Donald Bashford

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

65 papers	9,596 citations	38 h-index	68 g-index
68 ext. papers	10,228 ext. citations	6.4 avg, IF	6.03 L-index

#	Paper	IF	Citations
65	Exploring protein native states and large-scale conformational changes with a modified generalized born model. *Proteins: Structure, Function and Bioinformatics*, **2004**, 55, 383-94	4.2	1728
64	Generalized born models of macromolecular solvation effects. *Annual Review of Physical Chemistry*, **2000**, 51, 129-52	15.7	977
63	pKa's of ionizable groups in proteins: atomic detail from a continuum electrostatic model. *Biochemistry*, **1990**, 29, 10219-25	3.2	957
62	Modification of the Generalized Born Model Suitable for Macromolecules. *Journal of Physical Chemistry B*, **2000**, 104, 3712-3720	3.4	830
61	Electrostatic calculations of the pKa values of ionizable groups in bacteriorhodopsin. *Journal of Molecular Biology*, **1992**, 224, 473-86	6.5	517
60	Determinants of a protein fold. Unique features of the globin amino acid sequences. *Journal of Molecular Biology*, **1987**, 196, 199-216	6.5	455
59	Effective Born radii in the generalized Born approximation: the importance of being perfect. *Journal of Computational Chemistry*, **2002**, 23, 1297-304	3.5	364
58	Multiple-site titration curves of proteins: an analysis of exact and approximate methods for their calculation. *The Journal of Physical Chemistry*, **1991**, 95, 9556-9561		274
57	Density Functional/Poisson-Boltzmann Calculations of Redox Potentials for Iron-Sulfur Clusters. *Journal of the American Chemical Society*, **1994**, 116, 11898-11914	16.4	272
56	Electrostatic calculations of side-chain pK(a) values in myoglobin and comparison with NMR data for histidines. *Biochemistry*, **1993**, 32, 8045-56	3.2	226
55	Calculation of Redox Potentials and pKa Values of Hydrated Transition Metal Cations by a Combined Density Functional and Continuum Dielectric Theory. *Inorganic Chemistry*, **1996**, 35, 4694-4702	5.1	215
54	An object-oriented programming suite for electrostatic effects in biological molecules An experience report on the MEAD project. *Lecture Notes in Computer Science*, **1997**, 233-240	0.9	176
53	Incorporating Solvation Effects into Density Functional Electronic Structure Calculations. *The Journal of Physical Chemistry*, **1994**, 98, 11059-11068		158
52	Identification and characterization of the first small molecule inhibitor of MDMX. *Journal of Biological Chemistry*, **2010**, 285, 10786-96	5.4	152
51	Structure and Dynamics of Self-Assembling Peptide Nanotubes and the Channel-Mediated Water Organization and Self-Diffusion. A Molecular Dynamics Study. *Journal of the American Chemical Society*, **1995**, 117, 9151-9158	16.4	152
50	Catalysis and sulfa drug resistance in dihydropteroate synthase. *Science*, **2012**, 335, 1110-4	33.3	147
49	Macroscopic electrostatic models for protonation states in proteins. *Frontiers in Bioscience - Landmark*, **2004**, 9, 1082-99	2.8	120

48	Incorporating Protein Environments in Density Functional Theory: A Self-Consistent Reaction Field Calculation of Redox Potentials of [2Fe2S] Clusters in Ferredoxin and Phthalate Dioxygenase Reductase. *Journal of Physical Chemistry A*, **1998**, 102, 6311-6324	2.8	112
47	pK(a) Calculations suggest storage of an excess proton in a hydrogen-bonded water network in bacteriorhodopsin. *Journal of Molecular Biology*, **2001**, 312, 203-19	6.5	105
46	Disordered p27Kip1 exhibits intrinsic structure resembling the Cdk2/cyclin A-bound conformation. *Journal of Molecular Biology*, **2005**, 353, 1118-28	6.5	90
45	Calculations of electrostatic interactions and pKas in the active site of Escherichia coli thioredoxin. *Biochemistry*, **1998**, 37, 10298-306	3.2	76
44	A theoretical study of the UV/visible absorption and emission solvatochromic properties of solvent-sensitive dyes. *ChemPhysChem*, **2003**, 4, 1084-94	3.2	75
43	CuZn Superoxide Dismutase Geometry Optimization, Energetics, and Redox Potential Calculations by Density Functional and Electrostatic Methods. *Inorganic Chemistry*, **1999**, 38, 940-950	5.1	75
42	HLA-DRB1*07:01 is associated with a higher risk of asparaginase allergies. *Blood*, **2014**, 124, 1266-76	2.2	70
41	Diffusion-collision model for the folding kinetics of myoglobin. *Proteins: Structure, Function and Bioinformatics*, **1988**, 4, 211-27	4.2	67
40	Density Functional and Electrostatic Calculations of Manganese Superoxide Dismutase Active Site Complexes in Protein Environments. *Inorganic Chemistry*, **1999**, 38, 929-939	5.1	64
39	Use of 1H NMR spectroscopy and computer simulations To analyze histidine pKa changes in a protein tyrosine phosphatase: experimental and theoretical determination of electrostatic properties in a small protein. *Biochemistry*, **1997**, 36, 11984-94	3.2	63
38	Proton affinity changes driving unidirectional proton transport in the bacteriorhodopsin photocycle. *Journal of Molecular Biology*, **2003**, 332, 1183-93	6.5	59
37	Electrostatic effects in biological molecules. *Current Opinion in Structural Biology*, **1991**, 1, 175-184	8.1	58
36	Protonation states and pH titration in the photocycle of photoactive yellow protein. *Biochemistry*, **2000**, 39, 1100-13	3.2	55
35	Photoisomerization and proton transfer in photoactive yellow protein. *Journal of the American Chemical Society*, **2003**, 125, 8186-94	16.4	54
34	Dynamics of a type VI reverse turn in a linear peptide in aqueous solution. *Folding & Design*, **1997**, 2, 35-46		51
33	Structural details, pathways, and energetics of unfolding apomyoglobin. *Journal of Molecular Biology*, **2003**, 325, 555-67	6.5	50
32	Stabilization of Charges and Protonation States in the Active Site of the Protein Tyrosine Phosphatases:A Computational Study *Journal of Physical Chemistry B*, **2000**, 104, 11321-11333	3.4	49
31	Density-Functional and Electrostatic Calculations for a Model of a Manganese Superoxide Dismutase Active Site in Aqueous Solution. *The Journal of Physical Chemistry*, **1996**, 100, 13498-13505		42

30	Density functional study of the mechanism of a tyrosine phosphatase: I. Intermediate formation. *Journal of the American Chemical Society*, **2002**, 124, 10225-35	16.4	41
29	Multiple-site ligand binding to flexible macromolecules: Separation of global and local conformational change and an iterative mobile clustering approach. *Journal of Computational Chemistry*, **1999**, 20, 1091-1111	3.5	40
28	Thermodynamics of a reverse turn motif. Solvent effects and side-chain packing. *Journal of Molecular Biology*, **1997**, 270, 305-17	6.5	38
27	Density Functional Vertical Self-Consistent Reaction Field Theory for Solvatochromism Studies of Solvent-Sensitive Dyes. *Journal of Physical Chemistry A*, **2004**, 108, 3545-3555	2.8	38
26	Brownian dynamics simulation of protein folding: a study of the diffusion-collision model. *Biopolymers*, **1987**, 26, 481-506	2.2	34
25	Diffusion-collision model for the folding kinetics of the lambda-repressor operator-binding domain. *Journal of Biomolecular Structure and Dynamics*, **1984**, 1, 1243-55	3.6	32
24	Incomplete folding upon binding mediates Cdk4/cyclin D complex activation by tyrosine phosphorylation of inhibitor p27 protein. *Journal of Biological Chemistry*, **2011**, 286, 30142-51	5.4	31
23	Ligand binding mode prediction by docking: mdm2/mdmx inhibitors as a case study. *Journal of Chemical Information and Modeling*, **2014**, 54, 648-59	6.1	30
22	Density functional theory analysis of structure, energetics, and spectroscopy for the Mn-Fe active site of Chlamydia trachomatis ribonucleotide reductase in four oxidation states. *Inorganic Chemistry*, **2010**, 49, 7266-81	5.1	29
21	A Computational Study of the Role of Solvation Effects in Reverse Turn Formation in the Tetrapeptides APGD and APGN. *Journal of the American Chemical Society*, **1997**, 119, 4964-4971	16.4	27
20	Monitoring Ligand-Induced Protein Ordering in Drug Discovery. *Journal of Molecular Biology*, **2016**, 428, 1290-1303	6.5	24
19	Implicit Solvent Electrostatics in Biomolecular Simulation **2006**, 263-295		24
18	Electrostatic coupling to pH-titrating sites as a source of cooperativity in protein-ligand binding. *Protein Science*, **1998**, 7, 2012-25	6.3	23
17	Analysis of the active-site mechanism of tyrosyl-DNA phosphodiesterase I: a member of the phospholipase D superfamily. *Journal of Molecular Biology*, **2012**, 415, 741-58	6.5	22
16	Model for proton transport coupled to protein conformational change: application to proton pumping in the bacteriorhodopsin photocycle. *Journal of the American Chemical Society*, **2006**, 128, 16778-90	16.4	22
15	Computational studies of the early intermediates of the bacteriorhodopsin photocycle. *Biophysical Chemistry*, **1995**, 56, 95-104	3.5	22
14	Identification and characterization of an allosteric inhibitory site on dihydropteroate synthase. *ACS Chemical Biology*, **2014**, 9, 1294-302	4.9	21
13	Experimental and DFT studies: novel structural modifications greatly enhance the solvent sensitivity of live cell imaging dyes. *Journal of Physical Chemistry A*, **2007**, 111, 10849-60	2.8	20

12	An analytical algorithm for the rapid determination of the solvent accessibility of points in a three-dimensional lattice around a solute molecule. *Journal of Computational Chemistry*, **1995**, 16, 743-757	3.5	20
11	On the role of the conserved aspartate in the hydrolysis of the phosphocysteine intermediate of the low molecular weight tyrosine phosphatase. *Journal of the American Chemical Society*, **2004**, 126, 12677-84	16.4	19
10	Solvation energy density occlusion approximation for evaluation of desolvation penalties in biomolecular interactions. *Proteins: Structure, Function and Bioinformatics*, **2001**, 43, 12-27	4.2	17
9	A fluid salt-bridging cluster and the stabilization of p53. *Journal of Molecular Biology*, **2007**, 373, 1334-47	6.5	15
8	Use of Broken-Symmetry Density Functional Theory To Characterize the IspH Oxidized State: Implications for IspH Mechanism and Inhibition. *Journal of Chemical Theory and Computation*, **2014**, 10, 3871-3884	6.4	13
7	Efficient aminoacylation of the tRNA(Ala) acceptor stem: dependence on the 2:71 base pair. *Rna*, **2002**, 8, 659-70	5.8	13
6	Broken-Symmetry DFT Computations for the Reaction Pathway of IspH, an Iron-Sulfur Enzyme in Pathogenic Bacteria. *Inorganic Chemistry*, **2015**, 54, 6439-61	5.1	11
5	Mössbauer properties of the diferric cluster and the differential iron(II)-binding affinity of the iron sites in protein R2 of class Ia Escherichia coli ribonucleotide reductase: a DFT/electrostatics study. *Dalton Transactions*, **2011**, 40, 11164-75	4.3	10
4	Quantitative structure-activity relationship (QSAR) for a series of novel cannabinoid derivatives using descriptors derived from semi-empirical quantum-chemical calculations. *Bioorganic and Medicinal Chemistry*, **2009**, 17, 2598-606	3.4	10
3	Performance of a docking/molecular dynamics protocol for virtual screening of nutlin-class inhibitors of Mdmx. *Journal of Molecular Graphics and Modelling*, **2017**, 74, 54-60	2.8	8
2	Fluctuation and rotation in diffusion-influenced monomolecular reactions. *Journal of Chemical Physics*, **1986**, 85, 6999-7010	3.9	4
1	Electrostatic Calculations of the pKa of Ionizable Groups in Bacteriorhodopsin. *Jerusalem Symposia on Quantum Chemistry and Biochemistry*, **1992**, 107-114		