James M Briggs

List of Publications by Year in descending order

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75 papers	4,519 citations	134610 34 h-index	116156 66 g-index
76 all docs	76 docs citations	76 times ranked	4419 citing authors

#	Article	IF	Citations
1	Antibody mix-and-read assays based on fluorescence intensity probes. MAbs, 2021, 13, 1980178.	2.6	0
2	Antibody mix-and-read assays based on fluorescence intensity probes. MAbs, 2021, 13, 1980178.	2.6	1
3	Impact of lymphomaâ€linked Asn11Tyr point mutation on the interaction between Bclâ€2 and a BH3 mimetic: Insights from molecular dynamics simulation. Chemical Biology and Drug Design, 2020, 95, 435-450.	1.5	2
4	Insights into the substrate binding specificity of quorum-quenching acylase PvdQ. Journal of Molecular Graphics and Modelling, 2019, 88, 104-120.	1.3	16
5	Discovery of vascular Rho kinase (ROCK) inhibitory peptides. Experimental Biology and Medicine, 2019, 244, 940-951.	1.1	2
6	Immobilization and unbinding investigation of the antigen-antibody complex using theoretical and experimental techniques. Journal of Molecular Graphics and Modelling, 2019, 86, 219-227.	1.3	3
7	Targeted reduction of the EGFR protein, but not inhibition of its kinase activity, induces mitophagy and death of cancer cells through activation of mTORC2 and Akt. Oncogenesis, 2018, 7, 5.	2.1	34
8	Structural mutation analysis of PTEN and its genotypeâ€phenotype correlations in endometriosis and cancer. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1625-1643.	1.5	37
9	Functional Implications of the spectrum of BCL2 mutations in Lymphoma. Mutation Research - Reviews in Mutation Research, 2016, 769, 1-18.	2.4	22
10	Inhibition of Cholera Toxin and Other AB Toxins by Polyphenolic Compounds. PLoS ONE, 2016, 11, e0166477.	1.1	32
11	Biophysical Characteristics of Cholera Toxin andEscherichia coliHeat-Labile Enterotoxin Structure and Chemistry Lead to Differential Toxicity. Journal of Physical Chemistry B, 2015, 119, 1048-1061.	1.2	16
12	New Insights into the Binding and Catalytic Mechanisms of Bacillus thuringiensis Lactonase: Insights into B. thuringiensis AiiA Mechanism. PLoS ONE, 2013, 8, e75395.	1.1	8
13	Pharmacophoreâ€Based Virtual Screening to Aid in the Identification of Unknown Protein Function. Chemical Biology and Drug Design, 2012, 80, 828-842.	1.5	10
14	Mechanistic role of NS4A and substrate in the activation of HCV NS3 protease. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2428-2443.	1.5	14
15	Computational insights into the interaction of the anthrax lethal factor with the Nâ€terminal region of its substrates. Proteins: Structure, Function and Bioinformatics, 2009, 75, 323-335.	1.5	10
16	Cluster analysis of hydration waters around the active sites of bacterial alanine racemase using a 2â€ns MD simulation. Biopolymers, 2008, 89, 210-219.	1.2	9
17	Molecular dynamics simulations of Factor Xa: Insight into conformational transition of its binding subsites. Biopolymers, 2008, 89, 1104-1113.	1.2	9
18	Simulation of pH-Dependent Properties of Proteins Using Mesoscopic Models. Reviews in Computational Chemistry, 2007, , 249-311.	1.5	9

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19	Dopamine D1 Receptor Agonist and D2 Receptor Antagonist Effects of the Natural Product (â^')â€“Stepholidine: Molecular Modeling and Dynamics Simulations. Biophysical Journal, 2007, 93, 1431-1441.	0.2	38
20	Hybrid Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulations of HIV-1 Integrase/Inhibitor Complexes. Biophysical Journal, 2007, 93, 3613-3626.	0.2	15
21	Dynamic Pharmacophore Model Optimization:Â Identification of Novel HIV-1 Integrase Inhibitors. Journal of Medicinal Chemistry, 2006, 49, 1684-1692.	2.9	89
22	Computed Pore Potentials of the Nicotinic Acetylcholine Receptor. Biophysical Journal, 2006, 91, 1325-1335.	0.2	8
23	Electrostatic Steering at Acetylcholine Binding Sites. Biophysical Journal, 2006, 91, 1302-1314.	0.2	24
24	Comparative molecular dynamics simulations of HIV-1 integrase and the T66I/M154I mutant: Binding modes and drug resistance to a diketo acid inhibitor. Proteins: Structure, Function and Bioinformatics, 2005, 59, 723-741.	1.5	41
25	The 1.9 Ã... Crystal Structure of Alanine Racemase from Mycobacterium tuberculosis Contains a Conserved Entryway into the Active Site,. Biochemistry, 2005, 44, 1471-1481.	1.2	86
26	Dynamic Receptor-Based Pharmacophore Model Development and Its Application in Designing Novel HIV-1 Integrase Inhibitors. Journal of Medicinal Chemistry, 2005, 48, 1496-1505.	2.9	73
27	Comparison of Multiple Molecular Dynamics Trajectories Calculated for the Drug-Resistant HIV-1 Integrase T66I/M154I Catalytic Domain. Biophysical Journal, 2005, 88, 3072-3082.	0.2	48
28	Large-Scale Conformational Dynamics of the HIV-1 Integrase Core Domain and Its Catalytic Loop Mutants. Biophysical Journal, 2005, 88, 3133-3146.	0.2	58
29	Cluster analysis of water molecules in alanine racemase and their putative structural role. Protein Engineering, Design and Selection, 2004, 17, 223-234.	1.0	31
30	HIV-1 integrase pharmacophore model derived from diverse classes of inhibitors. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 1447-1454.	1.0	44
31	Efficient 3D Database Screening for Novel HIV-1 IN Inhibitors. Journal of Chemical Information and Computer Sciences, 2004, 44, 1450-1455.	2.8	44
32	Prediction of HIV-1 Integrase/Viral DNA Interactions in the Catalytic Domain by Fast Molecular Docking. Journal of Medicinal Chemistry, 2004, 47, 821-828.	2.9	52
33	Molecular dynamics studies of alanine racemase: A structural model for drug design. Biopolymers, 2003, 70, 186-200.	1.2	19
34	Chargeâ€“Charge Interactions are Key Determinants of the pK Values of Ionizable Groups in Ribonuclease Sa (pI=3.5) and a Basic Variant (pI=10.2). Journal of Molecular Biology, 2003, 325, 1077-1092.	2.0	96
35	pK Values of Histidine Residues in Ribonuclease Sa: Effect of Salt and Net Charge. Journal of Molecular Biology, 2003, 325, 1093-1105.	2.0	37
36	Molecular Dynamics Studies of the Wild-Type and Double Mutant HIV-1 Integrase Complexed with the 5CITEP Inhibitor: Mechanism for Inhibition and Drug Resistance. Biophysical Journal, 2003, 84, 1450-1463.	0.2	78

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37	Brownian Dynamics Simulations of the Recognition of the Scorpion Toxin P05 with the Small-conductance Calcium-activated Potassium Channels. Journal of Molecular Biology, 2002, 318, 417-428.	2.0	45
38	Brownian Dynamics Simulations of the Recognition of the Scorpion Toxin Maurotoxin with the Voltage-Gated Potassium Ion Channels. Biophysical Journal, 2002, 83, 2370-2385.	0.2	49
39	The association between a negatively charged ligand and the electronegative binding pocket of its receptor. Biopolymers, 2002, 63, 247-260.	1.2	18
40	Chargeâ€“charge interactions are the primary determinants of the pK values of the ionizable groups in Ribonuclease T1. Biophysical Chemistry, 2002, 101-102, 211-219.	1.5	10
41	A structure-based design approach for the identification of novel inhibitors: application to an alanine racemase. Journal of Computer-Aided Molecular Design, 2002, 16, 935-953.	1.3	25
42	Brownian Dynamics Simulations of Interaction Between Scorpion Toxin Lq2 and Potassium Ion Channel. Biophysical Journal, 2001, 80, 1659-1669.	0.2	42
43	A Model for Enzymeâ”Substrate Interaction in Alanine Racemase. Journal of the American Chemical Society, 2001, 123, 2830-2834.	6.6	32
44	Comparative molecular field analysis (coMFA) study of epothilones-tubulin depolymerization inhibitors: pharmacophore development using 3D QSAR methods. , 2001, 15, 41-55.		30
45	Similarities in the HIV-1 and ASV integrase active sites upon metal cofactor binding. Biopolymers, 2000, 53, 308-315.	1.2	27
46	Effects of pore mutations and permeant ion concentration on the spontaneous gating activity of OmpC porin. Protein Engineering, Design and Selection, 2000, 13, 491-500.	1.0	26
47	Developing a Dynamic Pharmacophore Model for HIV-1 Integrase. Journal of Medicinal Chemistry, 2000, 43, 2100-2114.	2.9	271
48	Investigations on human immunodeficiency virus type 1 integrase/DNA binding interactions via molecular dynamics and electrostatics calculations. , 2000, 85, 123-131.		22
49	Poisson-Boltzmann model studies of molecular electrostatic properties of the cAMP-dependent protein kinase. European Biophysics Journal, 1999, 28, 457-467.	1.2	10
50	Molecular Dynamics Studies on the HIV-1 Integrase Catalytic Domain. Biophysical Journal, 1999, 76, 2999-3011.	0.2	78
51	Calculation of the pKa Values for the Ligands and Side Chains of Escherichia coli d-Alanine:d-Alanine Ligase. Journal of Medicinal Chemistry, 1999, 42, 109-117.	2.9	28
52	Prediction of pKas of Titratable Residues in Proteins Using a Poisson-Boltzmann Model of the Solute-Solvent System. Lecture Notes in Computational Science and Engineering, 1999, , 176-196.	0.1	2
53	Correlation between rate of enzyme-substrate diffusional encounter and average Boltzmann factor around active site. , 1998, 45, 355-360.		19
54	Rapid binding of a cationic active site inhibitor to wild type and mutant mouse acetylcholinesterase: Brownian dynamics simulation including diffusion in the active site gorge. Biopolymers, 1998, 46, 465-474.	1.2	58

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55	Brownian and Essential Dynamics Studies of the HIV-1 Integrase Catalytic Domain. Journal of Biomolecular Structure and Dynamics, 1998, 16, 733-745.	2.0	17
56	pKaShift Effects on Backbone Amide Base-Catalyzed Hydrogen Exchange Rates in Peptides. Journal of the American Chemical Society, 1998, 120, 3735-3738.	6.6	35
57	On the Mechanism of Acetylcholinesterase Action:Â The Electrostatically Induced Acceleration of the Catalytic Acylation Step. Journal of the American Chemical Society, 1997, 119, 8159-8165.	6.6	53
58	Electrostatic and non-electrostatic contributions to the binding free energies of anthracycline antibiotics to DNA. Journal of Molecular Biology, 1997, 274, 253-267.	2.0	104
59	Absolute Configuration of Bromochlorofluoromethane from Molecular Dynamics Simulation of Its Enantioselective Complexation by Cryptophane-C. Journal of the American Chemical Society, 1997, 119, 3818-3823.	6.6	74
60	On the variational approach to Poissonâ€“Boltzmann free energies. Chemical Physics Letters, 1997, 281, 135-139.	1.2	68
61	A 240-Fold Electrostatic Rate-Enhancement for Acetylcholinesteraseâ^'Substrate Binding Can Be Predicted by the Potential within the Active Site. Journal of the American Chemical Society, 1996, 118, 13069-13070.	6.6	36
62	Computing ionization states of proteins with a detailed charge model. Journal of Computational Chemistry, 1996, 17, 1633-1644.	1.5	139
63	Orientational steering in enzyme-substrate association: Ionic strength dependence of hydrodynamic torque effects. European Biophysics Journal, 1996, 24, 137-41.	1.2	37
64	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
65	Parallelization of Poissonâ€"Boltzmann and Brownian Dynamics Calculations. ACS Symposium Series, 1995, , 170-185.	0.5	6
66	Conservative and nonconservative mutations in proteins: Anomalous mutations in a transport receptor analyzed by free energy and quantum chemical calculations. Protein Science, 1995, 4, 387-393.	3.1	3
67	Simulation of enzymeâ€“substrate encounter with gated active sites. Nature Structural and Molecular Biology, 1994, 1, 65-69.	3.6	71
68	Quantification of Solvent Effects on the Acidities of Z and E Esters from Fluid Simulations. Journal of the American Chemical Society, 1994, 116, 10630-10638.	6.6	30
69	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
70	Monte Carlo simulations of liquid acetic acid and methyl acetate with the OPLS potential functions. The Journal of Physical Chemistry, 1991, 95, 3315-3322.	2.9	149
71	Monte Carlo simulations of liquid alkyl ethers with the OPLS potential functions. Journal of Computational Chemistry, 1990, 11, 958-971.	1.5	141
72	Relative partition coefficients for organic solutes from fluid simulations. The Journal of Physical Chemistry, 1990, 94, 1683-1686.	2.9	500

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73	A priori pKa calculations and the hydration of organic anions. Journal of the American Chemical Society, 1989, 111, 4190-4197.	6.6	138
74	Monte Carlo simulations of liquid acetonitrile with a three-site model. Molecular Physics, 1988, 63, 547-558.	0.8	227
75	A priori calculations of pKa's for organic compounds in water. The pKa of ethane. Journal of the American Chemical Society, 1987, 109, 6857-6858.	6.6	111