Nuria E Campillo

List of Publications by Citations

91 papers	2,197 citations	28 h-index	43 g-index
96 ext. papers	2,517 ext. citations	5.1 avg, IF	4.71 L-index

#	Paper	IF	Citations
91	COVID-19: Drug Targets and Potential Treatments. *Journal of Medicinal Chemistry*, **2020**, 63, 12359-12386	8.3	207
90	Tacrine-melatonin hybrids as multifunctional agents for Alzheimer's disease, with cholinergic, antioxidant, and neuroprotective properties. *ChemMedChem*, **2009**, 4, 828-41	3.7	132
89	Plant-based heterologous expression of Mal d 2, a thaumatin-like protein and allergen of apple (Malus domestica), and its characterization as an antifungal protein. *Journal of Molecular Biology*, **2003**, 329, 721-30	6.5	121
88	Directed mutagenesis alters the stereochemistry of catalysis by isolated ketoreductase domains from the erythromycin polyketide synthase. *Chemistry and Biology*, **2006**, 13, 277-85		89
87	Exploring the binding sites of glycogen synthase kinase 3. Identification and characterization of allosteric modulation cavities. *Journal of Medicinal Chemistry*, **2011**, 54, 8461-70	8.3	78
86	Homology models of the cannabinoid CB1 and CB2 receptors. A docking analysis study. *European Journal of Medicinal Chemistry*, **2005**, 40, 75-83	6.8	72
85	5-imino-1,2,4-thiadiazoles: first small molecules as substrate competitive inhibitors of glycogen synthase kinase 3. *Journal of Medicinal Chemistry*, **2012**, 55, 1645-61	8.3	61
84	Tau-Centric Multitarget Approach for Alzheimer's Disease: Development of First-in-Class Dual Glycogen Synthase Kinase 3 and Tau-Aggregation Inhibitors. *Journal of Medicinal Chemistry*, **2018**, 61, 7640-7656	8.3	53
83	Neuroprotective efficacy of quinazoline type phosphodiesterase 7 inhibitors in cellular cultures and experimental stroke model. *European Journal of Medicinal Chemistry*, **2012**, 47, 175-85	6.8	53
82	Synthesis, structural analysis, and biological evaluation of thioxoquinazoline derivatives as phosphodiesterase 7 inhibitors. *ChemMedChem*, **2009**, 4, 866-76	3.7	53
81	Elucidation of the molecular recognition of bacterial cell wall by modular pneumococcal phage endolysin CPL-1. *Journal of Biological Chemistry*, **2007**, 282, 24990-9	5.4	53
80	The origin of the serum resistance associated (SRA) gene and a model of the structure of the SRA polypeptide from Trypanosoma brucei rhodesiense. *Molecular and Biochemical Parasitology*, **2003**, 127, 79-84	1.9	46
79	Chagas disease: progress and new perspectives. *Current Medicinal Chemistry*, **2010**, 17, 423-52	4.3	45
78	Effect of phosphodiesterase 7 (PDE7) inhibitors in experimental autoimmune encephalomyelitis mice. Discovery of a new chemically diverse family of compounds. *Journal of Medicinal Chemistry*, **2012**, 55, 3274-84	8.3	43
77	Crystal structure of CbpF, a bifunctional choline-binding protein and autolysis regulator from Streptococcus pneumoniae. *EMBO Reports*, **2009**, 10, 246-51	6.5	43
76	p-Coumaric acid decarboxylase from Lactobacillus plantarum: structural insights into the active site and decarboxylation catalytic mechanism. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 1662-76	4.2	39
75	PDE7 inhibitors as new drugs for neurological and inflammatory disorders. *Expert Opinion on Therapeutic Patents*, **2008**, 18, 1127-1139	6.8	37

74	Subtly Modulating Glycogen Synthase Kinase 3 Allosteric Inhibitor Development and Their Potential for the Treatment of Chronic Diseases. *Journal of Medicinal Chemistry*, **2017**, 60, 4983-5001	8.3	36
73	Hybridizing Feature Selection and Feature Learning Approaches in QSAR Modeling for Drug Discovery. *Scientific Reports*, **2017**, 7, 2403	4.9	36
72	From dual binding site acetylcholinesterase inhibitors to allosteric modulators: A new avenue for disease-modifying drugs in Alzheimer's disease. *European Journal of Medicinal Chemistry*, **2017**, 139, 773-791	6.8	35
71	Artificial Neural Networks in ADMET Modeling: Prediction of BloodBrain Barrier Permeation. *QSAR and Combinatorial Science*, **2008**, 27, 586-594		35
70	Cpl-7, a lysozyme encoded by a pneumococcal bacteriophage with a novel cell wall-binding motif. *Journal of Biological Chemistry*, **2010**, 285, 33184-33196	5.4	34
69	Docking, synthesis, and NMR studies of mannosyl trisaccharide ligands for DC-SIGN lectin. *Organic and Biomolecular Chemistry*, **2008**, 6, 2743-54	3.9	34
68	Cannabinoid agonists showing BuChE inhibition as potential therapeutic agents for Alzheimer's disease. *European Journal of Medicinal Chemistry*, **2014**, 73, 56-72	6.8	33
67	In vivo anti-Chagas vinylthio-, vinylsulfinyl-, and vinylsulfonylbenzofuroxan derivatives. *Journal of Medicinal Chemistry*, **2007**, 50, 6004-15	8.3	32
66	Development of second generation amidinohydrazones, thio- and semicarbazones as Trypanosoma cruzi-inhibitors bearing benzofuroxan and benzimidazole 1,3-dioxide core scaffolds. *MedChemComm*, **2010**, 1, 216	5	30
65	An iterative structure-assisted approach to sequence alignment and comparative modeling **1999**, 37, 55-60		29
64	The value of selected in vitro and in silico methods to predict acute oral toxicity in a regulatory context: results from the European Project ACuteTox. *Toxicology in Vitro*, **2013**, 27, 1357-76	3.6	28
63	Interference of the complex between NCS-1 and Ric8a with phenothiazines regulates synaptic function and is an approach for fragile X syndrome. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E999-E1008	11.5	26
62	Cannabinoid system in neurodegeneration: new perspectives in Alzheimer's disease. *Mini-Reviews in Medicinal Chemistry*, **2009**, 9, 539-59	3.2	26
61	Ring Strain and Hydrogen Bond Acidity. *Journal of Organic Chemistry*, **1998**, 63, 7759-7763	4.2	25
60	Neural computational prediction of oral drug absorption based on CODES 2D descriptors. *European Journal of Medicinal Chemistry*, **2010**, 45, 930-40	6.8	24
59	Identification of new allosteric sites and modulators of AChE through computational and experimental tools. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2018**, 33, 1034-1047	5.6	21
58	Medicinal and Biological Chemistry (MBC) Library: An Efficient Source of New Hits. *Journal of Chemical Information and Modeling*, **2017**, 57, 2143-2151	6.1	20
57	Cannabinoid derivatives exert a potent anti-myeloma activity both in vitro and in vivo. *International Journal of Cancer*, **2017**, 140, 674-685	7.5	20

56	QSAR Classification Models for Predicting the Activity of Inhibitors of Beta-Secretase (BACE1) Associated with Alzheimer's Disease. *Scientific Reports*, **2019**, 9, 9102	4.9	19
55	Design, synthesis, and evaluation of potential inhibitors of nitric oxide synthase. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 6193-206	3.4	19
54	Active-site-mutagenesis study of rat liver betaine-homocysteine S-methyltransferase. *Biochemical Journal*, **2003**, 370, 945-52	3.8	19
53	Highly potent and selective aryl-1,2,3-triazolyl benzylpiperidine inhibitors toward butyrylcholinesterase in Alzheimer's disease. *Bioorganic and Medicinal Chemistry*, **2019**, 27, 931-943	3.4	19
52	Identification in silico and experimental validation of novel phosphodiesterase 7 inhibitors with efficacy in experimental autoimmune encephalomyelitis mice. *ACS Chemical Neuroscience*, **2012**, 3, 793-803	5.7	18
51	Novel arylpyrazino[2,3-c][1,2,6]thiadiazine 2,2-dioxides as inhibitors of platelet aggregation. 1. Synthesis and pharmacological evaluation. *Journal of Medicinal Chemistry*, **1999**, 42, 1698-704	8.3	18
50	From Bitopic Inhibitors to Multitarget Drugs for the Future Treatment of Alzheimer's Disease. *Current Medicinal Chemistry*, **2015**, 22, 3789-806	4.3	18
49	Novel bronchodilators: synthesis, transamination reactions, and pharmacology of a series of pyrazino[2,3-c][1,2,6]thiadiazine 2, 2-dioxides. *Journal of Medicinal Chemistry*, **2000**, 43, 4219-27	8.3	15
48	Mutagenicity of N-oxide containing heterocycles and related compounds: experimental and theoretical studies. *Current Topics in Medicinal Chemistry*, **2014**, 14, 1374-87	3	15
47	Leucine rich repeat kinase 2 (LRRK2) inhibitors based on indolinone scaffold: Potential pro-neurogenic agents. *European Journal of Medicinal Chemistry*, **2017**, 138, 328-342	6.8	14
46	Multitarget cannabinoids as novel strategy for Alzheimer disease. *Current Alzheimer Research*, **2013** , 10, 229-39	3	14
45	Chameleon-like behavior of indolylpiperidines in complex with cholinesterases targets: Potent butyrylcholinesterase inhibitors. *European Journal of Medicinal Chemistry*, **2018**, 145, 431-444	6.8	13
44	The role of cofactor binding in tryptophan accessibility and conformational stability of His-tagged D-amino acid oxidase from Trigonopsis variabilis. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2007**, 1774, 556-65	4	13
43	Unravelling the structure of the pneumococcal autolytic lysozyme. *Biochemical Journal*, **2005**, 391, 41-9	3.8	13
42	Cyclic Nucleotide-Specific Phosphodiesterases as Potential Drug Targets for Anti-Leishmania Therapy. *Antimicrobial Agents and Chemotherapy*, **2018**, 62,	5.9	12
41	Indazolylketones as new multitarget cannabinoid drugs. *European Journal of Medicinal Chemistry*, **2019**, 166, 90-107	6.8	12
40	Amidines bearing benzofuroxan or benzimidazole 1,3-dioxide core scaffolds as Trypanosoma cruzi-inhibitors: structural basis for their interactions with cruzipain. *MedChemComm*, **2012**, 3, 90-101	5	11
39	Solvent effect on the tautomerism of 4-aminopyrazino[2,3-c][1,2,6]thiadiazine 2,2-dioxides. *Journal of the Chemical Society Perkin Transactions II*, **1998**, 1889-1892		11

38	Glycogen synthase kinase 3 (GSK-3) inhibitors: a patent update (2016-2019). *Expert Opinion on Therapeutic Patents*, **2020**, 30, 863-872	6.8	11
37	Innovative Therapeutic Potential of Cannabinoid Receptors as Targets in Alzheimer's Disease and Less Well-Known Diseases. *Current Medicinal Chemistry*, **2019**, 26, 3300-3340	4.3	9
36	Host-Directed FDA-Approved Drugs with Antiviral Activity against SARS-CoV-2 Identified by Hierarchical In Silico/In Vitro Screening Methods. *Pharmaceuticals*, **2021**, 14,	5.2	9
35	Novel Imidazo[4,5-c][1,2,6]thiadiazine 2,2-dioxides as antiproliferative trypanosoma cruzi drugs: Computational screening from neural network, synthesis and in vivo biological properties. *European Journal of Medicinal Chemistry*, **2017**, 136, 223-234	6.8	8
34	On the Reactivity of 1H-Pyrazino[2,3-c][1,2,6]thiadiazine 2,2-Dioxide and Derivatives: Nucleophilic Substitution, Amination, Aldol-Type Condensation, Oxidation, and Hydrolysis. *Helvetica Chimica Acta*, **2003**, 86, 139-146	2	8
33	Novel arylpyrazino[2,3-c][1,2,6]thiadiazine 2,2-dioxides as platelet aggregation inhibitors. 2. Optimization by quantitative structure-activity relationships. *Journal of Medicinal Chemistry*, **1999**, 42, 3279-88	8.3	8
32	Computer-aided molecular design of pyrazolotriazines targeting glycogen synthase kinase 3. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2019**, 34, 87-96	5.6	8
31	New applications for known drugs: Human glycogen synthase kinase 3 inhibitors as modulators of Aspergillus fumigatus growth. *European Journal of Medicinal Chemistry*, **2016**, 116, 281-289	6.8	7
30	Towards discovery of new leishmanicidal scaffolds able to inhibit GSK-3. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2020**, 35, 199-210	5.6	7
29	Identification of potential inhibitors of protein-protein interaction useful to fight against Ebola and other highly pathogenic viruses. *Antiviral Research*, **2021**, 186, 105011	10.8	7
28	Synthesis and nematocide activity of S-glycopyranosyl-6,7-diarylthiolumazines. *Bioorganic and Medicinal Chemistry*, **2004**, 12, 4431-7	3.4	6
27	QSAR Modelling to Identify LRRK2 Inhibitors for Parkinson's Disease. *Journal of Integrative Bioinformatics*, **2019**, 16,	3.8	6
26	Identification of Niemann-Pick C1 protein as a potential novel SARS-CoV-2 intracellular target. *Antiviral Research*, **2021**, 194, 105167	10.8	6
25	Deciphering the Inhibition of the Neuronal Calcium Sensor 1 and the Guanine Exchange Factor Ric8a with a Small Phenothiazine Molecule for the Rational Generation of Therapeutic Synapse Function Regulators. *Journal of Medicinal Chemistry*, **2018**, 61, 5910-5921	8.3	5
24	Dissimilar interaction of CB1/CB2 with lipid bilayers as revealed by molecular dynamics simulation. *Physical Chemistry Chemical Physics*, **2011**, 13, 3660-8	3.6	5
23	A study of peculiar tautomerism of pyrido[2,3-c][1,2,6]thiadiazine 2,2-dioxide system. *Computational and Theoretical Chemistry*, **2004**, 678, 83-89		5
22	Unconventional Alkoxylation of Pyrazino[2,3-c][1,2,6]thiadiazine 2,2-Dioxides Mediated by N-Halosuccinimides. *European Journal of Organic Chemistry*, **2002**, 2002, 2109	3.2	5
21	A Novel Tetracyclic System Containing the 1,2,6-Thiadiazine Ring: Synthesis, Structural Assignment and Tautomeric Studies. *Heterocycles*, **1998**, 48, 1833	0.8	5

20	Activation of the Cannabinoid Type 2 Receptor by a Novel Indazole Derivative Normalizes the Survival Pattern of Lymphoblasts from Patients with Late-Onset Alzheimer's Disease. *CNS Drugs*, **2018**, 32, 579-591	6.7	4
19	Discovery of novel PDE4A inhibitors as potential agents against schistosomiasis. *Future Medicinal Chemistry*, **2019**, 11, 1703-1720	4.1	4
18	Unraveling phosphodiesterase surfaces. Identification of phosphodiesterase 7 allosteric modulation cavities. *European Journal of Medicinal Chemistry*, **2013**, 70, 781-8	6.8	4
17	Homology modelling and active-site-mutagenesis study of the catalytic domain of the pneumococcal phosphorylcholine esterase. *Bioorganic and Medicinal Chemistry*, **2005**, 13, 6404-13	3.4	4
16	COVID-19 Vaccine Race: Analysis of Age-Dependent Immune Responses against SARS-CoV-2 Indicates that more than Just One Strategy May Be Needed. *Current Medicinal Chemistry*, **2021**, 28, 3964-3979	4.3	4
15	Artificial Neural Networks Based on CODES Descriptors in Pharmacology: Identification of Novel Trypanocidal Drugs against Chagas Disease. *Current Computer-Aided Drug Design*, **2013**, 9, 130-140	1.4	4
14	QSAR Modelling for Drug Discovery: Predicting the Activity of LRRK2 Inhibitors for Parkinson Disease Using Cheminformatics Approaches. *Advances in Intelligent Systems and Computing*, **2019**, 63-70	0.4	3
13	Interaction studies between human alpha-tocopherol transfer protein and nitric oxide donor tocopherol analogues with LDL-protective activity. *Bioorganic and Medicinal Chemistry*, **2009**, 17, 8143-8	3.4	3
12	Novel bronchodilators in the treatment of asthma and COPD. *Expert Opinion on Therapeutic Patents* , **2002**, 12, 53-63	6.8	3
11	Targeting Cannabinoid Receptor Activation and BACE-1 Activity Counteracts TgAPP Mice Memory Impairment and Alzheimer's Disease Lymphoblast Alterations. *Molecular Neurobiology*, **2020**, 57, 1938-1951	6.2	3
10	Therapeutic approaches for the future treatment of Fragile X. *Current Opinion in Behavioral Sciences*, **2015**, 4, 6-21	4	2
9	Crystal structure of CbpF, a bifunctional choline-binding protein and autolysis regulator from Streptococcus pneumoniae. *EMBO Reports*, **2009**, 10, 413-413	6.5	2
8	The Tautomerism of 5-Amino-3-oxo-1,2,4-thiadiazole: An Experimental and Theoretical Study. *European Journal of Organic Chemistry*, **2007**, 2007, 5603-5608	3.2	2
7	Naphthoquinone as a New Chemical Scaffold for Leishmanicidal Inhibitors of Leishmania GSK-3. *Biomedicines*, **2022**, 10, 1136	4.8	2
6	Deciphering the enzymatic target of a new family of antischistosomal agents bearing a quinazoline scaffold using complementary computational tools. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2020**, 35, 511-523	5.6	1
5	Artificial Neural Networks Based on CODES Descriptors in Pharmacology: Identification of Novel Trypanocidal Drugs against Chagas Disease. *Current Computer-Aided Drug Design*, **2013**, 9, 130-140	1.4	1
4	Phosphoribosyltransferase superfamily: A comparative structural analysis. *Journal of Molecular Modeling*, **2001**, 7, 80-89	2	1
3	Chapter 7:In silico Tools for Target Identification and Drug Molecular Docking in Leishmania. *RSC Drug Discovery Series*, **2017**, 130-152	0.6	1

2	New cannabinoid receptor antagonists as pharmacological tool. *Bioorganic and Medicinal Chemistry*, **2020**, 28, 115672	3.4	1
1	AI in drug development: a multidisciplinary perspective. *Molecular Diversity*, **2021**, 25, 1461-1479	3.1	1