

Sonsoles MartÃ- n SantamarÃ- a

List of Publications by Year in descending order

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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	Chemistry of Lipidâ€¦A: At the Heart of Innate Immunity. <i>Chemistry - A European Journal</i> , 2015, 21, 500-519.	1.7	193
2	Potential anti-inflammatory, anti-adhesive, anti/estrogenic, and angiotensin-converting enzyme inhibitory activities of anthocyanins and their gut metabolites. <i>Genes and Nutrition</i> , 2012, 7, 295-306.	1.2	134
3	Guanidinium Receptors as Enantioselective Amino Acid Membrane Carriers. <i>Journal of the American Chemical Society</i> , 2003, 125, 8270-8284.	6.6	113
4	ET-18-OCH ₃ (Edelfosine): A Selective Antitumour Lipid Targeting Apoptosis Through Intracellular Activation of Fas / CD95 Death Receptor. <i>Current Medicinal Chemistry</i> , 2004, 11, 3163-3184.	1.2	113
5	Fluoridation of heteroaromatic iodonium saltsâ€”experimental evidence supporting theoretical prediction of the selectivity of the process. <i>Chemical Communications</i> , 2000, , 649-650.	2.2	89
6	The preferred conformation of Î±-fluoroamides. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999, , 2409-2411.	0.9	75
7	Computational Approaches to Toll-Like Receptor 4 Modulation. <i>Molecules</i> , 2016, 21, 994.	1.7	69
8	Minimizing the Entropy Penalty for Ligand Binding: Lessons from the Molecular Recognition of the Histo Bloodâ€”Group Antigens by Human Galectinâ€”3. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 7268-7272.	7.2	56
9	Pairing <i>Bacteroides vulgatus</i> LPS Structure with Its Immunomodulatory Effects on Human Cellular Models. <i>ACS Central Science</i> , 2020, 6, 1602-1616.	5.3	55
10	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. <i>Journal of the American Chemical Society</i> , 2003, 125, 16243-16260.	6.6	54
11	Structureâ€”Activity Relationship in Monosaccharide-Based Toll-Like Receptor 4 (TLR4) Antagonists. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 2895-2909.	2.9	51
12	Symmetric dithiodigalactoside: strategic combination of binding studies and detection of selectivity between a plant toxin and human lectins. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 5445.	1.5	47
13	Activation of Human Toll-like Receptor 4 (TLR4)â””Myeloid Differentiation Factor 2 (MD-2) by Hypoacylated Lipopolysaccharide from a Clinical Isolate of <i>Burkholderia cenocepacia</i> . <i>Journal of Biological Chemistry</i> , 2015, 290, 21305-21319.	1.6	47
14	Modulation of CD14 and TLR4â””MDâ””2 Activities by a Synthetic Lipid A Mimetic. <i>ChemBioChem</i> , 2014, 15, 250-258.	1.3	44
15	An ab initio and MNDO-d SCF-MO computational study of stereoelectronic control in extrusion reactions of R ₂ Iâ€”F iodine(III) intermediatesâ€”. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999, , 2707-2714.	0.9	43
16	Structural aspects of binding of Î±-linked digalactosides to human galectin-1. <i>Glycobiology</i> , 2011, 21, 1627-1641.	1.3	43
17	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> , 2018, 9, .	1.8	39
18	Double aromaticity and anti-aromaticity in small carbon rings. <i>Chemical Communications</i> , 2000, , 1503-1504.	2.2	38

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19	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> , 2004, 47, 4439-4452.	2.9	38
20	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> , 2000, , 1415-1417.	1.1	36
21	Di fluorocarbasaccharides: Restoring the exo-anomeric Effect. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 9597-9602.	7.2	36
22	Serine versus Threonine Glycosylation with GalNAc: Unexpected Selectivity in Their Molecular Recognition with Lectins. <i>Chemistry - A European Journal</i> , 2014, 20, 12616-12627.	1.7	36
23	Structure of micelle-bound adrenomedullin: A first step toward the analysis of its interactions with receptors and small molecules. <i>Biopolymers</i> , 2012, 97, 45-53.	1.2	35
24	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> , 2004, 43, 405-414.	1.2	34
25	Assessing Carbohydrate-Carbohydrate Interactions by NMR Spectroscopy: The Trisaccharide Epitope from the Marine Sponge <i>Microciona prolifera</i> . <i>ChemBioChem</i> , 2009, 10, 511-519.	1.3	32
26	Virtual Screening Approaches towards the Discovery of Toll-Like Receptor Modulators. <i>International Journal of Molecular Sciences</i> , 2016, 17, 1508.	1.8	32
27	Adrenomedullin: a new target for the design of small molecule modulators with promising pharmacological activities. <i>European Journal of Medicinal Chemistry</i> , 2005, 40, 737-750.	2.6	31
28	Antibiotic Capture by Bacterial Lipocalins Uncovers an Extracellular Mechanism of Intrinsic Antibiotic Resistance. <i>MBio</i> , 2017, 8, .	1.8	31
29	Potent Clicked-MMP2 Inhibitors: Synthesis, Molecular Modeling and Biological Exploration. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 4587.	1.5	29
30	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> , 2013, 135, 16418-16428.	6.6	28
31	Amphiphilic Guanidinocalixarenes Inhibit Lipopolysaccharide (LPS)- and Lectin-Stimulated Toll-like Receptor 4 (TLR4) Signaling. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 4882-4892.	2.9	28
32	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> , 1997, 62, 6424-6428.	1.7	27
33	Twist localisation in single, double and triple twisted Möbius cyclacenes. <i>Perkin Transactions II RSC</i> , 2000, , 2378-2381.	1.1	27
34	Möbius aromatics arising from a C ₁ C ₁ C ring component. <i>Chemical Communications</i> , 2000, , 1089-1090.	2.2	26
35	Gram-Negative Extremophile Lipopolysaccharides: Promising Source of Inspiration for a New Generation of Endotoxin Antagonists. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 4055-4073.	1.2	26
36	Insights into the key determinants of membrane protein topology enable the identification of new monotopic folds. <i>ELife</i> , 2018, 7, .	2.8	26

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37	Enhancing Potency and Selectivity of a DC-SIGN Glycomimetic Ligand by Fragment-Based Design: Structural Basis. <i>Chemistry - A European Journal</i> , 2019, 25, 14659-14668.	1.7	25
38	New scaffolds for the design of selective estrogen receptor modulators. <i>Organic and Biomolecular Chemistry</i> , 2008, 6, 3486.	1.5	24
39	Rational design of a Tn antigen mimic. <i>Chemical Communications</i> , 2011, 47, 5319.	2.2	24
40	Novel carboxylate-based glycolipids: TLR4 antagonism, MD-2 binding and self-assembly properties. <i>Scientific Reports</i> , 2019, 9, 919.	1.6	24
41	Unveiling Molecular Recognition of Sialoglycans by Human Siglec-10. <i>IScience</i> , 2020, 23, 101231.	1.9	24
42	Adrenomedullin: a new and promising target for drug discovery. <i>Expert Opinion on Therapeutic Targets</i> , 2006, 10, 303-317.	1.5	22
43	Type IV Coupling Proteins as Potential Targets to Control the Dissemination of Antibiotic Resistance. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 201.	1.6	21
44	Understanding the Antibacterial Resistance: Computational Explorations in Bacterial Membranes. <i>ACS Omega</i> , 2021, 6, 6041-6054.	1.6	21
45	Möbius and Hückel molecular orbitals arising from C ₁ C ₁ C components in annulene rings. <i>Perkin Transactions II RSC</i> , 2000, , 2372-2377.	1.1	20
46	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> , 2004, 47, 4471-4482.	2.9	19
47	Engineering O-Glycosylation Points in Non-extended Peptides: Implications for the Molecular Recognition of Short Tumor-Associated Glycopeptides. <i>Chemistry - A European Journal</i> , 2011, 17, 3105-3110.	1.7	19
48	Conformational Selection in Glycomimetics: Human Galectin-1 Only Recognizes <i>syn</i> -Type Conformations of 1,3-Linked Lactose and Its C-Glycosyl Derivative. <i>Chemistry - A European Journal</i> , 2013, 19, 14581-14590.	1.7	19
49	Glycomimetics Targeting Glycosyltransferases: Synthetic, Computational and Structural Studies of Less-Polar Conjugates. <i>Chemistry - A European Journal</i> , 2016, 22, 7215-7224.	1.7	19
50	Molecular bases for the association of FHR-1 with atypical hemolytic uremic syndrome and other diseases. <i>Blood</i> , 2021, 137, 3484-3494.	0.6	17
51	Modulation of Toll-Like Receptor 4. Insights from X-Ray Crystallography and Molecular Modeling. <i>Current Topics in Medicinal Chemistry</i> , 2015, 14, 2672-2683.	1.0	17
52	Regio- and diastereoselective dialkylolation of (4S)-2,4-dimethyl-2,4-dihydro-1H-pirazino[2,1-b]quinazoline-3,6-dione. <i>Tetrahedron</i> , 1997, 53, 16795-16802.	1.0	16
53	Selective Human Adenosine A ₃ Antagonists based on Pyrido[2,1-f]purine-2,4-diones: Novel Features of hA ₃ Antagonist Binding. <i>ChemMedChem</i> , 2008, 3, 111-119.	1.6	16
54	Conformational Plasticity in Glycomimetics: Fluorocarbamethylidopyranosides Mimic the Intrinsic Dynamic Behaviour of Natural Idose Rings. <i>Chemistry - A European Journal</i> , 2015, 21, 10513-10521.	1.7	16

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55	Insights into real-time chemical processes in a calcium sensor protein-directed dynamic library. <i>Nature Communications</i> , 2019, 10, 2798.	5.8	16
56	Characterisation of the Dynamic Interactions between Complex N-Glycans and Human CD22. <i>ChemBioChem</i> , 2020, 21, 129-140.	1.3	16
57	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. <i>Perkin Transactions II RSC</i> , 2000, , 2158-2161.	1.1	15
58	New Therapeutic Strategies for Osteoarthritis by Targeting Sialic Acid Receptors. <i>Biomolecules</i> , 2020, 10, 637.	1.8	15
59	(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> , 1999, 55, 1755-1762.	1.0	13
60	Synthesis, Biological Evaluation, and Three-Dimensional Quantitative Structure-Activity Relationship Study of Small-Molecule Positive Modulators of Adrenomedullin. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 4068-4075.	2.9	13
61	Glycolipid-based TLR4 Modulators and Fluorescent Probes: Rational Design, Synthesis, and Biological Properties. <i>Chemical Biology and Drug Design</i> , 2016, 88, 217-229.	1.5	13
62	Synthetic Glycolipids as Molecular Vaccine Adjuvants: Mechanism of Action in Human Cells and In Vivo Activity. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 12261-12272.	2.9	13
63	Full-Atom Model of the Agonist LPS-Bound Toll-Like Receptor 4 Dimer in a Membrane Environment. <i>Chemistry - A European Journal</i> , 2021, 27, 15406-15425.	1.7	12
64	Multisite-directed inhibitors of protein kinase CK2: new challenges. <i>Molecular and Cellular Biochemistry</i> , 2011, 356, 117-119.	1.4	11
65	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> , 2016, 196, 2309-2318.	0.4	10
66	Molecular Insight into the Regulation of Vimentin by Cysteine Modifications and Zinc Binding. <i>Antioxidants</i> , 2021, 10, 1039.	2.2	10
67	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> , 2011, 84, 49-64.	0.9	9
68	Bradyrhizobium 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> , 2018, 9, 1888.	2.2	9
69	Towards β^2 -selectivity in functional estrogen receptor antagonists. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 7334.	1.5	8
70	6-Shogaol (enexasogol) treatment improves experimental knee osteoarthritis exerting a pleiotropic effect over immune innate signalling responses in chondrocytes. <i>British Journal of Pharmacology</i> , 2022, 179, 5089-5108.	2.7	8
71	Diastereoselective Reactions in Glycine Templates Containing anent-Ardeemin Fragment. <i>Journal of Organic Chemistry</i> , 2002, 67, 2013-2018.	1.7	7
72	Small-Molecule Negative Modulators of Adrenomedullin: Design, Synthesis, and 3D-QSAR Study. <i>ChemMedChem</i> , 2008, 3, 1345-1355.	1.6	7

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73	Mimicking Chitin: Chemical Synthesis, Conformational Analysis, and Molecular Recognition of the β -D-GlcNAc6S Acetylchitopentaose Analogue. <i>Chemistry - A European Journal</i> , 2010, 16, 4239-4249.	1.7	7
74	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> , 1999, 64, 7233-7235.	1.7	3
75	New clicked full agonists of the estrogen receptor β . <i>RSC Advances</i> , 2013, 3, 3697.	1.7	3
76	Abacavir Increases Purinergic P2X7 Receptor Activation by ATP: Does a Pro-inflammatory Synergism Underlie Its Cardiovascular Toxicity?. <i>Frontiers in Pharmacology</i> , 2021, 12, 613449.	1.6	2
77	In the search of a new prototype in the design of CK2 inhibitors. <i>Arkivoc</i> , 2011, 2011, 54-71.	0.3	2
78	Chemistry of Lipid A: At the Heart of Innate Immunity. <i>Chemistry - A European Journal</i> , 2015, 21, 477-477.	1.7	1