Sonsoles MartÃ-n SantamarÃ-a

List of Publications by Year
in descending order

78 papers	2,466 citations	185998 28 h-index	233125 45 g-index
90 all docs	90 docs citations	90 times ranked	3612 citing authors

#	Article	IF	Citations
1	6â€Shogaol (enexasogoal) treatment improves experimental knee osteoarthritis exerting a pleiotropic effect over immune innate signalling responses in chondrocytes. British Journal of Pharmacology, 2022, 179, 5089-5108.	2.7	8
2	Understanding the Antibacterial Resistance: Computational Explorations in Bacterial Membranes. ACS Omega, 2021, 6, 6041-6054.	1.6	21
3	Abacavir Increases Purinergic P2X7 Receptor Activation by ATP: Does a Pro-inflammatory Synergism Underlie Its Cardiovascular Toxicity?. Frontiers in Pharmacology, 2021, 12, 613449.	1.6	2
4	Molecular Insight into the Regulation of Vimentin by Cysteine Modifications and Zinc Binding. Antioxidants, 2021, 10, 1039.	2.2	10
5	Molecular bases for the association of FHR-1 with atypical hemolytic uremic syndrome and other diseases. Blood, 2021, 137, 3484-3494.	0.6	17
6	Synthetic Glycolipids as Molecular Vaccine Adjuvants: Mechanism of Action in Human Cells and In Vivo Activity. Journal of Medicinal Chemistry, 2021, 64, 12261-12272.	2.9	13
7	Fullâ€Atom Model of the Agonist LPSâ€Bound Tollâ€like Receptor 4 Dimer in a Membrane Environment. Chemistry - A European Journal, 2021, 27, 15406-15425.	1.7	12
8	Characterisation of the Dynamic Interactions between Complex Nâ€Glycans and Human CD22. ChemBioChem, 2020, 21, 129-140.	1.3	16
9	Unveiling Molecular Recognition of Sialoglycans by Human Siglec-10. IScience, 2020, 23, 101231.	1.9	24
10	Pairing Bacteroides vulgatus LPS Structure with Its Immunomodulatory Effects on Human Cellular Models. ACS Central Science, 2020, 6, 1602-1616.	5.3	55
11	Type IV Coupling Proteins as Potential Targets to Control the Dissemination of Antibiotic Resistance. Frontiers in Molecular Biosciences, 2020, 7, 201.	1.6	21
12	New Therapeutic Strategies for Osteoarthritis by Targeting Sialic Acid Receptors. Biomolecules, 2020, 10, 637.	1.8	15
13	Enhancing Potency and Selectivity of a DCâ€SIGN Glycomimetic Ligand by Fragmentâ€Based Design: Structural Basis. Chemistry - A European Journal, 2019, 25, 14659-14668.	1.7	25
14	Novel carboxylate-based glycolipids: TLR4 antagonism, MD-2 binding and self-assembly properties. Scientific Reports, 2019, 9, 919.	1.6	24
15	Insights into real-time chemical processes in a calcium sensor protein-directed dynamic library. Nature Communications, 2019, 10, 2798.	5.8	16
16	Minimizing the Entropy Penalty for Ligand Binding: Lessons from the Molecular Recognition of the Histo Bloodâ€Group Antigens by Human Galectinâ€3. Angewandte Chemie - International Edition, 2019, 58, 7268-7272.	7.2	56
17	Structureâ€“Activity Relationship in Monosaccharide-Based Toll-Like Receptor 4 (TLR4) Antagonists. Journal of Medicinal Chemistry, 2018, 61, 2895-2909.	2.9	51
18	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, .	1.8	39

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19	Bradyrhizobium 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.	2.2	9
20	Insights into the key determinants of membrane protein topology enable the identification of new monotopic folds. ELife, 2018, 7, .	2.8	26
21	Amphiphilic Guanidinocalixarenes Inhibit Lipopolysaccharide (LPS)- and Lectin-Stimulated Toll-like Receptor 4 (TLR4) Signaling. Journal of Medicinal Chemistry, 2017, 60, 4882-4892.	2.9	28
22	Gramâ€Negative Extremophile Lipopolysaccharides: Promising Source of Inspiration for a New Generation of Endotoxin Antagonists. European Journal of Organic Chemistry, 2017, 2017, 4055-4073.	1.2	26
23	Antibiotic Capture by Bacterial Lipocalins Uncovers an Extracellular Mechanism of Intrinsic Antibiotic Resistance. MBio, 2017, 8, .	1.8	31
24	Virtual Screening Approaches towards the Discovery of Toll-Like Receptor Modulators. International Journal of Molecular Sciences, 2016, 17, 1508.	1.8	32
25	Computational Approaches to Toll-Like Receptor 4 Modulation. Molecules, 2016, 21, 994.	1.7	69
26	Glycomimetics Targeting Glycosyltransferases: Synthetic, Computational and Structural Studies of Lessâ€Polar Conjugates. Chemistry - A European Journal, 2016, 22, 7215-7224.	1.7	19
27	Glycolipidâ€based <scp>TLR</scp>4 Modulators and Fluorescent Probes: Rational Design, Synthesis, and Biological Properties. Chemical Biology and Drug Design, 2016, 88, 217-229.	1.5	13
28	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, 2309-2318.	0.4	10
29	Conformational Plasticity in Glycomimetics: Fluorocarbamethylâ€<scp>L</scp>â€idopyranosides Mimic the Intrinsic Dynamic Behaviour of Natural Idose Rings. Chemistry - A European Journal, 2015, 21, 10513-10521.	1.7	16
30	Activation of Human Toll-like Receptor 4 (TLR4)Â·Myeloid Differentiation Factor 2 (MD-2) by Hypoacylated Lipopolysaccharide from a Clinical Isolate of Burkholderia cenocepacia. Journal of Biological Chemistry, 2015, 290, 21305-21319.	1.6	47
31	Chemistry of Lipidâ€…A: At the Heart of Innate Immunity. Chemistry - A European Journal, 2015, 21, 477-477.	1.7	1
32	Chemistry of Lipidâ€…A: At the Heart of Innate Immunity. Chemistry - A European Journal, 2015, 21, 500-519.	1.7	193
33	Modulation of Toll-Like Receptor 4. Insights from X-Ray Crystallography and Molecular Modeling. Current Topics in Medicinal Chemistry, 2015, 14, 2672-2683.	1.0	17
34	Modulation of CD14 and TLR4â‹…MDâ€2 Activities by a Synthetic Lipid A Mimetic. ChemBioChem, 2014, 15, 250-258.	1.3	44
35	gemâ€Difluorocarbadisaccharides: Restoring the exoâ€Anomeric Effect. Angewandte Chemie - International Edition, 2014, 53, 9597-9602.	7.2	36
36	Serine versus Threonine Glycosylation with Î±â€Oâ€GalNAc: Unexpected Selectivity in Their Molecular Recognition with Lectins. Chemistry - A European Journal, 2014, 20, 12616-12627.	1.7	36

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37	Conformational Selection in Glycomimetics: Human Galectinâ€1 Only Recognizes synâ€Î¨â€Type Conformations of Î²â€1,3â€Linked Lactose and Its Câ€Glycosyl Derivative. Chemistry - A European Journal, 2013, 19, 14581-14590.	1.7	19
38	New clicked full agonists of the estrogen receptorÂÎ². RSC Advances, 2013, 3, 3697.	1.7	3
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, 16418-16428.	6.6	28
40	Towards Î²-selectivity in functional estrogen receptor antagonists. Organic and Biomolecular Chemistry, 2012, 10, 7334.	1.5	8
41	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.	1.2	134
42	Structure of micelleâ€bound adrenomedullin: A first step toward the analysis of its interactions with receptors and small molecules. Biopolymers, 2012, 97, 45-53.	1.2	35
43	Rational design of a Tn antigen mimic. Chemical Communications, 2011, 47, 5319.	2.2	24
44	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.	0.9	9
45	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.	1.5	47
46	Potent â€œClickedâ€•MMP2 Inhibitors: Synthesis, Molecular Modeling and Biological Exploration. Organic and Biomolecular Chemistry, 2011, 9, 4587.	1.5	29
47	Multisite-directed inhibitors of protein kinase CK2: new challenges. Molecular and Cellular Biochemistry, 2011, 356, 117-119.	1.4	11
48	Engineering Oâ€Glycosylation Points in Nonâ€extended Peptides: Implications for the Molecular Recognition of Short Tumorâ€Associated Glycopeptides. Chemistry - A European Journal, 2011, 17, 3105-3110.	1.7	19
49	Structural aspects of binding of Î±-linked digalactosides to human galectin-1. Glycobiology, 2011, 21, 1627-1641.	1.3	43
50	In the search of a new prototype in the design of CK2 inhibitors. Arkivoc, 2011, 2011, 54-71.	0.3	2
51	Mimicking Chitin: Chemical Synthesis, Conformational Analysis, and Molecular Recognition of the Î²(1â†'3) Nâ€Acetylchitopentaose Analogue. Chemistry - A European Journal, 2010, 16, 4239-4249.	1.7	7
52	Assessing Carbohydrateâ€“Carbohydrate Interactions by NMR Spectroscopy: The Trisaccharide Epitope from the Marine Sponge Microciona prolifera. ChemBioChem, 2009, 10, 511-519.	1.3	32
53	Selective Human Adenosine A₃ Antagonists based on Pyrido[2,1â€f]purineâ€2,4â€diones: Novel Features of hA₃ Antagonist Binding. ChemMedChem, 2008, 3, 111-119.	1.6	16
54	Smallâ€Molecule Negative Modulators of Adrenomedullin: Design, Synthesis, and 3Dâ€QSAR Study. ChemMedChem, 2008, 3, 1345-1355.	1.6	7

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55	New scaffolds for the design of selective estrogen receptor modulators. Organic and Biomolecular Chemistry, 2008, 6, 3486.	1.5	24
56	Adrenomedullin: a new and promising target for drug discovery. Expert Opinion on Therapeutic Targets, 2006, 10, 303-317.	1.5	22
57	Adrenomedullin: a new target for the design of small molecule modulators with promising pharmacological activities. European Journal of Medicinal Chemistry, 2005, 40, 737-750.	2.6	31
58	Synthesis, Biological Evaluation, and Three-Dimensional Quantitative Structureâ^'Activity Relationship Study of Small-Molecule Positive Modulators of Adrenomedullin. Journal of Medicinal Chemistry, 2005, 48, 4068-4075.	2.9	13
59	ET-18-OCH3 (Edelfosine): A Selective Antitumour Lipid Targeting Apoptosis Through Intracellular Activation of Fas / CD95 Death Receptor. Current Medicinal Chemistry, 2004, 11, 3163-3184.	1.2	113
60	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, 405-414.	1.2	34
61	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, 4471-4482.	2.9	19
62	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, 4439-4452.	2.9	38
63	Development of a New Family of Conformationally Restricted Peptides as Potent Nucleators of Î²-Turns. Design, Synthesis, Structure, and Biological Evaluation of a Î²-Lactam Peptide Analogue of Melanostatin. Journal of the American Chemical Society, 2003, 125, 16243-16260.	6.6	54
64	Guanidinium Receptors as Enantioselective Amino Acid Membrane Carriers. Journal of the American Chemical Society, 2003, 125, 8270-8284.	6.6	113
65	Diastereoselective Reactions in Glycine Templates Containing anent-Ardeemin Fragment. Journal of Organic Chemistry, 2002, 67, 2013-2018.	1.7	7
66	Double aromaticity and anti-aromaticity in small carbon rings. Chemical Communications, 2000, , 1503-1504.	2.2	38
67	HÃ¼ckel and MÃ¶bius aromaticity and trimerous transition state behaviour in the pericyclic reactions of [10], [14], [16] and [18]annulenesâ€Šâ€. Perkin Transactions II RSC, 2000, , 1415-1417.	1.1	36
68	MÃ¶bius aromatics arising from a Cî€†Cî€†C ring component. Chemical Communications, 2000, , 1089-1090.	2.2	26
69	An ab initio and MNDO-d SCFâ€“MO computational study of the extrusion reactions of R2Iâ€“F iodine(III) via dimeric, trimeric and tetrameric transition statesâ€Šâ€. Perkin Transactions II RSC, 2000, , 2158-2161.	1.1	15
70	MÃ¶bius and HÃ¼ckel molecular orbitals arising from Cî€†Cî€†C components in annulene ringsâ€Šâ€. Perkin Transactions II RSC, 2000, , 2372-2377.	1.1	20
71	Fluoridation of heteroaromatic iodonium saltsâ€”experimental evidence supporting theoretical prediction of the selectivity of the process. Chemical Communications, 2000, , 649-650.	2.2	89
72	Twist localisation in single, double and triple twisted MÃ¶bius cyclacenesâ€. Perkin Transactions II RSC, 2000, , 2378-2381.	1.1	27

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73	(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.	1.0	13
74	An ab initio and MNDO-d SCF-MO computational study of stereoelectronic control in extrusion reactions of R2Iâ€“F iodine(III) intermediatesâ€. Journal of the Chemical Society Perkin Transactions II, 1999, , 2707-2714.	0.9	43
75	The preferred conformation of Î±-fluoroamides. Journal of the Chemical Society Perkin Transactions II, 1999, , 2409-2411.	0.9	75
76	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.	1.7	3
77	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.	1.7	27
78	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.	1.0	16