Neysa Nevins

List of Publications by Year
in descending order

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30 papers	3,850 citations	394286 19 h-index	454834 30 g-index
32 all docs	32 docs citations	32 times ranked	5738 citing authors

#	Article	IF	Citations
1	Automated high throughput pKa and distribution coefficient measurements of pharmaceutical compounds for the SAMPL8 blind prediction challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 1141-1155.	1.3	6
2	Characterization ofP. falciparumdipeptidyl aminopeptidase 3 specificity identifies differences in amino acid preferences between peptideâ€based substrates and covalent inhibitors. FEBS Journal, 2019, 286, 3998-4023.	2.2	7
3	D3R Grand Challenge 3: blind prediction of proteinâ€“ligand poses and affinity rankings. Journal of Computer-Aided Molecular Design, 2019, 33, 1-18.	1.3	104
4	Design of amidobenzimidazole STING receptor agonists with systemic activity. Nature, 2018, 564, 439-443.	13.7	505
5	Allosteric Wip1 phosphatase inhibition through flap-subdomain interaction. Nature Chemical Biology, 2014, 10, 181-187.	3.9	172
6	The Amino-Acid Substituents of Dipeptide Substrates of Cathepsin C Can Determine the Rate-Limiting Steps of Catalysis. Biochemistry, 2012, 51, 7551-7568.	1.2	16
7	Druggability Assessment of Allosteric Proteins by Dynamics Simulations in the Presence of Probe Molecules. Journal of Chemical Theory and Computation, 2012, 8, 2435-2447.	2.3	138
8	Discovery of Novel Cyanamide-Based Inhibitors of Cathepsin C. ACS Medicinal Chemistry Letters, 2011, 2, 142-147.	1.3	46
9	Azepanone-based inhibitors of human cathepsin S: Optimization of selectivity via the P2 substituent. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 4409-4415.	1.0	12
10	Molecular Shape and Medicinal Chemistry: A Perspective. Journal of Medicinal Chemistry, 2010, 53, 3862-3886.	2.9	262
11	Antitumor activity of an allosteric inhibitor of centromere-associated protein-E. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 5839-5844.	3.3	197
12	ATP-competitive inhibitors of the mitotic kinesin KSP that function via an allosteric mechanism. Nature Chemical Biology, 2007, 3, 722-726.	3.9	97
13	Crossover Point between Dialkoxy Disulfides (ROSSOR) and Thionosulfites ((RO)2SS):Â Prediction, Synthesis, and Structure. Journal of the American Chemical Society, 2006, 128, 291-304.	6.6	25
14	A Critical Assessment of Docking Programs and Scoring Functions. Journal of Medicinal Chemistry, 2006, 49, 5912-5931.	2.9	1,429
15	Structure Activity Relationships of 5-, 6-, and 7-Methyl-Substituted Azepan-3-one Cathepsin K Inhibitors. Journal of Medicinal Chemistry, 2006, 49, 1597-1612.	2.9	66
16	Polyoxometalate HIV-1 Protease Inhibitors. A New Mode of Protease Inhibition. Journal of the American Chemical Society, 2001, 123, 886-897.	6.6	374
17	Analysis of fluorescently labeled substance P analogs: binding, imaging and receptor activation. , 2001, 1, 1.		26
18	Calculated conformer energies for organic molecules with multiple polar functionalities are method dependent: Taxol (case study). BMC Chemical Biology, 2001, 1, 2.	1.6	24

#	Article	IF	Citations
19	The Conformations of Taxol in Chloroform. Journal of the American Chemical Society, 2000, 122, 724-725.	6.6	71
20	A Test of the Single-Conformation Hypothesis in the Analysis of NMR Data for Small Polar Molecules:Â A Force Field Comparison. Journal of Organic Chemistry, 1999, 64, 3979-3986.	1.7	57
21	Molecular Mechanics (MM3) Calculations on Oxygen-Containing Phosphorus (Coordination IV) Compounds. Journal of Organic Chemistry, 1999, 64, 5350-5360.	1.7	18
22	On Pure Axial Monosubstituted Cyclohexanes. Journal of the American Chemical Society, 1998, 120, 12145-12146.	6.6	7
23	Inherently Hindered Rotation about a Disulfide Bond. Journal of the American Chemical Society, 1997, 119, 12685-12686.	6.6	25
24	Hartreeâ^'Fock and MÃ¸llerâ^'Plesset (MP2) Treatment of Oxygen-Containing Phosphorus Compounds. Journal of Organic Chemistry, 1997, 62, 5198-5207.	1.7	19
25	Molecular mechanics (MM4) calculations on alkenes. Journal of Computational Chemistry, 1996, 17, 669-694.	1.5	21
26	Molecular mechanics (MM4) calculations on conjugated hydrocarbons. Journal of Computational Chemistry, 1996, 17, 695-729.	1.5	22
27	Molecular mechanics (MM4) vibrational frequency calculations for alkenes and conjugated hydrocarbons. Journal of Computational Chemistry, 1996, 17, 730-746.	1.5	62
28	Ab Initio and Molecular Mechanics Calculations on the Inversion of Cs to C2 Conformations of 1,3-Cycloheptadiene. The Journal of Physical Chemistry, 1994, 98, 2056-2061.	2.9	11
29	Termination layer variations on the cleaved (0001) surface determined by scanning tunneling microscopy. Surface Science, 1993, 291, 395-401.	0.8	21
30	Chemical vapor transport of Nb3Sn. Materials Research Bulletin, 1990, 25, 257-263.	2.7	0