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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	Recognizing Pitfalls in Virtual Screening: A Critical Review. Journal of Chemical Information and Modeling, 2012, 52, 867-881.	5.4	358
2	How to Recognize and Workaround Pitfalls in QSAR Studies: A Critical Review. Current Medicinal Chemistry, 2009, 16, 4297-4313.	2.4	168
3	Preliminary screening of some tropical plants for anti-tyrosinase activity. Journal of Ethnopharmacology, 2002, 82, 155-158.	4.1	125
4	Adenosine receptors and their modulators. Pharmaceutica Acta Helvetiae, 1993, 68, 77-111.	1.2	115
5	Synthesis and Biological Testing of Purine Derivatives as Potential ATP-Competitive Kinase Inhibitors. Journal of Medicinal Chemistry, 2005, 48, 710-722.	6.4	89
6	Ethnopharmacology and bioinformatic combination for leads discovery: application to phospholipase A2 inhibitors. Phytochemistry, 2001, 58, 865-874.	2.9	85
7	Scaffold Diversity Analysis of Compound Data Sets Using an Entropyâ€Based Measure. QSAR and Combinatorial Science, 2009, 28, 1551-1560.	1.4	82
8	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
9	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
10	Antitubercular Isoniazid and Drug Resistance of Mycobacterium tuberculosis â€" A Review. Archiv Der Pharmazie, 2002, 335, 511-525.	4.1	56
11	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
12	Large Compound Databases for Structure-Activity Relationships Studies in Drug Discovery. Mini-Reviews in Medicinal Chemistry, 2007, 7, 851-860.	2.4	41
13	Prolyl isomerases in a minimal cell. FEBS Journal, 2000, 267, 3270-3280.	0.2	33
14	Reverse Pharmacognosy: Another Way to Harness the Generosity of Nature. Current Pharmaceutical Design, 2010, 16, 1682-1696.	1.9	31
15	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
16	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
17	Elucidating Isoniazid Resistance Using Molecular Modeling. Journal of Chemical Information and Modeling, 2009, 49, 97-107.	5.4	24
18	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

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19	Application of Drug Repositioning Strategy to TOFISOPAM. Current Medicinal Chemistry, 2008, 15, 3196-3203.	2.4	22
20	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
21	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
22	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
23	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
24	Structure-function analysis of two variants of mumps virus hemagglutinin-neuraminidase protein. Brazilian Journal of Infectious Diseases, 2009, 13, 24-34.	0.6	16
25	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
26	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
27	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
28	Analgesic effect of leaf extract from Ageratina glabrata in the hot plate test. Revista Brasileira De Farmacognosia, 2011, 21, 928-935.	1.4	13
29	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
30	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
31	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
32	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
33	How to Valorize Biodiversity? LetÊ¼s Go Hashing, Extracting, Filtering, Mining, Fishing. Planta Medica, 2015, 81, 436-449.	1.3	11
34	Modulating testosterone pathway: a new strategy to tackle male skin aging?. Clinical Interventions in Aging, 2012, 7, 351.	2.9	9
35	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
36	Binding of boswellic acids to functional proteins of the SARSâ€CoVâ€2 virus: Bioinformatic studies. Archiv Der Pharmazie, 2021, 354, e2100160.	4.1	9

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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	Integrating computational and mixture-based screening of combinatorial libraries. Journal of Molecular Modeling, 2011, 17, 1473-1482.	1.8	8
39	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
40	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
41	Identification of NavÎ²1 Residues Involved in the Modulation of the Sodium Channel Nav1.4. PLoS ONE, 2013, 8, e81995.	2.5	6
42	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
43	Induced fit for cytochrome P450 3A4 based on molecular dynamics. ADMET and DMPK, 2019, 7, 252-266.	2.1	5
44	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
45	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
46	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
47	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
48	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
49	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
50	Exploring electrostatic patterns of human, murine, equine and canine TLR4/MD-2 receptors. Innate Immunity, 2020, 26, 364-380.	2.4	2
51	Do It Yourselfâ€”Dock It Yourself: General Concepts and Practical Considerations for Beginners to Start Molecular Ligandâ€“Target Docking Simulations. , 2021, , 205-227.		2
52	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
53	Dapsone is not a Pharmacodynamic Lead Compound for its Aryl Derivatives. Current Computer-Aided Drug Design, 2020, 16, 327-339.	1.2	2
54	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

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55	Theoretical study of the stability and NMR spectroscopic properties of vanadium(V) complexes. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	1
56	Chemometric Models of Differential Amino Acids at the NavÎ± and NavÎ² Interface of Mammalian Sodium Channel Isoforms. Molecules, 2020, 25, 3551.	3.8	1
57	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
58	QSAR Applied to 4-Chloro-3-formylcoumarin Derivatives Targeting Human Thymidine Phosphorylase. Clinical Complementary Medicine and Pharmacology, 2022, 2, 100031.	1.5	1
59	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
60	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
61	Structure - Function Analysis of the Cytochromes P450, Responsible for Phenprocoumon Metabolism. Journal of the Mexican Chemical Society, 2018, 61, .	0.6	0
62	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