

<b>Part A. PERSONAL INFORMATION</b>		<b>CV date</b>	10/09/2021
First and Family name	Sonsoles Martín Santamaría		
Social Security, Passport, ID number	50087571B	Age	50
Researcher codes	Open Researcher and Contributor ID (ORCID**)	<a href="https://orcid.org/0000-0002-7679-0155">0000-0002-7679-0155</a>	
	SCOPUS Author ID (*)		
	WoS Researcher ID (*)	<a href="https://www.researcherid.org/rid/A-8035-2012">A-8035-2012</a>	

(\*) Optional (\*\*) Mandatory

### A.1. Current position

Name of University/Institution	Consejo Superior de Investigaciones Científicas		
Department	Centro de Investigaciones Biológicas Margarita Salas		
Address and Country	C/ Ramiro de Maeztu, 9. 28040-Madrid. Spain		
Phone number	(+34) 918373112 Ext. 4389	E-mail	<a href="mailto:smsantamaria@cib.csic.es">smsantamaria@cib.csic.es</a>
Current position	Staff Scientist (Científico Titular)	From	06/06/2014
Key words	Chemical biology, drug design, glycosciences, innate immunity, Toll-like receptors, molecular modeling, computational chemistry, molecular recognition.		

### A.2. Education

PhD, Licensed, Graduate	University	Year
Degree in Pharmacy	Universidad Complutense de Madrid	1993
PhD in Pharmacy	Universidad Complutense de Madrid	1998

### A.3. General indicators of quality of scientific production (see instructions)

3 research 6-year periods (sexenios): 1997-2002, 2003-08 y 2009-14.

Postdocs: 4; PhD Thesis: 7 (2007, 2011, 2012, 2017 (2), 2018 y 2019); current PhD students 2; Master students: 14; current Master students 1.

Relevant bibliometric indicators: -publications in Web of Science 93; -h-index 27; -sum of times cited 1814; -average citations per item 20.4; average citations per year 75.6

Updated information: <https://publons.com/researcher/2758271/sonsoles-martin-santamaria>

Maternity leaves: 2001, 2003, and 2005-06.

### Part B. CV SUMMARY (max. 3500 characters, including spaces)

The research interests of Sonsoles Martín Santamaría lie at the interface between Chemistry and Biology. The multidisciplinary character of her scientific trajectory started from Organic Synthesis and moved toward Computational Chemistry and Molecular Modelling.

◆ In 1998, SMS got her **PhD** at the **Dept. of Organic and Pharmaceutical Chemistry, Universidad Complutense de Madrid**, "Premio Extraordinario" (Prof Avendaño's group, FPU grant) in the design and synthesis of agents as MDR (multidrug resistance) working in heterocyclic chemistry and asymmetric synthesis of peptide mimetics. Publication: 3 *J. Org. Chem.* and 2 *Tetrahedron*.

◆ **Two distinct postdoctoral stays** followed the PhD period:

- **Dept. of Chemistry, Imperial College London** (Prof Rzepa's group, 1998-2000). Involvement in several collaborative projects addressing diverse mechanistic and reactivity problems of Chemistry with Computational Chemistry techniques: stereoelectronic control in extrusion reactions of R<sub>2</sub>I-F Intermediates, conformation of  $\alpha$ -fluoro-aminoacids, Möbius aromaticity, and transition states in Pd-catalyzed reactions. Publication of 9 research articles. Tutoring of 2 final-year projects and undergraduate teaching (Degree in Chemistry).



- **Dept. of Pharmacology, Universidad de Alcalá** (Prof Gago's group 2001-03). Studies of drug-receptor interactions and structural studies of compounds with biological interest by means of MD simulations, 3D-QSAR and docking techniques. Collaborative work with groups from Academia (Profs Camarasa, Luque, and de Mendoza) and industry (PharmaMar). Publication of 6 articles (2 *J. Am. Chem. Soc.*, 2 *J. Med. Chem.*, *Biochemistry*, *Curr. Med. Chem.*).

◆ In 2003, SMS obtained a [Ramón y Cajal contract](#) and, in 2004, moved to the **Dept. of Chemistry, Universidad San Pablo CEU**, where she was [Assistant Professor](#) of Organic and Pharmaceutical Chemistry from 2008-11, under the I3 Program, and [Associate Professor](#) from 2011-14. "Acreditación Nacional" from ANECA for "Profesor Titular" in 2010.

- 2004-11. Involvement in the research projects of the de Pascual-Teresa & Ramos' group, working in the design and synthesis of ligands interacting estrogen receptors, adrenomedullin and MMP-2 (12 articles published in *J. Med. Chem.*, *Eur. J. Med. Chem.*, *Org. Biomol. Chem.*, *Expert. Opin. Ther. Targets*, among others). Collaborative work with groups from Academia (8 articles published in *Chem. Eur. J.*, *Chem. Commun.*, *Org. Biomol. Chem.*, *ChemBioChem*, among others). 3 PhD co-supervised and defended.

- 2012-14. SMS starts her independent carrier as [PI of the Computational Chemical Biology group](#).

◆ In June 2014, SMS moves to the **Centro de Investigaciones Biológicas Margarita Salas of CSIC**, as [Científico Titular](#) and PI of the Computational Chemical Biology group. SMS has faced new challenges involving a significant leap in the quality and novelty of the research objectives. Since 2012, her team's efforts are devoted to the application of molecular modelling and computational chemistry to the understanding of ligand-receptor interactions and molecular recognition processes of innate immunity receptors, with relevance for drug design. 7 PhD supervised and defended; 2 PhD Thesis in progress. SMS is involved in postgraduate teaching in three Master programs, is Secretary General of the Royal Society of Chemistry of Spain (RSEQ), and Chair of the Division of Chemistry in Life Sciences of EuChemS.

## Part C. RELEVANT MERITS

### C.1. Publications (including books, selected 2016-21)

1: Editor: **S. Martín-Santamaría**. 2018. *Computational tools in Chemical Biology*. London. Chemical Biology series. Royal Society of Chemistry. ISBN 978-1-78262-700-5.

2: Matamoros-Recio A, Franco-Gonzalez JF, Perez-Regidor L, Billod JM, Guzman-Caldentey J, **Martín-Santamaría, S.\*** (6/6) Full-Atom Model of the Agonist LPS-bound Toll-like Receptor 4 Dimer in a Membrane Environment. *Chem. Eur. J.*, **2021**, *in press*.

3: Matamoros-Recio A, Franco-Gonzalez JF, Forgione RE, Torres-Mozas A, Silipo A, **Martín-Santamaría S.\*** (6/6) Understanding the Antibacterial Resistance: Computational Explorations in Bacterial Membranes. *ACS Omega* **2021**, *6*, 6041-54.

4: Di Lorenzo F, ..., **Martín-Santamaría S**, ..., Molinaro A. (9/15) Pairing *Bacteroides vulgatus* LPS Structure with Its Immunomodulatory Effects on Human Cellular Models. *ACS Cent Sci.* **2020**, *6*, 1602-16.

5: Di Carluccio C, ..., **Martín-Santamaría S,\*** Marchetti R,\* Silipo A.\* (14/16) Characterisation of the Dynamic Interactions between Complex N-Glycans and Human CD22. *ChemBioChem.* **2020**, *21*, 129-140.

6: Medve L, ..., **Martin-Santamaria S,\*** Bernardi A,\* Fieschi F.\* (10/12) Enhancing Potency and Selectivity of a DC-SIGN Glycomimetic Ligand by Fragment-Based Design: Structural Basis. *Chemistry, A Eur. J.* **2019**, *25*, 14659-68.

7. Entova S, Billod JM, Swiecicki JM, **Martín-Santamaría S**, Imperiali B. Insights into the key determinants of membrane protein topology enable the identification of new monotopic folds. *Elife.* **2018**, *7*, e40889.

8. Sestito SE, Facchini FA, Morbioli I, Billod JM, **Martin-Santamaria S**, Casnati A, Sansone F, Peri F. Amphiphilic Guanidinocalixarenes Inhibit Lipopolysaccharide (LPS)- and Lectin-Stimulated Toll-like Receptor 4 (TLR4) Signaling. *J. Med. Chem.* **2017**, *60*, 4882-92.

9. El-Halfawy OM, Klett J, Ingram RJ, Loutet SA, Murphy ME, **Martín-Santamaría S**, Valvano MA. Antibiotic Capture by Bacterial Lipocalins Uncovers an Extracellular Mechanism of Intrinsic Antibiotic Resistance. *mBio.* **2017**, *8*, e00225-17.

10. Ghirardello M, de Las Rivas M, Lacetera A, Delso I, Lira-Navarrete E, Tejero T, **Martín-Santamaría S,\*** Hurtado-Guerrero R,\* Merino P.\* Glycomimetics Targeting Glycosyltransferases:



Synthetic, Computational and Structural Studies of Less-Polar Conjugates. *Chem. Eur. J.*, **2016**, *22*, 7215-24.

## C.2. Research projects (selected, last 10 years)

1. Title: Computational approaches to mechanisms of innate immunity and bacterial resistance.  
Principal Investigator: **Sonsoles Martín Santamaría**.  
Funding institution: MINECO. Reference: PID2020-113588RB-I00  
Duration: 01/09/2021 - 31/08/2024. Financing: 120.000 EUR.
2. Title: Computational studies of innate immunity molecular mechanisms: Toll-like receptors.  
Principal Investigator: **Sonsoles Martín Santamaría**.  
Funding institution: MINECO. Reference: CTQ2017-88353-R  
Duration: 01/01/2018 - 31/12/2020 - Extended until 30/09/2021. Financing: 130.196 EUR.
3. Title: Multidisciplinary approach to blocking SARS-CoV-2 entry through antivirals and Decoy-ACE2 fragments.  
Coordinator (4 groups): MJ Pérez-Pérez (IQM). PI (CIB): **Sonsoles Martín Santamaría**.  
Funding institution: CSIC & PRACE & Fondo SUPERA Santander (PI: R. Geller, UV). References: CSIC-COV19-082, PRACE COVID-19-26, BlockAce.  
Duration: 27/04/2020 - 26/04/2021. Funding (total): 157.000 € + 150.000 € + computing time.
4. Title: El sistema del Complemento en salud y enfermedad (Complemento II-CM).  
Coordinator: S. Rodríguez de Córdoba, CIB-CSIC. PI (CCB group): **S. Martín Santamaría**.  
Funding institution: Comunidad de Madrid. Reference: S2017/BMD-3673.  
Duration: 01/05/2018 – 30/04/2022. Financing: 828.091,87 EUR.
5. Title: Molecular Pattern Recognition Receptors: Computational Chemistry Insights for Drug Design and Innate Immunity Modulation.  
Principal Investigator: **Sonsoles Martín Santamaría**.  
Funding institution: MINECO. Reference: CTQ2014-57141-R. Duration: 01/01/2015 - 31/12/2017 - Extended until 31/12/2018. Financing: 108.000 EUR (direct costs).
6. Title: TOLLerant. Toll-Like Receptor 4 activation and function in diseases: an integrated chemical-biology approach.  
Coordinator: Francesco Peri, IT. PI (CIB): **Sonsoles Martín Santamaría**.  
Funding institution: EC Commission - Horizon2020. Marie Skłodowska-Curie Actions. Reference: MSCA-ITN-2014-ETN-Tollerant. Duration: 01/01/2015 - 31/12/2018. Funding: € 3,122,539.38 (total). € 250,000 for CSIC (IP: SMS).
7. Title: Molecular recognition processes of therapeutic targets involved in immunity and bacterial infection. Computational chemistry approaches.  
PI: **Sonsoles Martín Santamaría**. Funding institution: MINECO. Reference: CTQ2011-22724  
Duration: 01/01/2012 - 31/12/2014 - Extended 31/12/2015. Funding: 84.000 EUR (direct costs).
8. Title: GLYCOPHARM. The Sugar Code: from (bio)chemical concept to clinics.  
Coordinator: Dolores Solís, IQFR-CSIC. PI (CSICd): **Sonsoles Martín Santamaría**  
Funding institution: EC-FP7- Marie Curie Actions. Reference: PITN-GA-2012-317297. Duration: 01/11/2012 – 31/10/2016. Financing: 3,005,458.30 € (Total); 239,881.62 € (CSICd partner).
9. Title: Microbial cell surface determinants of virulence as targets for new therapeutics in Cystic Fibrosis.  
Principal Investigator: Antonio Molinaro, IT (Chair). **Sonsoles Martín Santamaría** (Work group 2 leader and 2013-14 Grant Holder).  
Funding institution: EC FP7 COST Action. Ref: COST Action (BM1003). Duration: 01/05/2010 – 28/10/2014. Funding: 60.000 € (2011); 87.400 € (2012); 139.000 € (2013); 117.6000 € (2014).

## C.3. Contracts, technological or transfer merits

### C.4. Patents

### C.5. COMISSIONS OF TRUST:

\* 2013-18. Management Board of the Chemistry Panel. National Research Plan of Spain. Ministry of Economy of Spain (MINECO).



- \* 2009-12. Expert for proposal evaluation. Chemistry Panel. National Research Plan of Spain. Ministry of Economy of Spain (MINECO).
- \* 2008-2016. Expert and Vice-chair for proposal evaluation. Chemistry Panel. European Commission. Programmes Marie Curie IXF Fellowships, FP7 Marie Curie ITN Fellowships.
- \* 2015-19. Expert for proposal evaluation. Chemistry Panel. Andalusian Agency for Evaluation, Spain.
- \* 2008-20. Occasional reviewer for proposal evaluation. National Evaluation Agencies of Spain (MEC-FPU, Ramon y Cajal Program, ANEP), France, Poland, Portugal, Cyprus, Germany.
- \* 2021. Chemistry Panel Coordinator. Predoctoral Fellowships (FPU). Ministry of Education, Spain.

#### C.6. REVIEWER

*Chemistry-A Eur. J., Chem. Commun., J. Chem. Inf. Model., Org. Biomol. Chem., ChemMedChem, MedChemComm., ACS Omega, Mol. BioSys., PhysChemChemPhys, RSC-Advances, PLOS ONE, J. Comput.-Aided Mol. Des.*

#### C.7. MEMBERSHIPS & SERVICES TO SCIENTIFIC SOCIETIES

- \* Royal Spanish Chemical Society of Spain (RSEQ). Secretary General since 2018. Associate Editor Journal "Anales de Química" (2009-12 and 2015-17). Web page Coordinator (2012-17). Division of "Chemical Biology": Co-founder; Secretary (2011-2016); President (2016-19).
- \* European Chemical Society (EuChemS). Chair of the Division of "Chemistry for Life Sciences". Since 2017.
- \* Spanish Society of Biochemistry and Molecular Biology (SEBBM, since 2014; Coordinator of the WP "Chemical Biology" 2016-18).
- \* Spanish Society of Therapeutic Chemistry (member since 1995).
- \* American Chemical Society (2012-18).
- \* Women in Theoretical/Computational Chemistry (since 2014).

#### C.8. OTHER

\* **Invited speaker in national and international conferences:** 25 invited speaker and 2 as plenary speaker. Selected are (2015-20 period), 2020: III Glycobasque Symposium; 2019: 42nd Conference of the Spanish Society of Biochemistry and Molecular Biology SEBBM; Translocation-transfer JPIAMR Virtual research network Kick-off meeting; 2018: 28th International Carbohydrate Conference, X Spanish Drug Discovery Network; 2017: 19th EUROCARB; Barluenga Lectureship workshop; XXXIII Meeting Reference Network in Theoretical and Computational Chemistry; Spanish-Japanese Symposium on Modern Synthetic Methodology; 2016: Japan-France-Spain Joint Symposium on Theoretical and Computational Science of Complex Systems; 2015: ICIQ-FIFC Spain-Japan Joint Symposium on Theoretical and Computational Chemistry of Complex Systems.

\* **Conferences by invitation to national and international universities and research institutions** (including USA and Japan). Selected are (2015-20 period, 2020: Center of Biotechnology and Plant Genomics (CBGP-UPM); 2019: National Royal Academy of Pharmacy, ES; University of Valencia, ES; 2018: University of Osaka, JP; 2017: University of Basque Country, ES; 2016: Institute of Chemical Research of Catalonia (ICIQ); University of Osaka, JP; 2015: University of La Rioja; University of the Basque Country.

\* Member of **scientific and/or organizing committees** of 17 national and international conferences, several symposia, 2 training schools from European projects, 1 summer school of the UIMP.

#### **Chair of the following scientific meetings:**

2021. Chair of EuChemS session at EFMC-ISMC International Symposium on Medicinal Chemistry.

2019. Joint ECBS/EuChemS Conference (6<sup>th</sup> European Chemical Biology Symposium & Meeting of the "Chemistry in Life Sciences" Division of EuChemS). Madrid, ES.

<https://congresosalcala.fgua.es/ecbs2019euchems/>

2016 III Biennial Meeting of the Chemical Biology Division of the RSEQ, Madrid, ES.

2016 Chair of Topic session "In Silico Methods in Life Sciences". 6th EuChemS Chemistry Conference. Sevilla, ES.

2015 Chair of the Joint Spanish-Japanese Symposium: Computational Approaches for the Study of Chemical and Biological Systems. Madrid, ES.

2015 Chair of the symposium "Chemical Biology". XXXV Biennial Meetings of the Royal Spanish Society of Chemistry. La Coruña, ES.