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List of Publications by Year
in descending order

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62 papers	1,806 citations	361413 20 h-index	276875 41 g-index
64 all docs	64 docs citations	64 times ranked	2830 citing authors

#	Article	IF	Citations
1	Computational Molecular Characterization of the Interaction of Acetylcholine and the NMDA Receptor to Explain the Direct Glycine-Competitive Potentiation of NMDA-Mediated Neuronal Currents. ACS Chemical Neuroscience, 2022, 13, 229-244.	3.5	2
2	QSAR Applied to 4-Chloro-3-formylcoumarin Derivatives Targeting Human Thymidine Phosphorylase. Clinical Complementary Medicine and Pharmacology, 2022, 2, 100031.	1.5	1
3	Allosteric Binding of MDMA to the Human Serotonin Transporter (hSERT) via Ensemble Binding Space Analysis with Î”G Calculations, Induced Fit Docking and Monte Carlo Simulations. Molecules, 2022, 27, 2977.	3.8	1
4	Are vanadium complexes druggable against the main protease Mpro of SARS-CoV-2? â€“ A computational approach. Inorganica Chimica Acta, 2021, 519, 120287.	2.4	15
5	Interaction between a Novel Oligopeptide Fragment of the Human Neurotrophin Receptor TrkB Ectodomain D5 and the C-Terminal Fragment of Tetanus Neurotoxin. Molecules, 2021, 26, 3988.	3.8	1
6	Induced fit, ensemble binding space docking and Monte Carlo simulations of MDMA â€˜ecstasyâ€™ and 3D pharmacophore design of MDMA derivatives on the human serotonin transporter (hSERT). Heliyon, 2021, 7, e07784.	3.2	5
7	Binding of boswellic acids to functional proteins of the SARSâ€CoVâ€2 virus: Bioinformatic studies. Archiv Der Pharmazie, 2021, 354, e2100160.	4.1	9
8	Do It Yourselfâ€”Dock It Yourself: General Concepts and Practical Considerations for Beginners to Start Molecular Ligandâ€“Target Docking Simulations. , 2021, , 205-227.		2
9	Exploring electrostatic patterns of human, murine, equine and canine TLR4/MD-2 receptors. Innate Immunity, 2020, 26, 364-380.	2.4	2
10	Five Novel Non-Sialic Acid-Like Scaffolds Inhibit In Vitro H1N1 and H5N2 Neuraminidase Activity of Influenza a Virus. Molecules, 2020, 25, 4248.	3.8	8
11	Chemometric Models of Differential Amino Acids at the NavÎ± and NavÎ²2 Interface of Mammalian Sodium Channel Isoforms. Molecules, 2020, 25, 3551.	3.8	1
12	Dapsone is not a Pharmacodynamic Lead Compound for its Aryl Derivatives. Current Computer-Aided Drug Design, 2020, 16, 327-339.	1.2	2
13	Theoretical study of the stability and NMR spectroscopic properties of vanadium(V) complexes. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	1
14	Substrate structure-activity relationship reveals a limited lipopolysaccharide chemotype range for intestinal alkaline phosphatase. Journal of Biological Chemistry, 2019, 294, 19405-19423.	3.4	12
15	Induced fit for cytochrome P450 3A4 based on molecular dynamics. ADMET and DMPK, 2019, 7, 252-266.	2.1	5
16	Interaction with St. John's wort due to exposure with blackcurrant aroma? How not to present a case report of an adverse event. Die Pharmazie, 2019, 74, 595-597.	0.5	0
17	Structure - Function Analysis of the Cytochromes P450, Responsible for Phenprocoumon Metabolism. Journal of the Mexican Chemical Society, 2018, 61, .	0.6	0
18	Mefloquine inhibits voltage dependent Nav1.4 channel by overlapping the local anaesthetic binding site. European Journal of Pharmacology, 2017, 796, 215-223.	3.5	7

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19	Synthesis, in vitro and in vivo giardicidal activity of nitrothiazole-NSAID chimeras displaying broad antiprotozoal spectrum. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 3490-3494.	2.2	19
20	Characterization of specific allosteric effects of the Na+ channel Î²1 subunit on the Nav1.4 isoform. European Biophysics Journal, 2017, 46, 485-494.	2.2	4
21	Why Antidiabetic Vanadium Complexes are Not in the Pipeline of â€œBig Pharmaâ€•Drug Research? A Critical Review. Current Medicinal Chemistry, 2016, 23, 2874-2891.	2.4	78
22	Antiprotozoal Nitazoxanide Derivatives: Synthesis, Bioassays and QSAR Study Combined with Docking for Mechanistic Insight. Current Computer-Aided Drug Design, 2015, 11, 21-31.	1.2	11
23	Predicting a double mutant in the twilight zone of low homology modeling for the skeletal muscle voltage-gated sodium channel subunit beta-1 (Na v 1.4 Î²1). Computational and Structural Biotechnology Journal, 2015, 13, 229-240.	4.1	4
24	11-Keto-Î²-Boswellic Acids Prevent Development of Autoimmune Reactions, Insulitis and Reduce Hyperglycemia During Induction of Multiple Low-Dose Streptozotocin (MLD-STZ) Diabetes in Mice. Hormone and Metabolic Research, 2015, 47, 463-469.	1.5	26
25	How to Valorize Biodiversity? LetÊ¼s Go Hashing, Extracting, Filtering, Mining, Fishing. Planta Medica, 2015, 81, 436-449.	1.3	11
26	Interference of Boswellic Acids with the Ligand Binding Domain of the Glucocorticoid Receptor. Journal of Chemical Information and Modeling, 2014, 54, 978-986.	5.4	15
27	Theoretical study of the structure, IR and NMR of the bis-peroxo-oxovanadate species containing-histidine peptides. Inorganica Chimica Acta, 2014, 420, 149-158.	2.4	9
28	REVIEWING AND IDENTIFYING AMINO ACIDS OF HUMAN, MURINE, CANINE AND EQUINE TLR4 / MD-2 RECEPTOR COMPLEXES CONFERRING ENDOTOXIC INNATE IMMUNITY ACTIVATION BY LPS/LIPID A, OR ANTAGONISTIC EFFECTS BY ERITORAN, IN CONTRAST TO SPECIES-DEPENDENT MODULATION BY LIPID IVA. Computational and Structural Biotechnology Journal, 2013, 5, e201302012.	4.1	25
29	THREE-DIMENSIONAL MAPPING OF DIFFERENTIAL AMINO ACIDS OF HUMAN, MURINE, CANINE AND EQUINE TLR4/MD-2 RECEPTOR COMPLEXES CONFERRING ENDOTOXIC ACTIVATION BY LIPID A, ANTAGONISM BY ERITORAN AND SPECIES-DEPENDENT ACTIVITIES OF LIPID IVA IN THE MAMMALIAN LPS SENSOR SYSTEM. Computational and Structural Biotechnology Journal, 2013, 7, e201305003.	4.1	20
30	Identification of NavÎ²1 Residues Involved in the Modulation of the Sodium Channel Nav1.4. PLoS ONE, 2013, 8, e81995.	2.5	6
31	Recognizing Pitfalls in Virtual Screening: A Critical Review. Journal of Chemical Information and Modeling, 2012, 52, 867-881.	5.4	358
32	Modulating testosterone pathway: a new strategy to tackle male skin aging?. Clinical Interventions in Aging, 2012, 7, 351.	2.9	9
33	A proline mimetic for enantioselective aldol reaction: a quantum chemical study of a catalytic reaction with a sterically hindered <scp>l</scp>â€prolinamide derivative. Journal of Physical Organic Chemistry, 2012, 25, 971-978.	1.9	3
34	Pharmacophore Design of p38α MAP Kinase Inhibitors with Either 2,4,5-Trisubstituted or 1,2,4,5-Tetrasubstituted Imidazole Scaffold. Current Medicinal Chemistry, 2011, 18, 1526-1539.	2.4	22
35	Analgesic effect of leaf extract from Ageratina glabrata in the hot plate test. Revista Brasileira De Farmacognosia, 2011, 21, 928-935.	1.4	13
36	Integrating computational and mixture-based screening of combinatorial libraries. Journal of Molecular Modeling, 2011, 17, 1473-1482.	1.8	8

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37	Elucidation of the fragmentation pathways of different phosphatidylinositol phosphate species (PIPx) using IRMPD implemented on a FT-ICR MS. Analytical and Bioanalytical Chemistry, 2010, 398, 2843-2851.	3.7	8
38	Reverse Pharmacognosy: Another Way to Harness the Generosity of Nature. Current Pharmaceutical Design, 2010, 16, 1682-1696.	1.9	31
39	Chimeric design, synthesis, and biological assays of a new nonpeptide insulin-mimetic vanadium compound to inhibit protein tyrosine phosphatase 1B. Drug Design, Development and Therapy, 2010, 4, 231-42.	4.3	5
40	Structure-function analysis of two variants of mumps virus hemagglutinin-neuraminidase protein. Brazilian Journal of Infectious Diseases, 2009, 13, 24-34.	0.6	16
41	How to Recognize and Workaround Pitfalls in QSAR Studies: A Critical Review. Current Medicinal Chemistry, 2009, 16, 4297-4313.	2.4	168
42	Scaffold Diversity Analysis of Compound Data Sets Using an Entropyâ€Based Measure. QSAR and Combinatorial Science, 2009, 28, 1551-1560.	1.4	82
43	Elucidating Isoniazid Resistance Using Molecular Modeling. Journal of Chemical Information and Modeling, 2009, 49, 97-107.	5.4	24
44	Antidiabetic Bis-Maltolato-OxoVanadium(IV): conversion of inactive trans- to bioactive cis-BMOV for possible binding to target PTP-1B. Drug Design, Development and Therapy, 2009, 2, 221-31.	4.3	12
45	Application of Drug Repositioning Strategy to TOFISOPAM. Current Medicinal Chemistry, 2008, 15, 3196-3203.	2.4	22
46	Large Compound Databases for Structure-Activity Relationships Studies in Drug Discovery. Mini-Reviews in Medicinal Chemistry, 2007, 7, 851-860.	2.4	41
47	Synthesis, Biological Testing, and Binding Mode Prediction of 6,9-Diarylpurin-8-ones as p38 MAP Kinase Inhibitors. Journal of Medicinal Chemistry, 2007, 50, 2060-2066.	6.4	23
48	In silico analysis identifies a C3HC4-RING finger domain of a putative E3 ubiquitin-protein ligase located at the C-terminus of a polyglutamine-containing protein. Brazilian Journal of Medical and Biological Research, 2007, 40, 293-299.	1.5	2
49	Isoniazid is Not a Lead Compound for its Pyridyl Ring Derivatives,Isonicotinoyl Amides, Hydrazides, and Hydrazones: A Critical Review. Current Medicinal Chemistry, 2006, 13, 2205-2219.	2.4	59
50	Are Vanadium Compounds Drugable? Structures and Effects of Antidiabetic Vanadium Compounds: A Critical Review. Mini-Reviews in Medicinal Chemistry, 2005, 5, 995-1008.	2.4	46
51	Synthesis and Biological Testing of Purine Derivatives as Potential ATP-Competitive Kinase Inhibitors. Journal of Medicinal Chemistry, 2005, 48, 710-722.	6.4	89
52	On the Restricted and Combined Use of RÃ¼denbergâ€™s Approximations in Molecular Orbital Theories of Hartree-Fock Type. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2003, 58, 756-784.	1.5	14
53	On RÃ¼denbergâ€™s Integral Approximations and Their Unrestricted and Combined Use in Crystal Orbital Theories of Hartree-Fock Type. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2003, 58, 785-800.	1.5	4
54	Preliminary screening of some tropical plants for anti-tyrosinase activity. Journal of Ethnopharmacology, 2002, 82, 155-158.	4.1	125

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55	Antitubercular Isoniazid and Drug Resistance of Mycobacterium tuberculosis â€" A Review. Archiv Der Pharmazie, 2002, 335, 511-525.	4.1	56
56	Ethnopharmacology and bioinformatic combination for leads discovery: application to phospholipase A2 inhibitors. Phytochemistry, 2001, 58, 865-874.	2.9	85
57	Prolyl isomerases in a minimal cell. FEBS Journal, 2000, 267, 3270-3280.	0.2	33
58	Molecular Modeling Study on Dapsone and Sulfonamides Comparing Structures and Properties with Respect to Anti-Leprosy Activity. Journal of Molecular Modeling, 1997, 3, 332-337.	1.8	11
59	Homology Modelling of a Newly Discovered Thioredoxin Protein and Analysis of the Force Field and Electrostatic Properties. Journal of Molecular Modeling, 1997, 3, 359-363.	1.8	4
60	Adenosine receptors and their modulators. Pharmaceutica Acta Helvetiae, 1993, 68, 77-111.	1.2	115
61	Antidiabetic Bis-Maltolato-OxoVanadium(IV): Conversion of inactive trans- to bioactive cis-BMOV for possible binding to target PTP-1B. Drug Design, Development and Therapy, 0, , 221.	4.3	16
62	An in silico approach to primaquine binding to Trp756 in the external vestibule of sodium channel Nav 1.4. Journal of Receptor, Ligand and Channel Research, 0, , 41.	0.7	0