

# Sonsoles Martn Santamara

## List of Publications by Citations

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77  
papers

1,936  
citations

26  
h-index

40  
g-index

90  
ext. papers

2,205  
ext. citations

6  
avg, IF

4.38  
L-index

#	Paper	IF	Citations
77	Chemistry of lipid A: at the heart of innate immunity. <i>Chemistry - A European Journal</i> , <b>2015</b> , 21, 500-19	4.8	147
76	Potential anti-inflammatory, anti-adhesive, anti/estrogenic, and angiotensin-converting enzyme inhibitory activities of anthocyanins and their gut metabolites. <i>Genes and Nutrition</i> , <b>2012</b> , 7, 295-306	4.3	115
75	Guanidinium receptors as enantioselective amino acid membrane carriers. <i>Journal of the American Chemical Society</i> , <b>2003</b> , 125, 8270-84	16.4	105
74	ET-18-OCH <sub>3</sub> (edelfosine): a selective antitumour lipid targeting apoptosis through intracellular activation of Fas/CD95 death receptor. <i>Current Medicinal Chemistry</i> , <b>2004</b> , 11, 3163-84	4.3	94
73	Fluoridation of heteroaromatic iodonium salts: experimental evidence supporting theoretical prediction of the selectivity of the process. <i>Chemical Communications</i> , <b>2000</b> , 649-650	5.8	81
72	The preferred conformation of $\beta$ -fluoroamides. <i>Journal of the Chemical Society Perkin Transactions II</i> , <b>1999</b> , 2409-2411		66
71	Computational Approaches to Toll-Like Receptor 4 Modulation. <i>Molecules</i> , <b>2016</b> , 21,	4.8	49
70	Development of a new family of conformationally restricted peptides as potent nucleators of beta-turns. Design, synthesis, structure, and biological evaluation of a beta-lactam peptide analogue of melanostatin. <i>Journal of the American Chemical Society</i> , <b>2003</b> , 125, 16243-60	16.4	48
69	Symmetric dithiodigalactoside: strategic combination of binding studies and detection of selectivity between a plant toxin and human lectins. <i>Organic and Biomolecular Chemistry</i> , <b>2011</b> , 9, 5445-55 <sup>9</sup>	4.8	46
68	Structural aspects of binding of linked digalactosides to human galectin-1. <i>Glycobiology</i> , <b>2011</b> , 21, 1627-38	4.8	40
67	Modulation of CD14 and TLR4/MD-2 activities by a synthetic lipid A mimetic. <i>ChemBioChem</i> , <b>2014</b> , 15, 250-8	3.8	39
66	Minimizing the Entropy Penalty for Ligand Binding: Lessons from the Molecular Recognition of the Histo Blood-Group Antigens by Human Galectin-3. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 7268-7272	16.4	38
65	An ab initio and MNDO-d SCF-MO computational study of stereoelectronic control in extrusion reactions of R <sub>2</sub> I iodine(III) intermediates. <i>Journal of the Chemical Society Perkin Transactions II</i> , <b>1999</b> , 2707-2714		38
64	Activation of Human Toll-like Receptor 4 (TLR4)/Myeloid Differentiation Factor 2 (MD-2) by Hypoacylated Lipopolysaccharide from a Clinical Isolate of Burkholderia cenocepacia. <i>Journal of Biological Chemistry</i> , <b>2015</b> , 290, 21305-19	5.4	36
63	Structural basis for the binding of didemnins to human elongation factor eEF1A and rationale for the potent antitumor activity of these marine natural products. <i>Journal of Medicinal Chemistry</i> , <b>2004</b> , 47, 4439-52	8.3	36
62	Double aromaticity and anti-aromaticity in small carbon rings. <i>Chemical Communications</i> , <b>2000</b> , 1503-1504	4.8	35
61	Structure-Activity Relationship in Monosaccharide-Based Toll-Like Receptor 4 (TLR4) Antagonists. <i>Journal of Medicinal Chemistry</i> , <b>2018</b> , 61, 2895-2909	8.3	32

60	Serine versus threonine glycosylation with $\beta$ D-GalNAc: unexpected selectivity in their molecular recognition with lectins. <i>Chemistry - A European Journal</i> , <b>2014</b> , 20, 12616-27	4.8	32
59	Role of histidine-85 in the catalytic mechanism of thymidine phosphorylase as assessed by targeted molecular dynamics simulations and quantum mechanical calculations. <i>Biochemistry</i> , <b>2004</b> , 43, 405-14	3.2	31
58	Assessing carbohydrate-carbohydrate interactions by NMR spectroscopy: the trisaccharide epitope from the marine sponge <i>Microciona prolifera</i> . <i>ChemBioChem</i> , <b>2009</b> , 10, 511-9	3.8	29
57	Hückel and Möbius aromaticity and trimerous transition state behaviour in the pericyclic reactions of [10], [14], [16] and [18]annulenes. <i>Perkin Transactions II RSC</i> , <b>2000</b> , 1415-1417		29
56	gem-Difluorocarbadisaccharides: restoring the exo-anomeric effect. <i>Angewandte Chemie - International Edition</i> , <b>2014</b> , 53, 9597-602	16.4	28
55	Structure of micelle-bound adrenomedullin: a first step toward the analysis of its interactions with receptors and small molecules. <i>Biopolymers</i> , <b>2012</b> , 97, 45-53	2.2	28
54	Adrenomedullin: a new target for the design of small molecule modulators with promising pharmacological activities. <i>European Journal of Medicinal Chemistry</i> , <b>2005</b> , 40, 737-50	6.8	28
53	Amphiphilic Guanidinocalixarenes Inhibit Lipopolysaccharide (LPS)- and Lectin-Stimulated Toll-like Receptor 4 (TLR4) Signaling. <i>Journal of Medicinal Chemistry</i> , <b>2017</b> , 60, 4882-4892	8.3	26
52	Interactions of bacterial cell division protein FtsZ with C8-substituted guanine nucleotide inhibitors. A combined NMR, biochemical and molecular modeling perspective. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 16418-28	16.4	26
51	Potent "clicked" MMP2 inhibitors: synthesis, molecular modeling and biological exploration. <i>Organic and Biomolecular Chemistry</i> , <b>2011</b> , 9, 4587-99	3.9	25
50	Regio- and Diastereoselective Alkylation of 2-Substituted 2,4-Dihydro-1H-pyrazino[2,1-b]quinazoline-3,6-diones. <i>Journal of Organic Chemistry</i> , <b>1997</b> , 62, 6424-6428	4.2	25
49	New scaffolds for the design of selective estrogen receptor modulators. <i>Organic and Biomolecular Chemistry</i> , <b>2008</b> , 6, 3486-96	3.9	24
48	Twist localisation in single, double and triple twisted Möbius cyclacenes. <i>Perkin Transactions II RSC</i> , <b>2000</b> , 2378-2381		24
47	Antibiotic Capture by Bacterial Lipocalins Uncovers an Extracellular Mechanism of Intrinsic Antibiotic Resistance. <i>MBio</i> , <b>2017</b> , 8,	7.8	23
46	Pairing LPS Structure with Its Immunomodulatory Effects on Human Cellular Models. <i>ACS Central Science</i> , <b>2020</b> , 6, 1602-1616	16.8	23
45	Virtual Screening Approaches towards the Discovery of Toll-Like Receptor Modulators. <i>International Journal of Molecular Sciences</i> , <b>2016</b> , 17,	6.3	22
44	Antagonistic Pleiotropy in the Bifunctional Surface Protein FadL (OmpP1) during Adaptation of <i>Haemophilus influenzae</i> to Chronic Lung Infection Associated with Chronic Obstructive Pulmonary Disease. <i>MBio</i> , <b>2018</b> , 9,	7.8	22
43	Möbius aromatics arising from a CCC ring component. <i>Chemical Communications</i> , <b>2000</b> , 1089-1090	5.8	21

42	Rational design of a Tn antigen mimic. <i>Chemical Communications</i> , <b>2011</b> , 47, 5319-21	5.8	20
41	Engineering O-glycosylation points in non-extended peptides: implications for the molecular recognition of short tumor-associated glycopeptides. <i>Chemistry - A European Journal</i> , <b>2011</b> , 17, 3105-10	4.8	19
40	Glycomimetics Targeting Glycosyltransferases: Synthetic, Computational and Structural Studies of Less-Polar Conjugates. <i>Chemistry - A European Journal</i> , <b>2016</b> , 22, 7215-24	4.8	19
39	Gram-Negative Extremophile Lipopolysaccharides: Promising Source of Inspiration for a New Generation of Endotoxin Antagonists. <i>European Journal of Organic Chemistry</i> , <b>2017</b> , 2017, 4055-4073	3.2	18
38	Möbius and Hückel molecular orbitals arising from CCC components in annulene rings. <i>Perkin Transactions II RSC</i> , <b>2000</b> , 2372-2377		18
37	Conformational selection in glycomimetics: human galectin-1 only recognizes syn-type conformations of $\beta$ 1,3-linked lactose and its C-glycosyl derivative. <i>Chemistry - A European Journal</i> , <b>2013</b> , 19, 14581-90	4.8	17
36	Adrenomedullin: a new and promising target for drug discovery. <i>Expert Opinion on Therapeutic Targets</i> , <b>2006</b> , 10, 303-17	6.4	17
35	Novel carboxylate-based glycolipids: TLR4 antagonism, MD-2 binding and self-assembly properties. <i>Scientific Reports</i> , <b>2019</b> , 9, 919	4.9	16
34	Modulation of binding strength in several classes of active site inhibitors of acetylcholinesterase studied by comparative binding energy analysis. <i>Journal of Medicinal Chemistry</i> , <b>2004</b> , 47, 4471-82	8.3	16
33	Regio- and diastereoselective dialkylation of (4S)-2,4-dimethyl-2,4-dihydro-1H-pyrazino[2,1-b]quinazoline-3,6-dione. <i>Tetrahedron</i> , <b>1997</b> , 53, 16795-16802	2.4	15
32	Selective human adenosine A3 antagonists based on pyrido[2,1-f]purine-2,4-diones: novel features of hA3 antagonist binding. <i>ChemMedChem</i> , <b>2008</b> , 3, 111-9	3.7	15
31	Enhancing Potency and Selectivity of a DC-SIGN Glycomimetic Ligand by Fragment-Based Design: Structural Basis. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 14659-14668	4.8	14
30	An ab initio and MNDO-d SCFMO computational study of the extrusion reactions of R2I <sub>2</sub> iodine(III) via dimeric, trimeric and tetrameric transition states. <i>Perkin Transactions II RSC</i> , <b>2000</b> , 2158-2161		14
29	Conformational Plasticity in Glycomimetics: Fluorocarbamethyl-L-idopyranosides Mimic the Intrinsic Dynamic Behaviour of Natural Idose Rings. <i>Chemistry - A European Journal</i> , <b>2015</b> , 21, 10513-21	4.8	13
28	Synthesis, biological evaluation, and three-dimensional quantitative structure-activity relationship study of small-molecule positive modulators of adrenomedullin. <i>Journal of Medicinal Chemistry</i> , <b>2005</b> , 48, 4068-75	8.3	13
27	Modulation of toll-like receptor 4. Insights from x-ray crystallography and molecular modeling. <i>Current Topics in Medicinal Chemistry</i> , <b>2014</b> , 14, 2672-83	3	13
26	Insights into the key determinants of membrane protein topology enable the identification of new monotopic folds. <i>ELife</i> , <b>2018</b> , 7,	8.9	13
25	Unveiling Molecular Recognition of Sialoglycans by Human Siglec-10. <i>IScience</i> , <b>2020</b> , 23, 101231	6.1	13

24	Characterisation of the Dynamic Interactions between Complex N-Glycans and Human CD22. <i>ChemBioChem</i> , <b>2020</b> , 21, 129-140	3.8	12
23	Multisite-directed inhibitors of protein kinase CK2: new challenges. <i>Molecular and Cellular Biochemistry</i> , <b>2011</b> , 356, 117-9	4.2	11
22	Glycolipid-based TLR4 Modulators and Fluorescent Probes: Rational Design, Synthesis, and Biological Properties. <i>Chemical Biology and Drug Design</i> , <b>2016</b> , 88, 217-29	2.9	10
21	(4S)-2,4-Dimethyl-2,4-dihydro-3,6-dioxo-(1H)-pyrazino[2,1-b]quinazolyl tosylate as an electrophilic glycine template. <i>Tetrahedron</i> , <b>1999</b> , 55, 1755-1762	2.4	10
20	Molecular Basis of the Functional Differences between Soluble Human Versus Murine MD-2: Role of Val135 in Transfer of Lipopolysaccharide from CD14 to MD-2. <i>Journal of Immunology</i> , <b>2016</b> , 196, 2309-18	5.3	8
19	gem-Difluorocarbadisaccharides: Restoring the exo-Anomeric Effect. <i>Angewandte Chemie</i> , <b>2014</b> , 126, 9751-9756	3.6	8
18	Towards selectivity in functional estrogen receptor antagonists. <i>Organic and Biomolecular Chemistry</i> , <b>2012</b> , 10, 7334-46	3.9	8
17	Structural studies on the interaction of saccharides and glycomimetics with galectin-1: A 3D perspective using a combined molecular modeling and NMR approach. <i>Pure and Applied Chemistry</i> , <b>2011</b> , 84, 49-64	2.1	8
16	Insights into real-time chemical processes in a calcium sensor protein-directed dynamic library. <i>Nature Communications</i> , <b>2019</b> , 10, 2798	17.4	7
15	Mimicking chitin: chemical synthesis, conformational analysis, and molecular recognition of the beta(1->3) N-acetylchitopentaose analogue. <i>Chemistry - A European Journal</i> , <b>2010</b> , 16, 4239-49	4.8	7
14	Understanding the Antibacterial Resistance: Computational Explorations in Bacterial Membranes. <i>ACS Omega</i> , <b>2021</b> , 6, 6041-6054	3.9	7
13	New Therapeutic Strategies for Osteoarthritis by Targeting Sialic Acid Receptors. <i>Biomolecules</i> , <b>2020</b> , 10,	5.9	6
12	Small-molecule negative modulators of adrenomedullin: design, synthesis, and 3D-QSAR study. <i>ChemMedChem</i> , <b>2008</b> , 3, 1345-55	3.7	6
11	Diastereoselective reactions in glycine templates containing an ent-ardeemin fragment. <i>Journal of Organic Chemistry</i> , <b>2002</b> , 67, 2013-8	4.2	6
10	Type IV Coupling Proteins as Potential Targets to Control the Dissemination of Antibiotic Resistance. <i>Frontiers in Molecular Biosciences</i> , <b>2020</b> , 7, 201	5.6	6
9	Lipid A: Immunological Properties and Molecular Basis of Its Binding to the Myeloid Differentiation Protein-2/Toll-Like Receptor 4 Complex. <i>Frontiers in Immunology</i> , <b>2018</b> , 9, 1888	8.4	6
8	Molecular bases for the association of FHR-1 with atypical hemolytic uremic syndrome and other diseases. <i>Blood</i> , <b>2021</b> , 137, 3484-3494	2.2	4
7	New clicked full agonists of the estrogen receptor $\beta$ . <i>RSC Advances</i> , <b>2013</b> , 3, 3697	3.7	2

6	Synthesis and Stereochemistry of 11,11a-Dihydro Derivatives of (4S)-2,4-Dimethyl-2,4-dihydro-1H-pyrazino[2,1-b]quinazoline-3,6-diones. A New Transannular Rearrangement Proposal. <i>Journal of Organic Chemistry</i> , <b>1999</b> , 64, 7233-7235	4.2	2
5	Synthetic Glycolipids as Molecular Vaccine Adjuvants: Mechanism of Action in Human Cells and In Vivo Activity. <i>Journal of Medicinal Chemistry</i> , <b>2021</b> , 64, 12261-12272	8.3	2
4	Abacavir Increases Purinergic P2X7 Receptor Activation by ATP: Does a Pro-inflammatory Synergism Underlie Its Cardiovascular Toxicity?. <i>Frontiers in Pharmacology</i> , <b>2021</b> , 12, 613449	5.6	1
3	Molecular Insight into the Regulation of Vimentin by Cysteine Modifications and Zinc Binding. <i>Antioxidants</i> , <b>2021</b> , 10,	7.1	1
2	Full-Atom Model of the Agonist LPS-Bound Toll-like Receptor 4 Dimer in a Membrane Environment. <i>Chemistry - A European Journal</i> , <b>2021</b> , 27, 15406-15425	4.8	1
1	Chemistry of Lipid A: At the Heart of Innate Immunity. <i>Chemistry - A European Journal</i> , <b>2015</b> , 21, 477-477	4.8	0