (8)** "The Use of Samarium Enolates, a Novel Alternative in the Addition Reactions to Imines. Synthesis of 3-Aminoesters, Amides and Enantiopure 3,4-Diaminoester" J.M. Concellón, H. Rodríguez-Solla, C. Simal *Adv. Synth. Catal.* **2009**, *351*, 1238-1242 (*Synfacts* **2009**, *9*, 1013). (IF₂₀₀₉ = 5.187). <https://doi.org/10.1002/adsc.200900189>

- (7) "Addition Reactions of Chloro- or Iodomethylithium to Imines. Synthesis of Enantiopure Aziridines and β -Chloroamines" J.M. Concellón, H. Rodríguez-Solla, P.L. Bernad, C. Simal *J. Org. Chem.* **2009**, 74, 2452-2459. (IF₂₀₀₉ = 4.219). <https://doi.org/10.1021/jo802596y>
- (6) "General, Stereoselective Synthesis of (Z)- β,γ -Unsaturated Nitriles Promoted by Samarium Diiodide" J.M. Concellón, H. Rodríguez-Solla, C. Simal, D. Santos, N.R. Paz *Org. Lett.* **2008**, 10, 4549-4552. (IF₂₀₀₈ = 5.128). <https://doi.org/10.1021/ol801752m>
- (5) "Addition Reactions of Iodomethylithium to Imines. A Direct and Efficient Synthesis of Aziridines and Enantiopure Amino Aziridines" J.M. Concellón, H. Rodríguez-Solla, C. Simal *Org. Lett.* **2008**, 10, 4457-4460 (*Synfacts* **2009**, 2, 0196). (IF₂₀₀₈ = 5.128). <https://doi.org/10.1021/ol801607r>
- (4) "Amidine catalysed O- to C-carboxyl transfer of heterocyclic carbonate derivatives" C. Joannesse, C. Simal, C. Concellón, J.E. Thomson, A.M.Z. Slawin, A.D. Smith *Org. Biomol. Chem.* **2008**, 6, 2900-2907. (IF₂₀₀₈ = 3.550). <https://doi.org/10.1039/b805850d>
- (3) "The First Cyclopropanation Reaction of Unmasked α,β -Unsaturated Carboxylic Acid: Direct and Complete Stereospecific Synthesis of Cyclopropanecarboxylic Acids Promoted by Sm/CHI₃" J.M. Concellón, H. Rodríguez-Solla, C. Simal *Org. Lett.* **2007**, 9, 2685-2688. (IF₂₀₀₇ = 4.802). <https://doi.org/10.1021/ol0709174>
- (2) "A Convenient Synthesis of (Z)-Allylsilanes with Good Stereoselectivity Promoted by Samarium Diiodide" J.M. Concellón, H. Rodríguez-Solla, C. Simal, C. Gómez *Synlett* **2007**, 1, 75-78. (IF₂₀₀₇ = 2.006). <https://doi.org/10.1055/s-2006-958436>
- (1) "Photoinduced Metalation of Nonactivated C-Cl Bonds with Samarium Diiodide: Synthesis of Alkenes with High (Z)-Selectivity through β -Elimination Reactions" J.M. Concellón, H. Rodríguez-Solla, C. Simal, M. Huerta *Org. Lett.* **2005**, 7, 5833-5835. (IF₂₀₀₅ = 4.368). <https://doi.org/10.1021/ol0523392>

CONFERENCES

23rd Panhellenic Chemistry Conference, "Rational design, synthesis and evaluation of mitoxantrone conjugated with mutated Gonadotropin Releasing Hormone (GnRH) for the treatment of hormone-dependent cancer", 25-28 September 2024, Athens (Greece).

37th European Peptide Symposium, "Rational design, synthesis and evaluation of mitoxantrone conjugated with mutated Gonadotropin Releasing Hormone (GnRH) for the treatment of hormone-dependent cancer" and "Analysis of Mannan (polymannose) Conjugated with 35-55 Immunodominant Epitope of Myelin Oligodendrocyte Glycoprotein for the Treatment of Multiple Sclerosis", 25-29 August 2024, Florence (Italy).

XXXI International Conference on Polyphenols (ICP2023), "Identification and Quantification of Major Phenolic Compounds from Different Strawberry Genotypes Using Liquid Chromatography", 3-6 July 2023, Nantes (France).

19th Hellenic Symposium on Medicinal Chemistry (HSMC-19), "Valuation of phenolic and volatile profiles from strawberry genotypes using chromatographic techniques" and "Characterization of secondary metabolites in hydroalcoholic extracts from leaves of *Salvia Pomifera* Subsp. *Calycina*", 9-11 March 2023, Patras (Greece).

36th European Peptide Symposium, "Design and synthesis of Gonadotropin Releasing Hormone (GnRH) peptide analogues conjugated with anthraquinone for selective immunosuppression", 28 August-2 September 2022, Barcelona (Spain).

70th International Congress and Annual Meeting of the Society for Medicinal Plant and Natural Product (GA) , "Optimization of Extraction Conditions and Identification of Organic Volatile Compounds from Strawberry Genotypes", 28-31 August 2022, Thessaloniki (Greece).
22nd Panhellenic Chemistry Conference , "Design and Synthesis of an Anthraquinone Analog-Conjugated Peptide", December 2016, Thessaloniki (Greece).
34th European Peptide Symposium , "Design and Synthesis of a Bioactive Peptide Conjugated with Anthraquinone: Targeting Selective Immunosuppression" and "Theoretical prediction of the binding energy of a proposed non peptide mimetic molecule with the T cell receptor (TCR), involve in multiple sclerosis", 4-9 September 2016, Leipzig (Germany).
18th European Symposium on Organic Chemistry (ESOC) , "Sulfoxide-Directed Enantioselective Synthesis of Functionalized Tetrahydropyridines", 7-12 July 2013, Marseille (France).
Marie Curie Researchers Symposium: SCIENCE–Passion, Mission, Responsibilities , "Organocatalytic Synthesis of δ -Lactams using Isothioureas", 25-27 September 2011, Warsaw (Poland).
242nd ACS National Meeting , "Organocatalytic Functionalization of Carboxylic Acids using Isothioureas", 28 August – 1 September 2011, Denver (USA).
XXXIII Spanish Royal Society of Chemistry Meeting (RSEQ) , "Organocatalytic Functionalization of Carboxylic Acids using Isothioureas", 25-28 July 2011, Valencia (Spain).
The British Association for Cancer Research (BARC) , "Small Molecule Inhibition of PIM Kinase Function", January 2010, Edinburgh (UK).
14th IUPAC International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis OMCOS 14 , "Stereospecific Cyclopropanation of Highly Substituted α,β -Enamides or Acids Promoted by CrCl_2 or $\text{Sm}/\text{CH}_3\text{I}$ and "Stereoselective Synthesis of Cyclopropyl Amides, Ketones and Acids", 2-6 August 2007, Nara (Japan).
XXX Spanish Royal Society of Chemistry Meeting (RSEQ) , "Synthesis of Olefins and α,β -unsaturated Ketones using Samarium Diiodide", 19-23 September 2007, Lugo (Spain).
230th ACS National Meeting , "New Applications of Transition Metal-based Single Electron Reducing Agents in Organic Synthesis: Samarium Diiodide-promoted β -Elimination Reactions", 28 August – 1 September 2005, Washington (USA).

REVIEWING ACTIVITIES

2022-present	<i>Reviewer</i> in the <i>European Journal of Medicinal Chemistry</i> and <i>Advanced Synthesis & Catalysis</i> (Wiley-VCH GmbH). <i>Translator</i> (Chapter 2: "Stereochemistry") for the Greek edition of "<i>Advanced Organic Chemistry</i>" by David E. Lewis (Oxford University Press). Broken Hill Publishers Ltd., 2025. Member of PhD Examination Committees. Organic and Inorganic Chemistry Department, Faculty of Chemistry, University of Oviedo (Spain). Member of PhD Examination Committees. Department of Chemistry, University of Patras (Greece).
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TEACHING ACTIVITIES	
2023 - present	Assistant Professor – <i>Undergraduate Courses</i> : “Structure and Reactivity in Organic Chemistry” (1 st year); “Spectroscopy of Organic Compounds-Experimental Organic Chemistry I” (2 nd year); “Chemistry of Heterocyclic Compounds and Biomolecules” (2 nd year); “Experimental Organic Chemistry II” (3 rd year). Department of Chemistry, University of Patras (Greece) <i>Graduate Courses</i> : “Organic Synthesis of Drugs”. MSc Program “Medicinal Chemistry and Chemical Biology”, University of Patras (Greece)
2008 - 2009	Teaching Assistant – “Experimentation in Organic Chemistry” (3 rd year, 75 hours), Faculty of Chemistry, University of Oviedo (Spain)
2007 - 2008	Teaching Assistant – “Experimentation in Organic Chemistry” (3 rd year, 75 hours), Faculty of Chemistry, University of Oviedo (Spain)
2006 - 2007	Teaching Assistant – “Experimentation in Organic Chemistry” (3 rd year, 75 hours), Faculty of Chemistry, University of Oviedo (Spain)

SUPERVISION OF GRADUATE STUDENTS & POSTDOCTORAL FELLOWS (*)	
(*) “Co-supervision from a Senior Postdoc position”	
2023 - present	2 MSc Students/ 3 Undergraduate Students Department of Chemistry, University of Patras (Greece)
2022 – 2023^(*)	1 Postdoc/ 1 PhD/ 3 MSc Students/ 4 Undergraduate Students Department of Pharmacy, University of Patras (Greece)
2015 - 2017^(*)	3 PhD/ 2 MSc Students/ 2 Undergraduate Students Department of Chemistry, University of Patras (Greece)
2012 - 2014^(*)	2 Undergraduate Students Institute of General Organic Chemistry-Spanish National Research Council (Spain)
2010 - 2012^(*)	3 PhD Students/ 2 Undergraduate Students School of Chemistry and Centre for Biomolecular Sciences, University of St Andrews (UK)

FELLOWSHIPS and AWARDS	
2015 - 2017	Marie Curie CLARÍN-COFUND Postdoctoral Fellowship awarded by FICYT (Foundation for the Promotion of Applied Scientific Research and Technology in Asturias, Spain) and co-financed by the EU (<i>Outgoing Grant</i> ; ref. ACA14-24)
2012 - 2014	JA-E-DOC Postdoctoral Fellowship awarded by the Spanish Ministry of Science and Innovation (ref. JAEDOC100)
2010 - 2012	Marie Curie Postdoctoral Intra-European Fellowship (IEF) awarded by the EU (ref. IsoCatPIEF-GA-2009-2536)
2010	PhD Distinction Award , University of Oviedo (Spain)
2005 - 2009	Predocctoral Fellowship FPI awarded by the Spanish Ministry of Education and Science (ref. BES-2005-9084)

RESEARCH GRANTS			
Project Title	Funding source	Period	Role of the PI
(1) "Development of new strawberry cultivars improved in terms of aroma and taste using chemical and genetic markers – STRAWBERRY"	EPAnEK (T2EΔK-01924)	2021-2023	Postdoctoral Researcher
(2) "Printable low-cost solar panels from Perovskites – PrintWin"	EPAnEK (T1EDK-01082)	2018-2021 (2 years)	Postdoctoral Researcher
(3) "A novel combined approach for the Immunotherapy of Multiple Sclerosis"	GSRI (ISR-3148O-P)	2014-2015	Postdoctoral Researcher
(4) "Rational design and synthesis of cyclic peptides and non-peptide mimetics as well as cyclodextrin conjugates for the immunotherapy of multiple sclerosis"	FICYT (Spain) (ACA14-24)	2014-2016	Postdoctoral Researcher
(5) "New molecular entities and catalysts-based transition metals complexes"	Spanish Ministry of Science and Innovation (CTQ2013-46459-C2-2-P)	2014-2016	Postdoctoral Researcher
(6) "Pre-clinical and Toxicology Evaluation of Immunodominant Myelin Peptides/Mimetics Conjugated with Mannan towards Clinical Phase I-II Studies: A Potential Therapeutic Vaccine Drug in the Treatment of Multiple Sclerosis (MS)"	EYΔE - ETAK (09SYN21-609)	2011-2015	Postdoctoral Researcher
(7) "Cancer Research UK 5 Year Drug Discovery Programme Grant"	Cancer Research UK (C17468/A9332)	2008-2013 (1 year)	Postdoctoral Researcher
(8) "Methods and strategies in synthesis of enantiopure bioactive molecules with sulfoxides and sulfonamides"	Spanish Ministry of Science and Innovation (CTQ2009-07752)	2009-2012	Postdoctoral Researcher
(9) "IsoCat (Isothioureas as organocatalysts)"	EU (PIEF-GA-2009-253604)	2010-2012	Postdoctoral Researcher
(10) "Highly selective reactions promoted by SmI_2 , CrCl_2 or Mn : elimination processes, cyclopropanation, heterocyclization and ring-opening of epoxides and aziridines"	Regional Ministry of Culture and Tourism of Asturias (Spain) (FC-08-IB08-028)	2010-2012	Predoctoral Researcher
(11) "New economic processes based on electron transfer of stoichiometric and catalytic amounts of SmI_2 , CrCl_2 or Mn , and their application in diastereoselective synthesis of organic compounds"	Spanish Ministry of Education and Science (CTQ2007-61132)	2007-2010	Predoctoral Researcher

(12) "Novel stereoselective transformations promoted by SmI_2 or CrCl_2 and synthesis of enantiopure functionalized amino compounds"	Spanish Ministry of Education and Science (CTQ2004-01191/BQU)	2004-2007	Predoctoral Researcher
(13) "Highly selective elimination and C-C bond-forming reactions mediated by SmI_2 . Preparation of enantiopure compounds"	Spanish Ministry of Science and Technology (MCT-01-BQU3807)	2001-2004	Predoctoral Researcher

SCIENTIFIC ACHIEVEMENTS - OVERVIEW

- ORCID / Scopus ID: 0000-0002-7096-4281 / 10939131000
- N° of Publications: 32
- Average of Impact Factor (2023) >6
- Total citations: > 1500 (google scholar); >1200 (WOS);
- *h*-index: 18 / *i*10-index: 24 (google scholar); 16 (Scopus)

Assistant Professor Carmen Simal Fernández (appointed in 2023) earned her PhD in Chemistry (Organic Chemistry) from the University of Oviedo (Spain) in 2009, awarded *Cum Laude* and the PhD Extraordinary Award. Her doctoral research focused on the development of novel stereoselective transformations mediated by samarium diiodide. During her PhD, she undertook four international research stays at leading European universities (Bristol, St Andrews, Athens, and Oxford), enhancing her expertise in advanced synthetic methodologies. Following her PhD, she joined the University of Oxford as a Postdoctoral Research Fellow (2009–2010), working on the design of small organic molecules for cancer therapy. She was subsequently awarded a Marie Curie Intra-European Fellowship at the University of St Andrews (2010–2012), where she investigated isothioureia-based organocatalysis and enantioselective Lewis-base catalysis. Her scientific excellence was later recognized by the Spanish National Research Council (CSIC) through a JAE-Doc Fellowship (2012–2015), enabling her to explore new methodologies in asymmetric synthesis using chiral sulfoxides. From 2015 to 2017, as a Clarín–COFUND Postdoctoral Fellow at the University of Patras, she contributed to the rational design and synthesis of peptide and non-peptide mimetics targeting autoimmune diseases such as multiple sclerosis. She subsequently broadened her research scope into Materials Chemistry at the University of Peloponnese (2020–2021), developing organic additive-assisted perovskite solar cells, and into Analytical and Natural Products Chemistry (University of Patras, 2021–2022), where she coordinated studies on strawberry genotypes through chromatographic profiling (GC-MS, LC-MS/HPLC).

Her multidisciplinary research combines **Organic and Medicinal Chemistry**, with complementary contributions to Materials Science and Analytical Chemistry. Her current research interests focus on the **design and synthesis of bioactive compounds**, particularly **flavonoids, organometallic hybrids, and targeted drug conjugates**, as potential next-generation therapeutics for **cancer, autoimmune diseases, and antimicrobial resistance**.

