Rosa Maria Vitale

List of Publications by Year in descending order

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71 papers 1,790 citations

257101 24 h-index 276539 41 g-index

76 all docs 76 docs citations

76 times ranked 2757 citing authors

#	Article	IF	CITATIONS
1	Carbonic Anhydrase Inhibitors:  X-ray and Molecular Modeling Study for the Interaction of a Fluorescent Antitumor Sulfonamide with Isozyme II and IX. Journal of the American Chemical Society, 2006, 128, 8329-8335.	6.6	200
2	Carbonic Anhydrase Inhibitors: Hypoxia-Activatable Sulfonamides Incorporating Disulfide Bonds that Target the Tumor-Associated Isoform IXâ€. Journal of Medicinal Chemistry, 2006, 49, 5544-5551.	2.9	100
3	Structure, conformation and biological activity of a novel lipodepsipeptide from Pseudomonas corrugata: cormycin A1. Biochemical Journal, 2004, 384, 25-36.	1.7	86
4	Preclinical Development of a Novel Class of CXCR4 Antagonist Impairing Solid Tumors Growth and Metastases. PLoS ONE, 2013, 8, e74548.	1.1	76
5	Rare Casbane Diterpenoids from the Hainan Soft Coral <i>Sinularia depressa</i> . Journal of Natural Products, 2010, 73, 133-138.	1.5	70
6	Insights into the Structural Basis of the GADD45 \hat{i}^2 -mediated Inactivation of the JNK Kinase, MKK7/JNKK2. Journal of Biological Chemistry, 2007, 282, 19029-19041.	1.6	66
7	Structure–activity relationships and molecular modelling of new 5-arylidene-4-thiazolidinone derivatives as aldose reductase inhibitors and potential anti-inflammatory agents. European Journal of Medicinal Chemistry, 2014, 81, 1-14.	2.6	63
8	Identification and characterization of phytocannabinoids as novel dual PPARα \hat{I}^3 agonists by a computational and in vitro experimental approach. Biochimica Et Biophysica Acta - General Subjects, 2019, 1863, 586-597.	1.1	55
9	The Endocannabinoid System and PPARs: Focus on Their Signalling Crosstalk, Action and Transcriptional Regulation. Cells, 2021, 10, 586.	1.8	55
10	Minimalist Hybrid Ligand/Receptor-Based Pharmacophore Model for CXCR4 Applied to a Small-Library of Marine Natural Products Led to the Identification of Phidianidine A as a New CXCR4 Ligand Exhibiting Antagonist Activity. ACS Chemical Biology, 2013, 8, 2762-2770.	1.6	54
11	Gadd $45\hat{l}^2$ forms a Homodimeric Complex that Binds Tightly to MKK7. Journal of Molecular Biology, 2008, 378, 97-111.	2.0	49
12	Carbonic Anhydrase Inhibitors: Bioreductive Nitro-Containing Sulfonamides with Selectivity for Targeting the Tumor Associated Isoforms IX and XII. Journal of Medicinal Chemistry, 2008, 51, 3230-3237.	2.9	49
13	Nitroxyl Peptides as Catalysts of Enantioselective Oxidations. Chemistry - A European Journal, 2002, 8, 84-93.	1.7	48
14	Probing the Dimeric Structure of Porcine Aminoacylase 1 by Mass Spectrometric and Modeling Procedures. Biochemistry, 2003, 42, 4430-4443.	1.2	47
15	Avarol derivatives as competitive AChE inhibitors, non hepatotoxic and neuroprotective agents for Alzheimer's disease. European Journal of Medicinal Chemistry, 2016, 122, 326-338.	2.6	43
16	Beneficial Effects of Akkermansia muciniphila Are Not Associated with Major Changes in the Circulating Endocannabinoidome but Linked to Higher Mono-Palmitoyl-Glycerol Levels as New PPARα Agonists. Cells, 2021, 10, 185.	1.8	43
17	Molecular modeling study for the binding of zonisamide and topiramate to the human mitochondrial carbonic anhydrase isoform VA. Bioorganic and Medicinal Chemistry, 2007, 15, 4152-4158.	1.4	37
18	N-Oleoyl-glycine reduces nicotine reward and withdrawal in mice. Neuropharmacology, 2019, 148, 320-331.	2.0	37

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19	The (Poly)Pharmacology of Cannabidiol in Neurological and Neuropsychiatric Disorders: Molecular Mechanisms and Targets. International Journal of Molecular Sciences, 2021, 22, 4876.	1.8	37
20	Structure and Absolute Stereochemistry of Syphonoside, a Unique Macrocyclic Glycoterpenoid from Marine Organisms. Journal of Organic Chemistry, 2007, 72, 5625-5630.	1.7	31
21	Structural Analysis of BldR from Sulfolobus solfataricus Provides Insights into the Molecular Basis of Transcriptional Activation in Archaea by MarR Family Proteins. Journal of Molecular Biology, 2009, 388, 559-569.	2.0	31
22	Structural Features of Distinctin Affecting Peptide Biological and Biochemical Properties. Biochemistry, 2008, 47, 7888-7899.	1.2	29
23	Converting the Highly Amyloidogenic Human Calcitonin into a Powerful Fibril Inhibitor by Three-dimensional Structure Homology with a Non-amyloidogenic Analogue. Journal of Biological Chemistry, 2011, 286, 2707-2718.	1.6	29
24	Tetrahydroisoquinoline-Derived Urea and 2,5-Diketopiperazine Derivatives as Selective Antagonists of the Transient Receptor Potential Melastatin 8 (TRPM8) Channel Receptor and Antiprostate Cancer Agents. Journal of Medicinal Chemistry, 2016, 59, 5661-5683.	2.9	29
25	Fishing for Targets of Alien Metabolites: A Novel Peroxisome Proliferator-Activated Receptor (PPAR) Agonist from a Marine Pest. Marine Drugs, 2018, 16, 431.	2.2	27
26	Air oxidation method employed for the disulfide bond formation of natural and synthetic peptides. Amino Acids, 2015, 47, 1507-1515.	1.2	24
27	Structural features of the inactive and active states of the melanin-concentrating hormone receptors: Insights from molecular simulations. Proteins: Structure, Function and Bioinformatics, 2004, 56, 430-448.	1.5	22
28	Molecular modeling and functional characterization of the monomeric primase–polymerase domain from the <i>Sulfolobusâ€∫solfataricus</i>) plasmid pIT3. FEBS Journal, 2008, 275, 4389-4402.	2.2	21
29	Carbonic Anhydrase Inhibitors. Comparison of Aliphatic Sulfamate/Bis-sulfamate Adducts with Isozymes II and IX as a Platform for Designing Tight-Binding, More Isoform-Selective Inhibitors. Journal of Medicinal Chemistry, 2009, 52, 5990-5998.	2.9	21
30	Structure–activity relationships of fraxamoside as an unusual xanthine oxidase inhibitor. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 345-354.	2.5	21
31	A SPR strategy for high-throughput ligand screenings based on synthetic peptides mimicking a selected subdomain of the target protein: A proof of concept on HER2 receptor. Bioorganic and Medicinal Chemistry, 2009, 17, 7015-7020.	1.4	20
32	Identification and Characterization of Cannabimovone, a Cannabinoid from Cannabis sativa, as a Novel PPARÎ ³ Agonist via a Combined Computational and Functional Study. Molecules, 2020, 25, 1119.	1.7	20
33	Cannabitwinol, a Dimeric Phytocannabinoid from Hemp, <i>Cannabis sativa</i> L., Is a Selective Thermo-TRP Modulator. Journal of Natural Products, 2020, 83, 2727-2736.	1.5	19
34	N-palmitoyl-D-glucosamine, A Natural Monosaccharide-Based Glycolipid, Inhibits TLR4 and Prevents LPS-Induced Inflammation and Neuropathic Pain in Mice. International Journal of Molecular Sciences, 2021, 22, 1491.	1.8	19
35	Ac10 c: a medium-ring, cycloaliphatic $\hat{Cl}_{\pm},\hat{l}_{\pm}$ -disubstituted glycine. Incorporation into model peptides and preferred conformation. Chemical Biology and Drug Design, 2001, 57, 307-315.	1.2	16
36	X-ray Diffraction Analysis and Conformational Energy Computations of \hat{I}^2 -Turn and 310-Helical Peptides Based on \hat{I}^2 -Amino Acids with an Olefinic Side Chain. Implications for Ring-Closing Metathesis. Macromolecules, 2002, 35, 4204-4209.	2.2	16

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37	Interactions of GFAP with ceftriaxone and phenytoin: SRCD and molecular docking and dynamic simulation. Biochimica Et Biophysica Acta - General Subjects, 2016, 1860, 2239-2248.	1.1	15
38	Neuroglobin–prion protein interaction: what's the function?. Journal of Peptide Science, 2011, 17, 387-391.	0.8	14
39	<i>In Silico</i> Identification and Experimental Validation of Novel Anti-Alzheimer's Multitargeted Ligands from a Marine Source Featuring a "2-Aminoimidazole plus Aromatic Group―Scaffold. ACS Chemical Neuroscience, 2018, 9, 1290-1303.	1.7	14
40	Patatin-like lipolytic acyl hydrolases and galactolipid metabolism in marine diatoms of the genus Pseudo-nitzschia. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2019, 1864, 181-190.	1.2	13
41	2-Pentadecyl-2-oxazoline ameliorates memory impairment and depression-like behaviour in neuropathic mice: possible role of adrenergic alpha2- and H3 histamine autoreceptors. Molecular Brain, 2021, 14, 28.	1.3	13
42	Elongation of the Hydrophobic Chain as a Molecular Switch: Discovery of Capsaicin Derivatives and Endogenous Lipids as Potent Transient Receptor Potential Vanilloid Channel 2 Antagonists. Journal of Medicinal Chemistry, 2018, 61, 8255-8281.	2.9	11
43	In Silico Identification and Experimental Validation of (â^')-Muqubilin A, a Marine Norterpene Peroxide, as PPARα/γ-RXRα Agonist and RARα Positive Allosteric Modulator. Marine Drugs, 2019, 17, 110.	2.2	11
44	Design, Synthesis and In Vitro Experimental Validation of Novel TRPV4 Antagonists Inspired by Labdane Diterpenes. Marine Drugs, 2020, 18, 519.	2.2	11
45	Biosynthesis of the Novel Endogenous 15-Lipoxygenase Metabolites N-13-Hydroxy-octodecadienoyl-ethanolamine and 13-Hydroxy-octodecadienoyl-glycerol by Human Neutrophils and Eosinophils. Cells, 2021, 10, 2322.	1.8	11
46	Potent Cytotoxic Analogs of Amphidinolides from the Atlantic Octocoral Stragulum bicolor. Marine Drugs, 2019, 17, 58.	2.2	10
47	Conformational Features of Human Melanin-Concentrating Hormone: An NMR and Computational Analysis. ChemBioChem, 2003, 4, 73-81.	1.3	8
48	Structural characterization of the functional regions in the archaeal protein Sso7d. Proteins: Structure, Function and Bioinformatics, 2007, 67, 189-197.	1.5	8
49	Identification and Characterization of Cannabidiol as an OX1R Antagonist by Computational and In Vitro Functional Validation. Biomolecules, 2021, 11, 1134.	1.8	8
50	Cî±-Methyl,Cî±-allylglycine (Mag) Homooligomers. Macromolecules, 2001, 34, 4263-4269.	2.2	6
51	Chaperone-like effect of ceftriaxone on HEWL aggregation: A spectroscopic and computational study. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 1317-1326.	1.1	6
52	Identification of the hydantoin alkaloids parazoanthines as novel CXCR4 antagonists by computational and in vitro functional characterization. Bioorganic Chemistry, 2020, 105, 104337.	2.0	4
53	The Combined Effect of Branching and Elongation on the Bioactivity Profile of Phytocannabinoids. Part I: Thermo-TRPs. Biomedicines, 2021, 9, 1070.	1.4	3
54	Spectroscopy data of ceftriaxone-lysozyme interaction and computational studies. Data in Brief, 2018, 18, 1808-1818.	0.5	2

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55	FAAH-Catalyzed C–C Bond Cleavage of a New Multitarget Analgesic Drug. ACS Chemical Neuroscience, 2019, 10, 424-437.	1.7	2
56	Discovery of a Remarkable Methyl Shift Effect in the Vanilloid Activity of Triterpene Amides. Journal of Natural Products, 2020, 83, 3476-3481.	1.5	2
57	Chapter 6. Natural Compounds and Synthetic Drugs Targeting the Ionotropic Cannabinoid Members of Transient Receptor Potential (TRP) Channels. RSC Drug Discovery Series, 2020, , 201-300.	0.2	2
58	Synthetic peptides mimicking the interleukin-6/gp 130 interaction: a two-helix bundle system. Design and conformational studies. Journal of Peptide Science, 2003, 9, 90-105.	0.8	1
59	Site-directed mutagenesis and molecular modelling studies show the role of Asp82 and cysteines in rat acylase 1, a member of the M20 family. Biochemical and Biophysical Research Communications, 2005, 330, 540-546.	1.0	1
60	Gadd $45\hat{l}^2$ dimerization does not affect MKK7 binding. Advances in Experimental Medicine and Biology, 2009, 611, 367-368.	0.8	1
61	Allyl-Based, CÎ \pm -Methylated Î \pm -Amino Acids in the Side-Chain to Side-Chain Ring-Closing Metathesis Reaction of Î 2 -Turn/310-Helical Peptides. , 2001, , 371-372.		1
62	Computational Methods in Mass Spectrometry-Based Protein 3D Studies. , 2011, , .		0
63	332 A New CXCR4 Receptor Antagonist – Effects on Cell Growth and Tumor Microenvironment in a Glioma Model. European Journal of Cancer, 2012, 48, S81.	1.3	0
64	P01.16 * MICROGLIA/MACROPHAGES AS CELLULAR TARGET OF NOVEL CXCR4 ANTAGONIST IN A GLIOMA MODEL. Neuro-Oncology, 2014, 16, ii30-ii30.	0.6	0
65	TOAC Peptides as Catalysts of Enantioselective Oxidations. , 2001, , 1065-1066.		0
66	Synthesis and NMR Characterization of Melanin-Concentrating Hormone., 2001,, 710-711.		0
67	Structural characterization of functionalized \hat{l}^2 -cyclodestrins. Acta Crystallographica Section A: Foundations and Advances, 2005, 61, c315-c315.	0.3	0
68	Self-association regions in the CARD of Bcl-10. Advances in Experimental Medicine and Biology, 2009, 611, 569-570.	0.8	0
69	Abstract 394: Rapid and persistant neutrophil mobilization by novel CXCR4 peptide antagonists. , 2011, , .		0
70	Abstract 4645: Preclinical development of RFF-1, a novel rational designed CXCL12 mimetic drug. , 2012, , .		0
71	Self-Inclusion Complexes of Monofunctionalized Beta-Cyclodextrins as Host–Guest Interaction Model Systems and Simple and Sensitive Testbeds for Implicit Solvation Methods. , 2015, , 271-296.		0