De-Xin Kong

List of Publications by Year
in descending order

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47	926	430442	476904
papers	citations	18 h-index	29 g-index

48	48	48	1555
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Accelerating the identification of subtype selective inhibitors via Three-Dimensional Biologically Relevant Spectrum (BRS-3D): The monoamine oxidase subtypes as a case study. Bioorganic Chemistry, 2021, 106, 104503.	2.0	1
2	Predicting lung adenocarcinoma disease progression using methylation-correlated blocks and ensemble machine learning classifiers. PeerJ, 2021, 9, e10884.	0.9	5
3	EnMCB: an R/bioconductor package for predicting disease progression based on methylation correlated blocks using ensemble models. Bioinformatics, 2021, 37, 4282-4284.	1.8	2
4	Identification of novel monoamine oxidase selective inhibitors employing a hierarchical ligand-based virtual screening strategy. Future Medicinal Chemistry, 2019, 11, 801-816.	1.1	4
5	Novel C7-Substituted Coumarins as Selective Monoamine Oxidase Inhibitors: Discovery, Synthesis and Theoretical Simulation. Molecules, 2019, 24, 4003.	1.7	9
6	Broad-spectrum monoclonal antibody and a sensitive multi-residue indirect competitive enzyme-linked immunosorbent assay for the antibacterial synergists in samples of animal origin. Food Chemistry, 2019, 280, 20-26.	4.2	20
7	Integrating Multifaceted Information to Predict Mycobacterium tuberculosis-Human Protein-Protein Interactions. Journal of Proteome Research, 2018, 17, 3810-3823.	1.8	8
8	Deciphering the Odorant Binding, Activation, and Discrimination Mechanism of Dhelobp21 from Dastarus Helophoroides. Scientific Reports, 2018, 8, 13506.	1.6	3
9	Cheminformatic Insight into the Differences between Terrestrial and Marine Originated Natural Products. Journal of Chemical Information and Modeling, 2018, 58, 1182-1193.	2.5	45
10	Theoretical Calculation and Experimental Verification Demonstrated the Impossibility of Finding Haptens Identifying Triphenylmethane Dyes and Their Leuco Metabolites Simultaneously. Molecules, 2018, 23, 663.	1.7	0
11	Quebrachitol: Global Status and Basic Research. Natural Products and Bioprospecting, 2017, 7, 113-122.	2.0	6
12	Comparative analyses of structural features and scaffold diversity for purchasable compound libraries. Journal of Cheminformatics, 2017, 9, 25.	2.8	25
13	Structural Transformation Detection Contributes to Screening of Behaviorally Active Compounds: Dynamic Binding Process Analysis of DhelOBP21 from Dastarcus helophoroides. Journal of Chemical Ecology, 2017, 43, 1033-1045.	0.9	27
14	Three-Dimensional Biologically Relevant Spectrum (BRS-3D): Shape Similarity Profile Based on PDB Ligands as Molecular Descriptors. Molecules, 2016, 21, 1554.	1.7	19
15	Structure-based discovery of two antiviral inhibitors targeting the NS3 helicase of Japanese encephalitis virus. Scientific Reports, 2016, 6, 34550.	1.6	20
16	Predicting subtype selectivity of dopamine receptor ligands with threeâ€dimensional biologically relevant spectrum. Chemical Biology and Drug Design, 2016, 88, 859-872.	1.5	10
17	Predicting Subtype Selectivity for Adenosine Receptor Ligands with Three-Dimensional Biologically Relevant Spectrum (BRS-3D). Scientific Reports, 2016, 6, 36595.	1.6	15
18	Predicting cancer-relevant proteins using an improved molecular similarity ensemble approach. Oncotarget, 2016, 7, 32394-32407.	0.8	4

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19	Structure-Based Analysis of the Ligand-Binding Mechanism for DhelOBP21, a C-minus Odorant Binding Protein, from Dastarcus helophoroides (Fairmaire; Coleoptera: Bothrideridae). International Journal of Biological Sciences, 2015, 11, 1281-1295.	2.6	40
20	Construction of a genomeâ€scale metabolic network of the plant pathogen Pectobacterium carotovorum provides new strategies for bactericide discovery. FEBS Letters, 2015, 589, 285-294.	1.3	18
21	Fluroxypyrâ€"a potential surrogate of 2,4-dichlorophenoxyacetic acid for retarding calyx senescence in postharvest citrus fruit. Postharvest Biology and Technology, 2015, 105, 17-25.	2.9	6
22	Drug Repurposing Based on Drugâ€"Drug Interaction. Chemical Biology and Drug Design, 2015, 85, 137-144.	1.5	15
23	Synthesis and biological evaluation of new simple indolic non peptidic HIV Protease inhibitors: The effect of different substitution patterns. Bioorganic and Medicinal Chemistry, 2014, 22, 4792-4802.	1.4	14
24	Exploring the Biologically Relevant Chemical Space for Drug Discovery. Journal of Chemical Information and Modeling, 2013, 53, 2820-2828.	2.5	39
25	Analysis of the Binding Sites of Porcine Sialoadhesin Receptor with PRRSV. International Journal of Molecular Sciences, 2013, 14, 23955-23979.	1.8	8
26	The Impact of Oxygen on Metabolic Evolution: A Chemoinformatic Investigation. PLoS Computational Biology, 2012, 8, e1002426.	1.5	23
27	Generic Immunoassay of Quinolones: Production and Characterization of Anti-pefloxacin Antibodies as Broad Selective Receptors. Food Analytical Methods, 2011, 4, 517-524.	1.3	12
28	Historical Variation of Structural Novelty in a Natural Product Library. Chemistry and Biodiversity, 2011, 8, 1968-1977.	1.0	24
29	Chemical Basis of Metabolic Network Organization. PLoS Computational Biology, 2011, 7, e1002214.	1.5	12
30	Marine natural products as sources of novel scaffolds: achievement and concern. Drug Discovery Today, 2010, 15, 884-886.	3.2	97
31	Chemoinformatics Approaches for Traditional Chinese Medicine Research and Case Application in Anticancer Drug Discovery. Current Drug Discovery Technologies, 2010, 7, 22-31.	0.6	18
32	How does oxygen rise drive evolution? Clues from oxygen-dependent biosynthesis of nuclear receptor ligands. Biochemical and Biophysical Research Communications, 2010, 391, 1158-1160.	1.0	21
33	Water in the Neck-Zipper Region of Kinesin. Chinese Physics Letters, 2009, 26, 078701.	1.3	2
34	Where is the hope for drug discovery? Let history tell the future. Drug Discovery Today, 2009, 14, 115-119.	3.2	128
35	Broad-Specific Antibodies for a Generic Immunoassay of Quinolone: Development of a Molecular Model for Selection of Haptens Based on Molecular Field-Overlapping. Analytical Chemistry, 2009, 81, 3246-3251.	3.2	34
36	Do Biologically Relevant Compounds Have More Chance To Be Drugs?. Journal of Chemical Information and Modeling, 2009, 49, 2376-2381.	2.5	22

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37	How Many Traditional Chinese Medicine Components Have Been Recognized by Modern Western Medicine? A Chemoinformatic Analysis and Implications for Finding Multicomponent Drugs. ChemMedChem, 2008, 3, 233-236.	1.6	37
38	Convergent Evolution of Medicines. ChemMedChem, 2008, 3, 1169-1171.	1.6	7
39	Excited-State pKa Values of Curcumin. Natural Product Communications, 2008, 3, 1934578X0800300.	0.2	0
40	Distribution patterns of small-molecule ligands in the protein universe and implications for origin of life and drug discovery. Genome Biology, 2007, 8, R176.	13.9	53
41	Density Functional Theory Methods as Powerful Tools to Elucidate Amino Acid Oxidation Mechanisms. A Case Study on Methionine Model Peptide. Journal of Physical Chemistry B, 2007, 111, 485-489.	1.2	14
42	COMPARISON OF THREE 3D-QSAR METHODS USING A NOVEL CLASS OF MURF INHIBITORS. Journal of Theoretical and Computational Chemistry, 2007, 06, 63-80.	1.8	6
43	Multiple pharmacological effects of olive oil phenols. Food Chemistry, 2007, 104, 1269-1271.	4.2	32
44	Characterization and expression of p23 gene in the amphioxus Branchiostoma belcheri. Comparative Biochemistry and Physiology - B Biochemistry and Molecular Biology, 2006, 145, 10-15.	0.7	8
45	Quantum study on photophysical and photochemical process of a new photosensitizer: hypomycin B. Journal of Photochemistry and Photobiology A: Chemistry, 2005, 170, 37-43.	2.0	1
46	Intramolecular H-bonding in the bay region of hypericin: an AM1 study. Dyes and Pigments, 2001, 51, 71-77.	2.0	7
47	Docking and QM/MM Studies of NS2B-NS3pro Inhibitors: a Molecular Target against the Dengue Virus. Journal of the Brazilian Chemical Society, 0, , .	0.6	5