Donald Bashford

List of Publications by Year
in descending order

65 papers	10,825 citations	87723 38 h-index	106150 65 g-index
68 all docs	68 docs citations	68 times ranked	9508 citing authors

#	Article	IF	Citations
1	Exploring protein native states and large-scale conformational changes with a modified generalized born model. Proteins: Structure, Function and Bioinformatics, 2004, 55, 383-394.	1.5	2,068
2	GENERALIZEDBORNMODELS OFMACROMOLECULARSOLVATIONEFFECTS. Annual Review of Physical Chemistry, 2000, 51, 129-152.	4.8	1,073
3	pKa's of ionizable groups in proteins: atomic detail from a continuum electrostatic model. Biochemistry, 1990, 29, 10219-10225.	1.2	1,045
4	Modification of the Generalized Born Model Suitable for Macromolecules. Journal of Physical Chemistry B, 2000, 104, 3712-3720.	1.2	973
5	Electrostatic calculations of the pKa values of ionizable groups in bacteriorhodopsin. Journal of Molecular Biology, 1992, 224, 473-486.	2.0	546
6	Determinants of a protein fold. Journal of Molecular Biology, 1987, 196, 199-216.	2.0	485
7	Effective Born radii in the generalized Born approximation: The importance of being perfect. Journal of Computational Chemistry, 2002, 23, 1297-1304.	1.5	412
8	Density Functional/Poisson-Boltzmann Calculations of Redox Potentials for Iron-Sulfur Clusters. Journal of the American Chemical Society, 1994, 116, 11898-11914.	6.6	305
9	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.	2.9	303
10	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.	1.9	238
11	Electrostatic calculations of side-chain pKa values in myoglobin and comparison with NMR data for histidines. Biochemistry, 1993, 32, 8045-8056.	1.2	237
12	Catalysis and Sulfa Drug Resistance in Dihydropteroate Synthase. Science, 2012, 335, 1110-1114.	6.0	210
13	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.	1.0	192
14	Incorporating Solvation Effects into Density Functional Electronic Structure Calculations. The Journal of Physical Chemistry, 1994, 98, 11059-11068.	2.9	171
15	Identification and Characterization of the First Small Molecule Inhibitor of MDMX. Journal of Biological Chemistry, 2010, 285, 10786-10796.	1.6	171
16	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.	6.6	163
17	Incorporating Protein Environments in Density Functional Theory:Â 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.	1.1	130
18	Macroscopic electrostatic models for protonation states in proteins. Frontiers in Bioscience - Landmark, 2004, 9, 1082.	3.0	126

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19	p K a calculations suggest storage of an excess proton in a hydrogen-bonded water network in bacteriorhodopsin 1 1Edited by G. von Heijne. Journal of Molecular Biology, 2001, 312, 203-219.	2.0	110
20	Disordered p27Kip1 Exhibits Intrinsic Structure Resembling the Cdk2/Cyclin A-bound Conformation. Journal of Molecular Biology, 2005, 353, 1118-1128.	2.0	103
21	CuZn Superoxide Dismutase Geometry Optimization, Energetics, and Redox Potential Calculations by Density Functional and Electrostatic Methods. Inorganic Chemistry, 1999, 38, 940-950.	1.9	90
22	A Theoretical Study of the UV/Visible Absorption and Emission Solvatochromic Properties of Solvent-Sensitive Dyes. ChemPhysChem, 2003, 4, 1084-1094.	1.0	84
23	HLA-DRB1*07:01 is associated with a higher risk of asparaginase allergies. Blood, 2014, 124, 1266-1276.	0.6	84
24	Calculations of Electrostatic Interactions and pKas in the Active Site of Escherichia coli Thioredoxin,. Biochemistry, 1998, 37, 10298-10306.	1.2	82
25	Density Functional and Electrostatic Calculations of Manganese Superoxide Dismutase Active Site Complexes in Protein Environments. Inorganic Chemistry, 1999, 38, 929-939.	1.9	72
26	Diffusion-collision model for the folding kinetics of myoglobin. Proteins: Structure, Function and Bioinformatics, 1988, 4, 211-227.	1.5	71
27	Use of1H NMR Spectroscopy and Computer Simulations To Analyze Histidine pKaChanges in a Protein Tyrosine Phosphatase:Â Experimental and Theoretical Determination of Electrostatic Properties in a Small Proteinâ€. Biochemistry, 1997, 36, 11984-11994.	1.2	68
28	Electrostatic effects in biological molecules. Current Opinion in Structural Biology, 1991, 1, 175-184.	2.6	63
29	Proton Affinity Changes Driving Unidirectional Proton Transport in the Bacteriorhodopsin Photocycle. Journal of Molecular Biology, 2003, 332, 1183-1193.	2.0	63
30	Dynamics of a type VI reverse turn in a linear peptide in aqueous solution. Folding & Design, 1997, 2, 35-46.	4.5	57
31	Protonation States and pH Titration in the Photocycle of Photoactive Yellow Proteinâ€. Biochemistry, 2000, 39, 1100-1113.	1.2	55
32	Photoisomerization and Proton Transfer in Photoactive Yellow Protein. Journal of the American Chemical Society, 2003, 125, 8186-8194.	6.6	54
33	Structural Details, Pathways, and Energetics of Unfolding Apomyoglobin. Journal of Molecular Biology, 2003, 325, 555-567.	2.0	52
34	Stabilization of Charges and Protonation States in the Active Site of the Protein Tyrosine Phosphatases:Â A Computational Studyâ€. Journal of Physical Chemistry B, 2000, 104, 11321-11333.	1.2	49
35	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.	2.9	47
36	Density Functional Vertical Self-Consistent Reaction Field Theory for Solvatochromism Studies of Solvent-Sensitive Dyes. Journal of Physical Chemistry A, 2004, 108, 3545-3555.	1.1	45

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37	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.	1.5	44
38	Density Functional Study of the Mechanism of a Tyrosine Phosphatase:Â I. Intermediate Formation. Journal of the American Chemical Society, 2002, 124, 10225-10235.	6.6	44
39	Thermodynamics of a reverse turn motif. Solvent effects and side-chain packing. Journal of Molecular Biology, 1997, 270, 305-317.	2.0	39
40	Diffusion-Collision Model for the Folding Kinetics of the Î»-Repressor Operator-Binding Domain. Journal of Biomolecular Structure and Dynamics, 1984, 1, 1243-1255.	2.0	38
41	Brownian dynamics simulation of protein folding: A study of the diffusion-collision model. Biopolymers, 1987, 26, 481-506.	1.2	37
42	Incomplete Folding upon Binding Mediates Cdk4/Cyclin D Complex Activation by Tyrosine Phosphorylation of Inhibitor p27 Protein. Journal of Biological Chemistry, 2011, 286, 30142-30151.	1.6	37
43	Ligand Binding Mode Prediction by Docking: Mdm2/Mdmx Inhibitors as a Case Study. Journal of Chemical Information and Modeling, 2014, 54, 648-659.	2.5	35
44	Identification and Characterization of an Allosteric Inhibitory Site on Dihydropteroate Synthase. ACS Chemical Biology, 2014, 9, 1294-1302.	1.6	34
45	Density Functional Theory Analysis of Structure, Energetics, and Spectroscopy for the Mnâ''Fe Active Site of Chlamydia trachomatis Ribonucleotide Reductase in Four Oxidation States. Inorganic Chemistry, 2010, 49, 7266-7281.	1.9	32
46	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.	6.6	29
47	Monitoring Ligand-Induced Protein Ordering in Drug Discovery. Journal of Molecular Biology, 2016, 428, 1290-1303.	2.0	29
48	Implicit Solvent Electrostatics in Biomolecular Simulation. , 2006, , 263-295.		29
49	Analysis of the Active-Site Mechanism of Tyrosyl-DNA Phosphodiesterase I: A Member of the Phospholipase D Superfamily. Journal of Molecular Biology, 2012, 415, 741-758.	2.0	28
50	Electrostatic coupling to pHâ€titrating sites as a source of cooperativity in proteinâ€ligand binding. Protein Science, 1998, 7, 2012-2025.	3.1	25
51	Experimental and DFT Studies:Â Novel Structural Modifications Greatly Enhance the Solvent Sensitivity of Live Cell Imaging Dyes. Journal of Physical Chemistry A, 2007, 111, 10849-10860.	1.1	25
52	Model for Proton Transport Coupled to Protein Conformational Change:Â Application to Proton Pumping in the Bacteriorhodopsin Photocycle. Journal of the American Chemical Society, 2006, 128, 16778-16790.	6.6	24
53	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.	1.5	23
54	Computational studies of the early intermediates of the bacteriorhodopsin photocycle. Biophysical Chemistry, 1995, 56, 95-104.	1.5	22

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55	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, 12677-12684.	6.6	22
56	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.	2.3	21
57	A Fluid Salt-bridging Cluster and the Stabilization of p53. Journal of Molecular Biology, 2007, 373, 1334-1347.	2.0	19
58	Broken-Symmetry DFT Computations for the Reaction Pathway of IspH, an Ironâ€“Sulfur Enzyme in Pathogenic Bacteria. Inorganic Chemistry, 2015, 54, 6439-6461.	1.9	18
59	Solvation energy density occlusion approximation for evaluation of desolvation penalties in biomolecular interactions. Proteins: Structure, Function and Bioinformatics, 2001, 43, 12-27.	1.5	17
60	Efficient aminoacylation of the tRNAAla acceptor stem: Dependence on the 2:71 base pair. Rna, 2002, 8, 659-670.	1.6	14
61	Quantitative structureâ€“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, 2598-2606.	1.4	12
62	MÃ¶ssbauer 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.	1.6	12
63	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.	1.3	12
64	Fluctuation and rotation in diffusionâ€influenced monomolecular reactions. Journal of Chemical Physics, 1986, 85, 6999-7010.	1.2	4
65	Electrostatic Calculations of the pK a â€™s of Ionizable Groups in Bacteriorhodopsin. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1992, , 107-114.	0.2	0