Anthony Nicholls

List of Publications by Year
in descending order

35 papers	13,644 citations	293460 24 h-index	425179 34 g-index
35 all docs	35 docs citations	35 times ranked	13510 citing authors

#	Article	IF	Citations
1	Virtual Screening in the Cloud: How Big Is Big Enough?. Journal of Chemical Information and Modeling, 2020, 60, 4274-4282.	2.5	50
2	Leaving us with fond memories, smiles, SMILES and, alas, tears: a tribute to David Weininger, 1952â€“2016. Journal of Computer-Aided Molecular Design, 2018, 32, 313-319.	1.3	1
3	Statistics in molecular modeling: a summary. Journal of Computer-Aided Molecular Design, 2016, 30, 279-280.	1.3	1
4	Confidence limits, error bars and method comparison in molecular modeling. Part 2: comparing methods. Journal of Computer-Aided Molecular Design, 2016, 30, 103-126.	1.3	29
5	The statistics of virtual screening and lead optimization. Journal of Computer-Aided Molecular Design, 2015, 29, 923-936.	1.3	12
6	JCAMD special series: statistics and molecular modeling. Journal of Computer-Aided Molecular Design, 2014, 28, 885-886.	1.3	1
7	Efficient calculation of SAMPL4 hydration free energies using OMEGA, SZYBKI, QUACPAC, and Zap TK. Journal of Computer-Aided Molecular Design, 2014, 28, 289-298.	1.3	13
8	Confidence limits, error bars and method comparison in molecular modeling. Part 1: The calculation of confidence intervals. Journal of Computer-Aided Molecular Design, 2014, 28, 887-918.	1.3	83
9	Call for Papers: GRC, CADD, and statistics, and all that. Journal of Computer-Aided Molecular Design, 2012, 26, 1097-1099.	1.3	0
10	The character of molecular modeling. Journal of Computer-Aided Molecular Design, 2012, 26, 103-105.	1.3	5
11	What Do We Know?: Simple Statistical Techniques that Help. Methods in Molecular Biology, 2011, 672, 531-581.	0.4	12
12	Molecular Shape and Medicinal Chemistry: A Perspective. Journal of Medicinal Chemistry, 2010, 53, 3862-3886.	2.9	262
13	SAMPL2 and continuum modeling. Journal of Computer-Aided Molecular Design, 2010, 24, 293-306.	1.3	20
14	The SAMPL2 blind prediction challenge: introduction and overview. Journal of Computer-Aided Molecular Design, 2010, 24, 259-279.	1.3	175
15	Analysis of SM8 and Zap TK calculations and their geometric sensitivity. Journal of Computer-Aided Molecular Design, 2010, 24, 335-342.	1.3	9
16	Integrated Continuum Dielectric Approaches To Treat Molecular Polarizability and the Condensed Phase: Refractive Index and Implicit Solvation. Journal of Chemical Theory and Computation, 2009, 5, 1785-1802.	2.3	18
17	The SAMP1 Solvation Challenge: Further Lessons Regarding the Pitfalls of Parametrization. Journal of Physical Chemistry B, 2009, 113, 4521-4532.	1.2	36
18	How to do an evaluation: pitfalls and traps. Journal of Computer-Aided Molecular Design, 2008, 22, 179-190.	1.3	126

#	Article	IF	Citations
19	What do we know and when do we know it?. Journal of Computer-Aided Molecular Design, 2008, 22, 239-255.	1.3	179
20	Recommendations for evaluation of computational methods. Journal of Computer-Aided Molecular Design, 2008, 22, 133-139.	1.3	269
21	Predicting Small-Molecule Solvation Free Energies: An Informal Blind Test for Computational Chemistry. Journal of Medicinal Chemistry, 2008, 51, 769-779.	2.9	248
22	Comparison of Shape-Matching and Docking as Virtual Screening Tools. Journal of Medicinal Chemistry, 2007, 50, 74-82.	2.9	826
23	A simple formula for dielectric polarisation energies: The Sheffield Solvation Model. Chemical Physics Letters, 2007, 441, 163-166.	1.2	28
24	Automated ligand placement and refinement with a combined force field and shape potential. Acta Crystallographica Section D: Biological Crystallography, 2006, 62, 741-749.	2.5	79
25	Small Molecule Shape-Fingerprints. Journal of Chemical Information and Modeling, 2005, 45, 673-684.	2.5	105
26	A Shape-Based 3-D Scaffold Hopping Method and Its Application to a Bacterial Proteinâ˜'Protein Interaction. Journal of Medicinal Chemistry, 2005, 48, 1489-1495.	2.9	556
27	Variable selection and model validation of 2D and 3D molecular descriptors›. Journal of Computer-Aided Molecular Design, 2004, 18, 451-474.	1.3	54
28	Gaussian docking functions. Biopolymers, 2003, 68, 76-90.	1.2	433
29	A smooth permittivity function for Poisson-Boltzmann solvation methods. Journal of Computational Chemistry, 2001, 22, 608-640.	1.5	306
30	The fast multipole boundary element method for molecular electrostatics: An optimal approach for large systems. Journal of Computational Chemistry, 1995, 16, 898-913.	1.5	147
31	A rapid method for calculating derivatives of solvent accessible surface areas of molecules. Journal of Computational Chemistry, 1995, 16, 1038-1044.	1.5	67
32	Classical electrostatics in biology and chemistry. Science, 1995, 268, 1144-1149.	6.0	2,743
33	Electrostatic contributions to solvation energies: comparison of free energy perturbation and continuum calculations. Journal of the American Chemical Society, 1991, 113, 1454-1455.	6.6	197
34	A rapid finite difference algorithm, utilizing successive over-relaxation to solve the Poisson-Boltzmann equation. Journal of Computational Chemistry, 1991, 12, 435-445.	1.5	1,194
35	Protein folding and association: Insights from the interfacial and thermodynamic properties of hydrocarbons. Proteins: Structure, Function and Bioinformatics, 1991, 11, 281-296.	1.5	5,360