Malcolm E Davis

List of Publications by Year
in descending order

22	3,109	393982 19	642321 23
papers	citations	h-index	g-index

23	23	23	1945
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Conserved Core Substructures in the Overlay of Proteinâ€“Ligand Complexes. Journal of Chemical Information and Modeling, 2011, 51, 1931-1941.	2.5	13
2	An Atomic and Molecular View of the Depth Dependence of the Free Energies of Solute Transfer from Water into Lipid Bilayers. Molecular Pharmaceutics, 2011, 8, 2204-2215.	2.3	22
3	DRUG DISCOVERY INTERFACE: Functional Group Dependence of Solute Partitioning to Various Locations within a DOPC Bilayer: A Comparison of Molecular Dynamics Simulations with Experiment. Journal of Pharmaceutical Sciences, 2011, 100, 2136-2146.	1.6	28
4	Proteinâ˜Ligand NOE Matching:Â A High-Throughput Method for Binding Pose Evaluation That Does Not Require Protein NMR Resonance Assignments. Journal of the American Chemical Society, 2006, 128, 7252-7263.	6.6	48
5	Solid-phase synthesis and SAR of 4-carboxy-2-azetidinone mechanism-based tryptase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 2233-2239.	1.0	63
6	Implementation of a six-dimensional search using theAMoRetranslation function for difficult molecular-replacement problems. Journal of Applied Crystallography, 1999, 32, 98-101.	1.9	32
7	Empirical free energy calculations: a blind test and further improvements to the method 1 1Edited by F. E. Cohen. Journal of Molecular Biology, 1997, 268, 401-411.	2.0	76
8	Finite difference Poisson-Boltzmann electrostatic calculations: Increased accuracy achieved by harmonic dielectric smoothing and charge antialiasing. Journal of Computational Chemistry, 1997, 18, 268-276.	1.5	70
9	Electrostatics and diffusion of molecules in solution: simulations with the University of Houston Brownian Dynamics program. Computer Physics Communications, 1995, 91, 57-95.	3.0	622
10	A Comparison of Particle-Particle, Particle-Mesh and Ewald Methods for Calculating Electrostatic Interactions in Periodic Molecular Systems. Molecular Simulation, 1994, 14, 11-20.	0.9	187
11	Simulation of enzymeâ€“substrate encounter with gated active sites. Nature Structural and Molecular Biology, 1994, 1, 65-69.	3.6	71
12	The inducible multipole solvation model: A new model for solvation effects on solute electrostatics. Journal of Chemical Physics, 1994, 100, 5149-5159.	1.2	38
13	Electrostatics in biomolecular structure and dynamics. [Erratum to document cited in CA112(25):231952j]. Chemical Reviews, 1993, 93, 1669-1669.	23.0	4
14	Brownian dynamics simulations of diffusional encounters between triose phosphate isomerase and glyceraldehyde phosphate: electrostatic steering of glyceraldehyde phosphate. The Journal of Physical Chemistry, 1993, 97, 233-237.	2.9	50
15	Computation of electrostatic forces on solvated molecules using the Poisson-Boltzmann equation. The Journal of Physical Chemistry, 1993, 97, 3591-3600.	2.9	324
16	Electrostatic energy calculations by a Finite-difference method: Rapid calculation of charge-solvent interaction energies. Journal of Computational Chemistry, 1992, 13, 768-771.	1.5	57
17	Solving the finite-difference non-linear Poisson-Boltzmann equation. Journal of Computational Chemistry, 1992, 13, 1114-1118.	1.5	98
18	Electrostatics and diffusion of molecules in solution: simulations with the University of Houston Brownian dynamics program. Computer Physics Communications, 1991, 62, 187-197.	3.0	457

#	Article	IF	Citations
19	Dielectric boundary smoothing in finite difference solutions of the poisson equation: An approach to improve accuracy and convergence. Journal of Computational Chemistry, 1991, 12, 909-912.	1.5	123
20	[22] Diffusion-controlled enzymatic reactions. Methods in Enzymology, 1991, 202, 473-497.	0.4	63
21	Electric-field distribution inside the bacterial photosynthetic reaction center of Rhodopseudomonas viridis. Chemical Physics Letters, 1990, 173, 246-252.	1.2	19
22	Electrostatics in biomolecular structure and dynamics. Chemical Reviews, 1990, 90, 509-521.	23.0	643