

# James M Briggs

## List of Publications by Year in descending order

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75  
papers

4,519  
citations

117625

34  
h-index

102487

66  
g-index

76  
all docs

76  
docs citations

76  
times ranked

3875  
citing authors

#	ARTICLE	IF	CITATIONS
1	Electrostatics and diffusion of molecules in solution: simulations with the University of Houston Brownian Dynamics program. <i>Computer Physics Communications</i> , 1995, 91, 57-95.	7.5	622
2	Relative partition coefficients for organic solutes from fluid simulations. <i>The Journal of Physical Chemistry</i> , 1990, 94, 1683-1686.	2.9	500
3	Developing a Dynamic Pharmacophore Model for HIV-1 Integrase. <i>Journal of Medicinal Chemistry</i> , 2000, 43, 2100-2114.	6.4	271
4	Monte Carlo simulations of liquid acetonitrile with a three-site model. <i>Molecular Physics</i> , 1988, 63, 547-558.	1.7	227
5	Monte Carlo simulations of liquid acetic acid and methyl acetate with the OPLS potential functions. <i>The Journal of Physical Chemistry</i> , 1991, 95, 3315-3322.	2.9	149
6	Monte Carlo simulations of liquid alkyl ethers with the OPLS potential functions. <i>Journal of Computational Chemistry</i> , 1990, 11, 958-971.	3.3	141
7	Computing ionization states of proteins with a detailed charge model. <i>Journal of Computational Chemistry</i> , 1996, 17, 1633-1644.	3.3	139
8	A priori pKa calculations and the hydration of organic anions. <i>Journal of the American Chemical Society</i> , 1989, 111, 4190-4197.	13.7	138
9	A priori calculations of pKa's for organic compounds in water. The pKa of ethane. <i>Journal of the American Chemical Society</i> , 1987, 109, 6857-6858.	13.7	111
10	Electrostatic and non-electrostatic contributions to the binding free energies of anthracycline antibiotics to DNA. <i>Journal of Molecular Biology</i> , 1997, 274, 253-267.	4.2	104
11	Charge-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). <i>Journal of Molecular Biology</i> , 2003, 325, 1077-1092.	4.2	96
12	Dynamic Pharmacophore Model Optimization: Identification of Novel HIV-1 Integrase Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 1684-1692.	6.4	89
13	The 1.9 Å... Crystal Structure of Alanine Racemase from <i>Mycobacterium tuberculosis</i> Contains a Conserved Entryway into the Active Site. <i>Biochemistry</i> , 2005, 44, 1471-1481.	2.5	86
14	Molecular Dynamics Studies on the HIV-1 Integrase Catalytic Domain. <i>Biophysical Journal</i> , 1999, 76, 2999-3011.	0.5	78
15	Molecular Dynamics Studies of the Wild-Type and Double Mutant HIV-1 Integrase Complexed with the 5CITEP Inhibitor: Mechanism for Inhibition and Drug Resistance. <i>Biophysical Journal</i> , 2003, 84, 1450-1463.	0.5	78
16	Absolute Configuration of Bromochlorofluoromethane from Molecular Dynamics Simulation of Its Enantioselective Complexation by Cryptophane-C. <i>Journal of the American Chemical Society</i> , 1997, 119, 3818-3823.	13.7	74
17	Dynamic Receptor-Based Pharmacophore Model Development and Its Application in Designing Novel HIV-1 Integrase Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 1496-1505.	6.4	73
18	Simulation of enzyme-substrate encounter with gated active sites. <i>Nature Structural and Molecular Biology</i> , 1994, 1, 65-69.	8.2	71

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19	On the variational approach to Poisson-Boltzmann free energies. <i>Chemical Physics Letters</i> , 1997, 281, 135-139.	2.6	68
20	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. <i>Biopolymers</i> , 1998, 46, 465-474.	2.4	58
21	Large-Scale Conformational Dynamics of the HIV-1 Integrase Core Domain and Its Catalytic Loop Mutants. <i>Biophysical Journal</i> , 2005, 88, 3133-3146.	0.5	58
22	On the Mechanism of Acetylcholinesterase Action: The Electrostatically Induced Acceleration of the Catalytic Acylation Step. <i>Journal of the American Chemical Society</i> , 1997, 119, 8159-8165.	13.7	53
23	Prediction of HIV-1 Integrase/Viral DNA Interactions in the Catalytic Domain by Fast Molecular Docking. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 821-828.	6.4	52
24	Brownian dynamics simulations of diffusional encounters between triose phosphate isomerase and glyceraldehyde phosphate: electrostatic steering of glyceraldehyde phosphate. <i>The Journal of Physical Chemistry</i> , 1993, 97, 233-237.	2.9	50
25	Brownian Dynamics Simulations of the Recognition of the Scorpion Toxin Maurotoxin with the Voltage-Gated Potassium Ion Channels. <i>Biophysical Journal</i> , 2002, 83, 2370-2385.	0.5	49
26	Comparison of Multiple Molecular Dynamics Trajectories Calculated for the Drug-Resistant HIV-1 Integrase T66I/M154I Catalytic Domain. <i>Biophysical Journal</i> , 2005, 88, 3072-3082.	0.5	48
27	Brownian Dynamics Simulations of the Recognition of the Scorpion Toxin P05 with the Small-conductance Calcium-activated Potassium Channels. <i>Journal of Molecular Biology</i> , 2002, 318, 417-428.	4.2	45
28	HIV-1 integrase pharmacophore model derived from diverse classes of inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2004, 14, 1447-1454.	2.2	44
29	Efficient 3D Database Screening for Novel HIV-1 IN Inhibitors. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 1450-1455.	2.8	44
30	Brownian Dynamics Simulations of Interaction Between Scorpion Toxin Lq2 and Potassium Ion Channel. <i>Biophysical Journal</i> , 2001, 80, 1659-1669.	0.5	42
31	Comparative molecular dynamics simulations of HIV-1 integrase and the T66I/M154I mutant: Binding modes and drug resistance to a diketo acid inhibitor. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 59, 723-741.	2.6	41
32	Dopamine D1 Receptor Agonist and D2 Receptor Antagonist Effects of the Natural Product ( $\alpha$ )-Stepholidine: Molecular Modeling and Dynamics Simulations. <i>Biophysical Journal</i> , 2007, 93, 1431-1441.	0.5	38
33	Oriental steering in enzyme-substrate association: Ionic strength dependence of hydrodynamic torque effects. <i>European Biophysics Journal</i> , 1996, 24, 137-41.	2.2	37
34	pK Values of Histidine Residues in Ribonuclease Sa: Effect of Salt and Net Charge. <i>Journal of Molecular Biology</i> , 2003, 325, 1093-1105.	4.2	37
35	Structural mutation analysis of PTEN and its genotype-phenotype correlations in endometriosis and cancer. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 1625-1643.	2.6	37
36	A 240-Fold Electrostatic Rate-Enhancement for Acetylcholinesterase's Substrate Binding Can Be Predicted by the Potential within the Active Site. <i>Journal of the American Chemical Society</i> , 1996, 118, 13069-13070.	13.7	36

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37	pKaShift Effects on Backbone Amide Base-Catalyzed Hydrogen Exchange Rates in Peptides. <i>Journal of the American Chemical Society</i> , 1998, 120, 3735-3738.	13.7	35
38	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. <i>Oncogenesis</i> , 2018, 7, 5.	4.9	34
39	A Model for Enzyme-Substrate Interaction in Alanine Racemase. <i>Journal of the American Chemical Society</i> , 2001, 123, 2830-2834.	13.7	32
40	Inhibition of Cholera Toxin and Other AB Toxins by Polyphenolic Compounds. <i>PLoS ONE</i> , 2016, 11, e0166477.	2.5	32
41	Cluster analysis of water molecules in alanine racemase and their putative structural role. <i>Protein Engineering, Design and Selection</i> , 2004, 17, 223-234.	2.1	31
42	Quantification of Solvent Effects on the Acidities of Z and E Esters from Fluid Simulations. <i>Journal of the American Chemical Society</i> , 1994, 116, 10630-10638.	13.7	30
43	Comparative molecular field analysis (coMFA) study of epothilones-tubulin depolymerization inhibitors: pharmacophore development using 3D QSAR methods. , 2001, 15, 41-55.		30
44	Calculation of the pKa Values for the Ligands and Side Chains of Escherichia coli d-Alanine:d-Alanine Ligase. <i>Journal of Medicinal Chemistry</i> , 1999, 42, 109-117.	6.4	28
45	Similarities in the HIV-1 and ASV integrase active sites upon metal cofactor binding. <i>Biopolymers</i> , 2000, 53, 308-315.	2.4	27
46	Effects of pore mutations and permeant ion concentration on the spontaneous gating activity of OmpC porin. <i>Protein Engineering, Design and Selection</i> , 2000, 13, 491-500.	2.1	26
47	A structure-based design approach for the identification of novel inhibitors: application to an alanine racemase. <i>Journal of Computer-Aided Molecular Design</i> , 2002, 16, 935-953.	2.9	25
48	Electrostatic Steering at Acetylcholine Binding Sites. <i>Biophysical Journal</i> , 2006, 91, 1302-1314.	0.5	24
49	Investigations on human immunodeficiency virus type 1 integrase/DNA binding interactions via molecular dynamics and electrostatics calculations. , 2000, 85, 123-131.		22
50	Functional Implications of the spectrum of BCL2 mutations in Lymphoma. <i>Mutation Research - Reviews in Mutation Research</i> , 2016, 769, 1-18.	5.5	22
51	Correlation between rate of enzyme-substrate diffusional encounter and average Boltzmann factor around active site. , 1998, 45, 355-360.		19
52	Molecular dynamics studies of alanine racemase: A structural model for drug design. <i>Biopolymers</i> , 2003, 70, 186-200.	2.4	19
53	The association between a negatively charged ligand and the electronegative binding pocket of its receptor. <i>Biopolymers</i> , 2002, 63, 247-260.	2.4	18
54	Brownian and Essential Dynamics Studies of the HIV-1 Integrase Catalytic Domain. <i>Journal of Biomolecular Structure and Dynamics</i> , 1998, 16, 733-745.	3.5	17

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55	Biophysical Characteristics of Cholera Toxin and Escherichia coli Heat-Labile Enterotoxin Structure and Chemistry Lead to Differential Toxicity. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1048-1061.	2.6	16
56	Insights into the substrate binding specificity of quorum-quenching acylase PvdQ. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 88, 104-120.	2.4	16
57	Hybrid Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulations of HIV-1 Integrase/Inhibitor Complexes. <i>Biophysical Journal</i> , 2007, 93, 3613-3626.	0.5	15
58	Mechanistic role of NS4A and substrate in the activation of HCV NS3 protease. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 2428-2443.	2.6	14
59	Poisson-Boltzmann model studies of molecular electrostatic properties of the cAMP-dependent protein kinase. <i>European Biophysics Journal</i> , 1999, 28, 457-467.	2.2	10
60	Charge-charge interactions are the primary determinants of the pK values of the ionizable groups in Ribonuclease T1. <i>Biophysical Chemistry</i> , 2002, 101-102, 211-219.	2.8	10
61	Computational insights into the interaction of the anthrax lethal factor with the N-terminal region of its substrates. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 75, 323-335.	2.6	10
62	Pharmacophore-Based Virtual Screening to Aid in the Identification of Unknown Protein Function. <i>Chemical Biology and Drug Design</i> , 2012, 80, 828-842.	3.2	10
63	Simulation of pH-Dependent Properties of Proteins Using Mesoscopic Models. <i>Reviews in Computational Chemistry</i> , 2007, , 249-311.	1.5	9
64	Cluster analysis of hydration waters around the active sites of bacterial alanine racemase using a MD simulation. <i>Biopolymers</i> , 2008, 89, 210-219.	2.4	9
65	Molecular dynamics simulations of Factor Xa: Insight into conformational transition of its binding subsites. <i>Biopolymers</i> , 2008, 89, 1104-1113.	2.4	9
66	Computed Pore Potentials of the Nicotinic Acetylcholine Receptor. <i>Biophysical Journal</i> , 2006, 91, 1325-1335.	0.5	8
67	New Insights into the Binding and Catalytic Mechanisms of Bacillus thuringiensis Lactonase: Insights into B. thuringiensis AiiA Mechanism. <i>PLoS ONE</i> , 2013, 8, e75395.	2.5	8
68	Parallelization of Poisson-Boltzmann and Brownian Dynamics Calculations. <i>ACS Symposium Series</i> , 1995, , 170-185.	0.5	6
69	Conservative and nonconservative mutations in proteins: Anomalous mutations in a transport receptor analyzed by free energy and quantum chemical calculations. <i>Protein Science</i> , 1995, 4, 387-393.	7.6	3
70	Immobilization and unbinding investigation of the antigen-antibody complex using theoretical and experimental techniques. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 86, 219-227.	2.4	3
71	Discovery of vascular Rho kinase (ROCK) inhibitory peptides. <i>Experimental Biology and Medicine</i> , 2019, 244, 940-951.	2.4	2
72	Impact of lymphoma-linked Asn11Tyr point mutation on the interaction between Bcl2 and a BH3 mimetic: Insights from molecular dynamics simulation. <i>Chemical Biology and Drug Design</i> , 2020, 95, 435-450.	3.2	2

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73	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.	0.3	2
74	Antibody mix-and-read assays based on fluorescence intensity probes. MAbs, 2021, 13, 1980178.	5.2	1
75	Antibody mix-and-read assays based on fluorescence intensity probes. MAbs, 2021, 13, 1980178.	5.2	0