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List of Publications by Year in descending order

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31
papers

1,367
citations

566801

15
h-index

454577

30
g-index

33
all docs

33
docs citations

33
times ranked

1717
citing authors

#	ARTICLE	IF	CITATIONS
1	Discovery of a Potent, Selective, and Efficacious Class of Reversible Î±-Ketoheterocycle Inhibitors of Fatty Acid Amide Hydrolase Effective as Analgesics. Journal of Medicinal Chemistry, 2005, 48, 1849-1856.	2.9	201
2	Structure-Guided Design, Synthesis, and Evaluation of Guanine-Derived Inhibitors of the eIF4E mRNA-Cap Interaction. Journal of Medicinal Chemistry, 2012, 55, 3837-3851.	2.9	179
3	Elucidation of Fatty Acid Amide Hydrolase Inhibition by Potent Î±-Ketoheterocycle Derivatives from Monte Carlo Simulations. Journal of the American Chemical Society, 2005, 127, 17377-17384.	6.6	163
4	Macrophomate Synthase: QM/MM Simulations Address the Diels-Alder versus Michael-Aldol Reaction Mechanism. Journal of the American Chemical Society, 2005, 127, 3577-3588.	6.6	108
5	Search for Non-Nucleoside Inhibitors of HIV-1 Reverse Transcriptase Using Chemical Similarity, Molecular Docking, and MM-GB/SA Scoring. Journal of Chemical Information and Modeling, 2007, 47, 2416-2428.	2.5	79
6	Extension of the PDDG/PM3 and PDDG/MNDO semiempirical molecular orbital methods to the halogens. Journal of Computational Chemistry, 2004, 25, 138-150.	1.5	76
7	Contributions of Conformational Compression and Preferential Transition State Stabilization to the Rate Enhancement by Chorismate Mutase. Journal of the American Chemical Society, 2003, 125, 6892-6899.	6.6	73
8	Synthetic and Theoretical Studies on the Reduction of Electron Withdrawing Group Conjugated Olefins Using the Hantzsch 1,4-Dihydropyridine Ester. Journal of Organic Chemistry, 2003, 68, 8815-8822.	1.7	70
9	Extension of the PDDG/PM3 Semiempirical Molecular Orbital Method to Sulfur, Silicon, and Phosphorus. Journal of Chemical Theory and Computation, 2005, 1, 817-823.	2.3	70
10	From Docking False-Positive to Active Anti-HIV Agent. Journal of Medicinal Chemistry, 2007, 50, 5324-5329.	2.9	65
11	Investigation of Solvent Effects for the Claisen Rearrangement of Chorismate to Prephenate: Mechanistic Interpretation via Near Attack Conformations. Journal of the American Chemical Society, 2003, 125, 6663-6672.	6.6	56
12	Improving MM-GB/SA Scoring through the Application of the Variable Dielectric Model. Journal of Chemical Theory and Computation, 2011, 7, 3859-3865.	2.3	39
13	Effects of Arg90 Neutralization on the Enzyme-Catalyzed Rearrangement of Chorismate to Prephenate. Journal of Chemical Theory and Computation, 2005, 1, 617-625.	2.3	28
14	On the application of simple explicit water models to the simulations of biomolecules. Brazilian Journal of Physics, 2004, 34, 126-136.	0.7	19
15	A molecular dynamics study of an L-type calcium channel model. Protein Engineering, Design and Selection, 2002, 15, 109-122.	1.0	18
16	Brain-wide mapping of c-fos expression in the single prolonged stress model and the effects of pretreatment with ACH-000029 or prazosin. Neurobiology of Stress, 2020, 13, 100226.	1.9	16
17	Molecular dynamics study on liquid 1-octanol. International Journal of Quantum Chemistry, 2000, 80, 999-1006.	1.0	14
18	Thermodynamic Analysis of Thrombin Inhibition by Benzamidine and p-Methylbenzamidine via Free-Energy Perturbations: Inspection of Intraperturbed-Group Contributions Using the Finite Difference Thermodynamic Integration (FDTI) Algorithm. Journal of Physical Chemistry B, 2002, 106, 466-476.	1.2	13

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19	Preclinical characterization of ACH-000029, a novel anxiolytic compound acting on serotonergic and alpha-adrenergic receptors. <i>Progress in Neuro-Psychopharmacology and Biological Psychiatry</i> , 2019, 95, 109707.	2.5	12
20	Thrombin Inhibition by Novel Benzamidine Derivatives: A Free-Energy Perturbation Study. <i>Journal of Medicinal Chemistry</i> , 2002, 45, 4995-5004.	2.9	11
21	Evaluating the relative free energy of hydration of new thrombin inhibitor candidates using the finite difference thermodynamic integration (FDTI) method. <i>International Journal of Quantum Chemistry</i> , 2001, 85, 713-726.	1.0	9
22	Discovery of ACH-000143: A Novel Potent and Peripherally Preferred Melatonin Receptor Agonist that Reduces Liver Triglycerides and Steatosis in Diet-Induced Obese Rats. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 1904-1929.	2.9	9
23	Investigation of the induced-fit mechanism and catalytic activity of the human cytomegalovirus protease homodimer via molecular dynamics simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003, 52, 483-491.	1.5	7
24	A molecular dynamics study on liquid 1-octanol. Part 3. Evaluating octanol/water partition coefficients of novel thrombin inhibitors via free-energy perturbations. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 542-553.	1.0	6
25	Synthesis of 12-membered macrocyclic templates and library analogs for PPI. <i>Tetrahedron Letters</i> , 2013, 54, 3298-3301.	0.7	6
26	The serotonergic and alpha-1 adrenergic receptor modulator ACH-000029 ameliorates anxiety-like behavior in a post-traumatic stress disorder model. <i>Neuropharmacology</i> , 2020, 164, 107912.	2.0	6
27	Molecular dynamics study on liquid 1-octanol. Part 2. Water-saturated 1-octanol solution*. <i>International Journal of Quantum Chemistry</i> , 2002, 90, 786-791.	1.0	5
28	Potential of mean force calculations on an L-type calcium channel model. <i>Protein Engineering, Design and Selection</i> , 2003, 16, 209-215.	1.0	3
29	Human Cytomegalovirus Protease: Why is the Dimer Required for Catalytic Activity?. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 278-288.	2.3	3
30	Design, synthesis and antihypertensive evaluation of novel codrugs with combined angiotensin type 1 receptor antagonism and neprilysin inhibition. <i>European Journal of Pharmaceutical Sciences</i> , 2021, 159, 105731.	1.9	3
31	Characterization and in silico Mutagenic Assessment of a New Betahistine Degradation Impurity. <i>Journal of the Brazilian Chemical Society</i> , 0, , .	0.6	0