Sonsoles Martn Santamara

List of Publications by Year in Descending Order

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	Abacavir Increases Purinergic P2X7 Receptor Activation by ATP: Does a Pro-inflammatory Synergism Underlie Its Cardiovascular Toxicity?. *Frontiers in Pharmacology*, **2021**, 12, 613449	5.6	1
76	Molecular Insight into the Regulation of Vimentin by Cysteine Modifications and Zinc Binding. *Antioxidants*, **2021**, 10,	7.1	1
75	Molecular bases for the association of FHR-1 with atypical hemolytic uremic syndrome and other diseases. *Blood*, **2021**, 137, 3484-3494	2.2	4
74	Understanding the Antibacterial Resistance: Computational Explorations in Bacterial Membranes. *ACS Omega*, **2021**, 6, 6041-6054	3.9	7
73	Synthetic Glycolipids as Molecular Vaccine Adjuvants: Mechanism of Action in Human Cells and In Vivo Activity. *Journal of Medicinal Chemistry*, **2021**, 64, 12261-12272	8.3	2
72	Full-Atom Model of the Agonist LPS-Bound Toll-like Receptor 4 Dimer in a Membrane Environment. *Chemistry - A European Journal*, **2021**, 27, 15406-15425	4.8	1
71	New Therapeutic Strategies for Osteoarthritis by Targeting Sialic Acid Receptors. *Biomolecules*, **2020**, 10,	5.9	6
70	Unveiling Molecular Recognition of Sialoglycans by Human Siglec-10. *IScience*, **2020**, 23, 101231	6.1	13
69	Pairing LPS Structure with Its Immunomodulatory Effects on Human Cellular Models. *ACS Central Science*, **2020**, 6, 1602-1616	16.8	23
68	Type IV Coupling Proteins as Potential Targets to Control the Dissemination of Antibiotic Resistance. *Frontiers in Molecular Biosciences*, **2020**, 7, 201	5.6	6
67	Characterisation of the Dynamic Interactions between Complex N-Glycans and Human CD22. *ChemBioChem*, **2020**, 21, 129-140	3.8	12
66	Novel carboxylate-based glycolipids: TLR4 antagonism, MD-2 binding and self-assembly properties. *Scientific Reports*, **2019**, 9, 919	4.9	16
65	Insights into real-time chemical processes in a calcium sensor protein-directed dynamic library. *Nature Communications*, **2019**, 10, 2798	17.4	7
64	Minimizing the Entropy Penalty for Ligand Binding: Lessons from the Molecular Recognition of the Histo Blood-Group Antigens by Human Galectin-3. *Angewandte Chemie - International Edition*, **2019**, 58, 7268-7272	16.4	38
63	Enhancing Potency and Selectivity of a DC-SIGN Glycomimetic Ligand by Fragment-Based Design: Structural Basis. *Chemistry - A European Journal*, **2019**, 25, 14659-14668	4.8	14
62	Structure-Activity Relationship in Monosaccharide-Based Toll-Like Receptor 4 (TLR4) Antagonists. *Journal of Medicinal Chemistry*, **2018**, 61, 2895-2909	8.3	32
61	Insights into the key determinants of membrane protein topology enable the identification of new monotopic folds. *ELife*, **2018**, 7,	8.9	13

60	Antagonistic Pleiotropy in the Bifunctional Surface Protein FadL (OmpP1) during Adaptation of Haemophilus influenzae to Chronic Lung Infection Associated with Chronic Obstructive Pulmonary Disease. *MBio*, **2018**, 9,	7.8	22
59	Lipid A: Immunological Properties and Molecular Basis of Its Binding to the Myeloid Differentiation Protein-2/Toll-Like Receptor 4 Complex. *Frontiers in Immunology*, **2018**, 9, 1888	8.4	6
58	Amphiphilic Guanidinocalixarenes Inhibit Lipopolysaccharide (LPS)- and Lectin-Stimulated Toll-like Receptor 4 (TLR4) Signaling. *Journal of Medicinal Chemistry*, **2017**, 60, 4882-4892	8.3	26
57	Gram-Negative Extremophile Lipopolysaccharides: Promising Source of Inspiration for a New Generation of Endotoxin Antagonists. *European Journal of Organic Chemistry*, **2017**, 2017, 4055-4073	3.2	18
56	Antibiotic Capture by Bacterial Lipocalins Uncovers an Extracellular Mechanism of Intrinsic Antibiotic Resistance. *MBio*, **2017**, 8,	7.8	23
55	Glycolipid-based TLR4 Modulators and Fluorescent Probes: Rational Design, Synthesis, and Biological Properties. *Chemical Biology and Drug Design*, **2016**, 88, 217-29	2.9	10
54	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. *Journal of Immunology*, **2016**, 196, 2309-18	5.3	8
53	Virtual Screening Approaches towards the Discovery of Toll-Like Receptor Modulators. *International Journal of Molecular Sciences*, **2016**, 17,	6.3	22
52	Computational Approaches to Toll-Like Receptor 4 Modulation. *Molecules*, **2016**, 21,	4.8	49
51	Glycomimetics Targeting Glycosyltransferases: Synthetic, Computational and Structural Studies of Less-Polar Conjugates. *Chemistry - A European Journal*, **2016**, 22, 7215-24	4.8	19
50	Activation of Human Toll-like Receptor 4 (TLR4)□Myeloid Differentiation Factor 2 (MD-2) by Hypoacylated Lipopolysaccharide from a Clinical Isolate of Burkholderia cenocepacia. *Journal of Biological Chemistry*, **2015**, 290, 21305-19	5.4	36
49	Chemistry of Lipid A: At the Heart of Innate Immunity. *Chemistry - A European Journal*, **2015**, 21, 477-477	4.8	0
48	Chemistry of lipid A: at the heart of innate immunity. *Chemistry - A European Journal*, **2015**, 21, 500-19	4.8	147
47	Conformational Plasticity in Glycomimetics: Fluorocarbamethyl-L-idopyranosides Mimic the Intrinsic Dynamic Behaviour of Natural Idose Rings. *Chemistry - A European Journal*, **2015**, 21, 10513-21	4.8	13
46	Modulation of CD14 and TLR4□MD-2 activities by a synthetic lipid A mimetic. *ChemBioChem*, **2014**, 15, 250-8	3.8	39
45	gem-Difluorocarbadisaccharides: restoring the exo-anomeric effect. *Angewandte Chemie - International Edition*, **2014**, 53, 9597-602	16.4	28
44	Serine versus threonine glycosylation with □O-GalNAc: unexpected selectivity in their molecular recognition with lectins. *Chemistry - A European Journal*, **2014**, 20, 12616-27	4.8	32
43	gem-Difluorocarbadisaccharides: Restoring the exo-Anomeric Effect. *Angewandte Chemie*, **2014**, 126, 9751-9756	3.6	8

42	Modulation of toll-like receptor 4. Insights from x-ray crystallography and molecular modeling. *Current Topics in Medicinal Chemistry*, **2014**, 14, 2672-83	3	13
41	Conformational selection in glycomimetics: human galectin-1 only recognizes syn- type conformations of 1,3-linked lactose and its C-glycosyl derivative. *Chemistry - A European Journal*, **2013**, 19, 14581-90	4.8	17
40	New clicked full agonists of the estrogen receptor *RSC Advances*, **2013**, 3, 3697	3.7	2
39	Interactions of bacterial cell division protein FtsZ with C8-substituted guanine nucleotide inhibitors. A combined NMR, biochemical and molecular modeling perspective. *Journal of the American Chemical Society*, **2013**, 135, 16418-28	16.4	26
38	Structure of micelle-bound adrenomedullin: a first step toward the analysis of its interactions with receptors and small molecules. *Biopolymers*, **2012**, 97, 45-53	2.2	28
37	Towards selectivity in functional estrogen receptor antagonists. *Organic and Biomolecular Chemistry*, **2012**, 10, 7334-46	3.9	8
36	Potential anti-inflammatory, anti-adhesive, anti/estrogenic, and angiotensin-converting enzyme inhibitory activities of anthocyanins and their gut metabolites. *Genes and Nutrition*, **2012**, 7, 295-306	4.3	115
35	Structural studies on the interaction of saccharides and glycomimetics with galectin-1: A 3D perspective using a combined molecular modeling and NMR approach. *Pure and Applied Chemistry*, **2011**, 84, 49-64	2.1	8
34	Symmetric dithiodigalactoside: strategic combination of binding studies and detection of selectivity between a plant toxin and human lectins. *Organic and Biomolecular Chemistry*, **2011**, 9, 5445-55	3.9	46
33	Potent "clicked" MMP2 inhibitors: synthesis, molecular modeling and biological exploration. *Organic and Biomolecular Chemistry*, **2011**, 9, 4587-99	3.9	25
32	Multisite-directed inhibitors of protein kinase CK2: new challenges. *Molecular and Cellular Biochemistry*, **2011**, 356, 117-9	4.2	11
31	Engineering O-glycosylation points in non-extended peptides: implications for the molecular recognition of short tumor-associated glycopeptides. *Chemistry - A European Journal*, **2011**, 17, 3105-10	4.8	19
30	Rational design of a Tn antigen mimic. *Chemical Communications*, **2011**, 47, 5319-21	5.8	20
29	Structural aspects of binding of linked digalactosides to human galectin-1. *Glycobiology*, **2011**, 21, 1627-41	3.8	40
28	Mimicking chitin: chemical synthesis, conformational analysis, and molecular recognition of the beta(1-->3) N-acetylchitopentaose analogue. *Chemistry - A European Journal*, **2010**, 16, 4239-49	4.8	7
27	Assessing carbohydrate-carbohydrate interactions by NMR spectroscopy: the trisaccharide epitope from the marine sponge Microciona prolifera. *ChemBioChem*, **2009**, 10, 511-9	3.8	29
26	New scaffolds for the design of selective estrogen receptor modulators. *Organic and Biomolecular Chemistry*, **2008**, 6, 3486-96	3.9	24
25	Selective human adenosine A3 antagonists based on pyrido[2,1-f]purine-2,4-diones: novel features of hA3 antagonist binding. *ChemMedChem*, **2008**, 3, 111-9	3.7	15

24	Small-molecule negative modulators of adrenomedullin: design, synthesis, and 3D-QSAR study. *ChemMedChem*, **2008**, 3, 1345-55	3.7	6
23	Adrenomedullin: a new and promising target for drug discovery. *Expert Opinion on Therapeutic Targets*, **2006**, 10, 303-17	6.4	17
22	Synthesis, biological evaluation, and three-dimensional quantitative structure-activity relationship study of small-molecule positive modulators of adrenomedullin. *Journal of Medicinal Chemistry*, **2005**, 48, 4068-75	8.3	13
21	Adrenomedullin: a new target for the design of small molecule modulators with promising pharmacological activities. *European Journal of Medicinal Chemistry*, **2005**, 40, 737-50	6.8	28
20	ET-18-OCH3 (edelfosine): a selective antitumour lipid targeting apoptosis through intracellular activation of Fas/CD95 death receptor. *Current Medicinal Chemistry*, **2004**, 11, 3163-84	4.3	94
19	Role of histidine-85 in the catalytic mechanism of thymidine phosphorylase as assessed by targeted molecular dynamics simulations and quantum mechanical calculations. *Biochemistry*, **2004**, 43, 405-14	3.2	31
18	Modulation of binding strength in several classes of active site inhibitors of acetylcholinesterase studied by comparative binding energy analysis. *Journal of Medicinal Chemistry*, **2004**, 47, 4471-82	8.3	16
17	Structural basis for the binding of didemnins to human elongation factor eEF1A and rationale for the potent antitumor activity of these marine natural products. *Journal of Medicinal Chemistry*, **2004**, 47, 4439-52	8.3	36
16	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. *Journal of the American Chemical Society*, **2003**, 125, 16243-60	16.4	48
15	Guanidinium receptors as enantioselective amino acid membrane carriers. *Journal of the American Chemical Society*, **2003**, 125, 8270-84	16.4	105
14	Diastereoselective reactions in glycine templates containing an ent-ardeemin fragment. *Journal of Organic Chemistry*, **2002**, 67, 2013-8	4.2	6
13	Double aromaticity and anti-aromaticity in small carbon rings. *Chemical Communications*, **2000**, 1503-1504	5.8	35
12	Hückel and Möbius aromaticity and trimerous transition state behaviour in the pericyclic reactions of [10], [14], [16] and [18]annulenes. *Perkin Transactions II RSC*, **2000**, 1415-1417		29
11	Möbius aromatics arising from a CCC ring component. *Chemical Communications*, **2000**, 1089-1090	5.8	21
10	An ab initio and MNDO-d SCF-MO computational study of the extrusion reactions of R2I-F iodine(III) via dimeric, trimeric and tetrameric transition states. *Perkin Transactions II RSC*, **2000**, 2158-2161		14
9	Möbius and Hückel molecular orbitals arising from CCC components in annulene rings. *Perkin Transactions II RSC*, **2000**, 2372-2377		18
8	Fluoridation of heteroaromatic iodonium salts-experimental evidence supporting theoretical prediction of the selectivity of the process. *Chemical Communications*, **2000**, 649-650	5.8	81
7	Twist localisation in single, double and triple twisted Möbius cyclacenes. *Perkin Transactions II RSC*, **2000**, 2378-2381		24

6	(4S)-2,4-Dimethyl-2,4-dihydro-3,6-dioxo-(1H)-pyrazino[2,1-b]quinazolyl tosylate as an electrophilic glycine template. *Tetrahedron*, **1999**, 55, 1755-1762	2.4	10
5	An ab initio and MNDO-d SCF-MO computational study of stereoelectronic control in extrusion reactions of R2IF iodine(III) intermediates. *Journal of the Chemical Society Perkin Transactions II*, **1999**, 2707-2714		38
4	The preferred conformation of Fluoroamides. *Journal of the Chemical Society Perkin Transactions II*, **1999**, 2409-2411		66
3	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. *Journal of Organic Chemistry*, **1999**, 64, 7233-7235	4.2	2
2	Regio- and Diastereoselective Alkylation of 2-Substituted 2,4-Dihydro-1H-pyrazino[2,1-b]quinazoline-3,6-diones. *Journal of Organic Chemistry*, **1997**, 62, 6424-6428	4.2	25
1	Regio- and diastereoselective dialkylation of (4S)-2,4-dimethyl-2,4-dihydro-1H-pirazino[2,1-b]quinazoline-3,6-dione. *Tetrahedron*, **1997**, 53, 16795-16802	2.4	15