Cristiano Ruch Werneck GuimarÃ£es

List of Publications by Year
in descending order

31 papers	1,367 citations	567281 15 h-index	454955 30 g-index
33 all docs	33 docs citations	33 times ranked	1717 citing authors

#	Article	IF	Citations
1	Discovery of ACH-000143: A Novel Potent and Peripherally Preferred Melatonin Receptor Agonist that Reduces Liver Triglycerides and Steatosis in Diet-Induced Obese Rats. Journal of Medicinal Chemistry, 2021, 64, 1904-1929.	6.4	9
2	Design, synthesis and antihypertensive evaluation of novel codrugs with combined angiotensin type 1 receptor antagonism and neprilysin inhibition. European Journal of Pharmaceutical Sciences, 2021, 159, 105731.	4.0	3
3	The serotonergic and alpha-1 adrenergic receptor modulator ACH-000029 ameliorates anxiety-like behavior in a post-traumatic stress disorder model. Neuropharmacology, 2020, 164, 107912.	4.1	6
4	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.	4.0	16
5	Preclinical characterization of ACH-000029, a novel anxiolytic compound acting on serotonergic and alpha-adrenergic receptors. Progress in Neuro-Psychopharmacology and Biological Psychiatry, 2019, 95, 109707.	4.8	12
6	Synthesis of 12-membered macrocyclic templates and library analogs for PPI. Tetrahedron Letters, 2013, 54, 3298-3301.	1.4	6
7	Structure-Guided Design, Synthesis, and Evaluation of Guanine-Derived Inhibitors of the eIF4E mRNAâ€“Cap Interaction. Journal of Medicinal Chemistry, 2012, 55, 3837-3851.	6.4	179
8	Improving MM-GB/SA Scoring through the Application of the Variable Dielectric Model. Journal of Chemical Theory and Computation, 2011, 7, 3859-3865.	5.3	39
9	From Docking False-Positive to Active Anti-HIV Agent. Journal of Medicinal Chemistry, 2007, 50, 5324-5329.	6.4	65
10	Human Cytomegalovirus Protease:â€‰ Why is the Dimer Required for Catalytic Activity?. Journal of Chemical Theory and Computation, 2007, 3, 278-288.	5.3	3
11	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.	5.4	79
12	A molecular dynamics study on liquid 1-octanol. Part 3. Evaluating octanol/water partition coefficients of novel thrombin inhibitors via free-energy perturbations. International Journal of Quantum Chemistry, 2005, 102, 542-553.	2.0	6
13	Macrophomate Synthase:Â QM/MM Simulations Address the Dielsâ^'Alder versus Michaelâ^'Aldol Reaction Mechanism. Journal of the American Chemical Society, 2005, 127, 3577-3588.	13.7	108
14	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.	13.7	163
15	Effects of Arg90 Neutralization on the Enzyme-Catalyzed Rearrangement of Chorismate to Prephenate. Journal of Chemical Theory and Computation, 2005, 1, 617-625.	5.3	28
16	Extension of the PDDG/PM3 Semiempirical Molecular Orbital Method to Sulfur, Silicon, and Phosphorus. Journal of Chemical Theory and Computation, 2005, 1, 817-823.	5.3	70
17	Discovery of a Potent, Selective, and Efficacious Class of Reversible Î±-Ketoheterocycle Inhibitors of Fatty Acid Amide Hydrolase Effective as Analgesicsâ^‡. Journal of Medicinal Chemistry, 2005, 48, 1849-1856.	6.4	201
18	On the application of simple explicit water models to the simulations of biomolecules. Brazilian Journal of Physics, 2004, 34, 126-136.	1.4	19

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19	Extension of the PDDG/PM3 and PDDG/MNDO semiempirical molecular orbital methods to the halogens. Journal of Computational Chemistry, 2004, 25, 138-150.	3.3	76
20	Investigation of the induced-fit mechanism and catalytic activity of the human cytomegalovirus protease homodimer via molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2003, 52, 483-491.	2.6	7
21	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.	13.7	73
22	Investigation of Solvent Effects for the Claisen Rearrangement of Chorismate to Prephenate:â€‰ Mechanistic Interpretation via Near Attack Conformations. Journal of the American Chemical Society, 2003, 125, 6663-6672.	13.7	56
23	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.	3.2	70
24	Potential of mean force calculations on an L-type calcium channel model. Protein Engineering, Design and Selection, 2003, 16, 209-215.	2.1	3
25	A molecular dynamics study of an L-type calcium channel model. Protein Engineering, Design and Selection, 2002, 15, 109-122.	2.1	18
26	Thrombin Inhibition by Novel Benzamidine Derivatives:Â A Free-Energy Perturbation Study. Journal of Medicinal Chemistry, 2002, 45, 4995-5004.	6.4	11
27	Thermodynamic Analysis of Thrombin Inhibition by Benzamidine andp-Methylbenzamidine via Free-Energy Perturbations:Â Inspection of Intraperturbed-Group Contributions Using the Finite Difference Thermodynamic Integration (FDTI) Algorithm. Journal of Physical Chemistry B, 2002, 106, 466-476.	2.6	13
28	Molecular dynamics study on liquid 1-octanol. Part 2. Water-saturated 1-octanol solution*. International Journal of Quantum Chemistry, 2002, 90, 786-791.	2.0	5
29	Evaluating the relative free energy of hydration of new thrombin inhibitor candidates using the finite difference thermodynamic integration (FDTI) method. International Journal of Quantum Chemistry, 2001, 85, 713-726.	2.0	9
30	Molecular dynamics study on liquid 1-octanol. International Journal of Quantum Chemistry, 2000, 80, 999-1006.	2.0	14
31	Characterization and in silico Mutagenic Assessment of a New Betahistine Degradation Impurity. Journal of the Brazilian Chemical Society, 0, , .	0.6	0