

Donald Bashford

List of Publications by Year in Descending Order

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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	Performance of a docking/molecular dynamics protocol for virtual screening of nutlin-class inhibitors of Mdmx. <i>Journal of Molecular Graphics and Modelling</i> , 2017 , 74, 54-60	2.8	8
64	Monitoring Ligand-Induced Protein Ordering in Drug Discovery. <i>Journal of Molecular Biology</i> , 2016 , 428, 1290-1303	6.5	24
63	Broken-Symmetry DFT Computations for the Reaction Pathway of IspH, an Iron-Sulfur Enzyme in Pathogenic Bacteria. <i>Inorganic Chemistry</i> , 2015 , 54, 6439-61	5.1	11
62	Ligand binding mode prediction by docking: mdm2/mdmx inhibitors as a case study. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 648-59	6.1	30
61	Identification and characterization of an allosteric inhibitory site on dihydropteroate synthase. <i>ACS Chemical Biology</i> , 2014 , 9, 1294-302	4.9	21
60	Use of Broken-Symmetry Density Functional Theory To Characterize the IspH Oxidized State: Implications for IspH Mechanism and Inhibition. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3871-3884	6.4	13
59	HLA-DRB1*07:01 is associated with a higher risk of asparaginase allergies. <i>Blood</i> , 2014 , 124, 1266-76	2.2	70
58	Analysis of the active-site mechanism of tyrosyl-DNA phosphodiesterase I: a member of the phospholipase D superfamily. <i>Journal of Molecular Biology</i> , 2012 , 415, 741-58	6.5	22
57	Catalysis and sulfa drug resistance in dihydropteroate synthase. <i>Science</i> , 2012 , 335, 1110-4	33.3	147
56	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. <i>Dalton Transactions</i> , 2011 , 40, 11164-75	4.3	10
55	Incomplete folding upon binding mediates Cdk4/cyclin D complex activation by tyrosine phosphorylation of inhibitor p27 protein. <i>Journal of Biological Chemistry</i> , 2011 , 286, 30142-51	5.4	31
54	Density functional theory analysis of structure, energetics, and spectroscopy for the Mn-Fe active site of Chlamydia trachomatis ribonucleotide reductase in four oxidation states. <i>Inorganic Chemistry</i> , 2010 , 49, 7266-81	5.1	29
53	Identification and characterization of the first small molecule inhibitor of MDMX. <i>Journal of Biological Chemistry</i> , 2010 , 285, 10786-96	5.4	152
52	Quantitative structure-activity relationship (QSAR) for a series of novel cannabinoid derivatives using descriptors derived from semi-empirical quantum-chemical calculations. <i>Bioorganic and Medicinal Chemistry</i> , 2009 , 17, 2598-606	3.4	10
51	Experimental and DFT studies: novel structural modifications greatly enhance the solvent sensitivity of live cell imaging dyes. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 10849-60	2.8	20
50	A fluid salt-bridging cluster and the stabilization of p53. <i>Journal of Molecular Biology</i> , 2007 , 373, 1334-476.5	16.4	15
49	Model for proton transport coupled to protein conformational change: application to proton pumping in the bacteriorhodopsin photocycle. <i>Journal of the American Chemical Society</i> , 2006 , 128, 16778-90	16.4	22

48	Implicit Solvent Electrostatics in Biomolecular Simulation 2006 , 263-295		24
47	Disordered p27Kip1 exhibits intrinsic structure resembling the Cdk2/cyclin A-bound conformation. <i>Journal of Molecular Biology</i> , 2005 , 353, 1118-28	6.5	90
46	Macroscopic electrostatic models for protonation states in proteins. <i>Frontiers in Bioscience - Landmark</i> , 2004 , 9, 1082-99	2.8	120
45	Exploring protein native states and large-scale conformational changes with a modified generalized born model. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004 , 55, 383-94	4.2	1728
44	On the role of the conserved aspartate in the hydrolysis of the phosphocysteine intermediate of the low molecular weight tyrosine phosphatase. <i>Journal of the American Chemical Society</i> , 2004 , 126, 12677-84	16.4	19
43	Density Functional Vertical Self-Consistent Reaction Field Theory for Solvatochromism Studies of Solvent-Sensitive Dyes. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 3545-3555	2.8	38
42	A theoretical study of the UV/visible absorption and emission solvatochromic properties of solvent-sensitive dyes. <i>ChemPhysChem</i> , 2003 , 4, 1084-94	3.2	75
41	Photoisomerization and proton transfer in photoactive yellow protein. <i>Journal of the American Chemical Society</i> , 2003 , 125, 8186-94	16.4	54
40	Structural details, pathways, and energetics of unfolding apomyoglobin. <i>Journal of Molecular Biology</i> , 2003 , 325, 555-67	6.5	50
39	Proton affinity changes driving unidirectional proton transport in the bacteriorhodopsin photocycle. <i>Journal of Molecular Biology</i> , 2003 , 332, 1183-93	6.5	59
38	Effective Born radii in the generalized Born approximation: the importance of being perfect. <i>Journal of Computational Chemistry</i> , 2002 , 23, 1297-304	3.5	364
37	Efficient aminoacylation of the tRNA(Ala) acceptor stem: dependence on the 2:71 base pair. <i>Rna</i> , 2002 , 8, 659-70	5.8	13
36	Density functional study of the mechanism of a tyrosine phosphatase: I. Intermediate formation. <i>Journal of the American Chemical Society</i> , 2002 , 124, 10225-35	16.4	41
35	Solvation energy density occlusion approximation for evaluation of desolvation penalties in biomolecular interactions. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001 , 43, 12-27	4.2	17
34	pK(a) Calculations suggest storage of an excess proton in a hydrogen-bonded water network in bacteriorhodopsin. <i>Journal of Molecular Biology</i> , 2001 , 312, 203-19	6.5	105
33	Generalized born models of macromolecular solvation effects. <i>Annual Review of Physical Chemistry</i> , 2000 , 51, 129-52	15.7	977
32	Protonation states and pH titration in the photocycle of photoactive yellow protein. <i>Biochemistry</i> , 2000 , 39, 1100-13	3.2	55
31	Modification of the Generalized Born Model Suitable for Macromolecules. <i>Journal of Physical Chemistry B</i> , 2000 , 104, 3712-3720	3.4	830

30	Stabilization of Charges and Protonation States in the Active Site of the Protein Tyrosine Phosphatases: [A Computational Study] <i>Journal of Physical Chemistry B</i> , 2000 , 104, 11321-11333	3.4	49
29	Multiple-site ligand binding to flexible macromolecules: Separation of global and local conformational change and an iterative mobile clustering approach. <i>Journal of Computational Chemistry</i> , 1999 , 20, 1091-1111	3.5	40
28	CuZn Superoxide Dismutase Geometry Optimization, Energetics, and Redox Potential Calculations by Density Functional and Electrostatic Methods. <i>Inorganic Chemistry</i> , 1999 , 38, 940-950	5.1	75
27	Density Functional and Electrostatic Calculations of Manganese Superoxide Dismutase Active Site Complexes in Protein Environments. <i>Inorganic Chemistry</i> , 1999 , 38, 929-939	5.1	64
26	Electrostatic coupling to pH-titrating sites as a source of cooperativity in protein-ligand binding. <i>Protein Science</i> , 1998 , 7, 2012-25	6.3	23
25	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. <i>Journal of Physical Chemistry A</i> , 1998 , 102, 6311-6324	2.8	112
24	Calculations of electrostatic interactions and pKas in the active site of Escherichia coli thioredoxin. <i>Biochemistry</i> , 1998 , 37, 10298-306	3.2	76
23	A Computational Study of the Role of Solvation Effects in Reverse Turn Formation in the Tetrapeptides APGD and APGN. <i>Journal of the American Chemical Society</i> , 1997 , 119, 4964-4971	16.4	27
22	An object-oriented programming suite for electrostatic effects in biological molecules An experience report on the MEAD project. <i>Lecture Notes in Computer Science</i> , 1997 , 233-240	0.9	176
21	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. <i>Biochemistry</i> , 1997 , 36, 11984-94	3.2	63
20	Thermodynamics of a reverse turn motif. Solvent effects and side-chain packing. <i>Journal of Molecular Biology</i> , 1997 , 270, 305-17	6.5	38
19	Dynamics of a type VI reverse turn in a linear peptide in aqueous solution. <i>Folding & Design</i> , 1997 , 2, 35-46		51
18	Calculation of Redox Potentials and pKa Values of Hydrated Transition Metal Cations by a Combined Density Functional and Continuum Dielectric Theory. <i>Inorganic Chemistry</i> , 1996 , 35, 4694-4702	5.1	215
17	Density-Functional and Electrostatic Calculations for a Model of a Manganese Superoxide Dismutase Active Site in Aqueous Solution. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 13498-13505		42
16	Structure and Dynamics of Self-Assembling Peptide Nanotubes and the Channel-Mediated Water Organization and Self-Diffusion. A Molecular Dynamics Study. <i>Journal of the American Chemical Society</i> , 1995 , 117, 9151-9158	16.4	152
15	An analytical algorithm for the rapid determination of the solvent accessibility of points in a three-dimensional lattice around a solute molecule. <i>Journal of Computational Chemistry</i> , 1995 , 16, 743-757	3.5	20
14	Computational studies of the early intermediates of the bacteriorhodopsin photocycle. <i>Biophysical Chemistry</i> , 1995 , 56, 95-104	3.5	22
13	Incorporating Solvation Effects into Density Functional Electronic Structure Calculations. <i>The Journal of Physical Chemistry</i> , 1994 , 98, 11059-11068		158

12	Density Functional/Poisson-Boltzmann Calculations of Redox Potentials for Iron-Sulfur Clusters. <i>Journal of the American Chemical Society</i> , 1994 , 116, 11898-11914	16.4	272
11	Electrostatic calculations of side-chain pK(a) values in myoglobin and comparison with NMR data for histidines. <i>Biochemistry</i> , 1993 , 32, 8045-56	3.2	226
10	Electrostatic calculations of the pKa values of ionizable groups in bacteriorhodopsin. <i>Journal of Molecular Biology</i> , 1992 , 224, 473-86	6.5	517
9	Electrostatic Calculations of the pKa of Ionizable Groups in Bacteriorhodopsin. <i>Jerusalem Symposia on Quantum Chemistry and Biochemistry</i> , 1992 , 107-114		
8	Electrostatic effects in biological molecules. <i>Current Opinion in Structural Biology</i> , 1991 , 1, 175-184	8.1	58
7	Multiple-site titration curves of proteins: an analysis of exact and approximate methods for their calculation. <i>The Journal of Physical Chemistry</i> , 1991 , 95, 9556-9561		274
6	pKa's of ionizable groups in proteins: atomic detail from a continuum electrostatic model. <i>Biochemistry</i> , 1990 , 29, 10219-25	3.2	957
5	Diffusion-collision model for the folding kinetics of myoglobin. <i>Proteins: Structure, Function and Bioinformatics</i> , 1988 , 4, 211-27	4.2	67
4	Determinants of a protein fold. Unique features of the globin amino acid sequences. <i>Journal of Molecular Biology</i> , 1987 , 196, 199-216	6.5	455
3	Brownian dynamics simulation of protein folding: a study of the diffusion-collision model. <i>Biopolymers</i> , 1987 , 26, 481-506	2.2	34
2	Fluctuation and rotation in diffusion-influenced monomolecular reactions. <i>Journal of Chemical Physics</i> , 1986 , 85, 6999-7010	3.9	4
1	Diffusion-collision model for the folding kinetics of the lambda-repressor operator-binding domain. <i>Journal of Biomolecular Structure and Dynamics</i> , 1984 , 1, 1243-55	3.6	32