Jeffry D Madura

List of Publications by Year
in descending order

129 papers	43,436 citations	126907 33 h-index	23533 111 g-index
138 all docs	138 docs citations	138 times ranked	37496 citing authors

#	Article	IF	Citations
1	Comparison of simple potential functions for simulating liquid water. Journal of Chemical Physics, 1983, 79, 926-935.	3.0	34,333
2	Optimized intermolecular potential functions for liquid hydrocarbons. Journal of the American Chemical Society, 1984, 106, 6638-6646.	13.7	2,069
3	Development of an improved four-site water model for biomolecular simulations: TIP4P-Ew. Journal of Chemical Physics, 2004, 120, 9665-9678.	3.0	1,747
4	Temperature and size dependence for Monte Carlo simulations of TIP4P water. Molecular Physics, 1985, 56, 1381-1392.	1.7	706
5	Electrostatics and diffusion of molecules in solution: simulations with the University of Houston Brownian Dynamics program. Computer Physics Communications, 1995, 91, 57-95.	7.5	622
6	Electrostatics and diffusion of molecules in solution: simulations with the University of Houston Brownian dynamics program. Computer Physics Communications, 1991, 62, 187-197.	7.5	457
7	Quantum and statistical mechanical studies of liquids. 25. Solvation and conformation of methanol in water. Journal of the American Chemical Society, 1983, 105, 1407-1413.	13.7	378
8	Ab initio and Monte Carlo calculations for a nucleophilic addition reaction in the gas phase and in aqueous solution. Journal of the American Chemical Society, 1986, 108, 2517-2527.	13.7	185
9	Electronic origins and consequences of pyramidalization of asymmetric alkenes in ground and triplet excited states. Journal of the American Chemical Society, 1983, 105, 5980-5988.	13.7	97
10	Molecular dynamics simulation with a continuum electrostatic model of the solvent. Journal of Computational Chemistry, 1995, 16, 1081-1095.	3.3	96
11	Family 18 chitinaseâ€“oligosaccharide substrate interaction: subsite preference and anomer selectivity of Serratia marcescens chitinase A. Biochemical Journal, 2003, 376, 87-95.	3.7	91
12	Antifreeze Proteins at the Ice/Water Interface: Three Calculated Discriminating Properties for Orientation of Type I Proteins. Biophysical Journal, 2007, 93, 1442-1451.	0.5	90
13	Molecular recognition and binding of thermal hysteresis proteins to ice. , 2000, 13, 101-113.		88
14	Effect of a Bound Non-Nucleoside RT Inhibitor on the Dynamics of Wild-Type and Mutant HIV-1 Reverse Transcriptase. Journal of the American Chemical Society, 2005, 127, 17253-17260.	13.7	74
15	Fischer route to pyrido[3,2-g]indoles. A novel receptor for urea derivatives. Journal of the American Chemical Society, 1990, 112, 4549-4550.	13.7	73
16	Dopamine transporter comparative molecular modeling and binding site prediction using the LeuT_{Aa} leucine transporter as a template. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1033-1046.	2.6	72
17	Photonic crystal protein hydrogel sensor materials enabled by conformationally induced volume phase transition. Chemical Science, 2016, 7, 4557-4562.	7.4	72
18	Simulation of enzymeâ€“substrate encounter with gated active sites. Nature Structural and Molecular Biology, 1994, 1, 65-69.	8.2	71

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19	Biological Applications of Electrostatic Calculations and Brownian Dynamics Simulations. Reviews in Computational Chemistry, 2007, , 229-267.	1.5	70
20	[22] Diffusion-controlled enzymatic reactions. Methods in Enzymology, 1991, 202, 473-497.	1.0	63
21	Interactions of the D- and L-Forms of Winter Flounder Antifreeze Peptide with the {201} Planes of Ice. Journal of the American Chemical Society, 1994, 116, 417-418.	13.7	63
22	Global Transitions of Proteins Explored by a Multiscale Hybrid Methodology: Application to Adenylate Kinase. Biophysical Journal, 2013, 105, 1643-1652.	0.5	63
23	Effects of truncating long-range interactions in aqueous ionic solution simulations. Chemical Physics Letters, 1988, 150, 105-108.	2.6	59
24	Scanning electron microscopy and molecular modeling of inhibition of calcium oxalate monohydrate crystal growth by citrate and phosphocitrate. Calcified Tissue International, 1995, 56, 297-304.	3.1	51
25	Gibbs free energies of formation of pcdds: Evaluation of estimation methods and application for predicting dehalogenation pathways. Environmental Toxicology and Chemistry, 1996, 15, 824-836.	4.3	51
26	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
27	Kinetic and Mechanistic Studies of Prolyl Oligopeptidase from the Hyperthermophile Pyrococcus furiosus. Journal of Biological Chemistry, 2001, 276, 19310-19317.	3.4	50
28	Water under high pressure. Molecular Physics, 1988, 64, 325-336.	1.7	46
29	Docking of sulfonamides to carbonic anhydrase II and IV. Journal of Molecular Graphics and Modelling, 2000, 18, 283-289.	2.4	45
30	CoMFA 3D-QSAR Analysis of HIV-1 RT Nonnucleoside Inhibitors, TIBO Derivatives Based on Docking Conformation and Alignment. Journal of Chemical Information and Computer Sciences, 2004, 44, 2167-2178.	2.8	45
31	Monoamine Transporter Structure, Function, Dynamics, and Drug Discovery: A Computational Perspective. AAPS Journal, 2012, 14, 820-831.	4.4	39
32	Homology Modeling of Glycosyl Hydrolase Family 18 Enzymes and Proteins. Journal of Chemical Information and Computer Sciences, 1997, 37, 999-1005.	2.8	38
33	Structure modeling, ligand binding, and binding affinity calculation (LR-MM-PBSA) of human heparanase for inhibition and drug design. Proteins: Structure, Function and Bioinformatics, 2006, 65, 580-592.	2.6	37
34	Receptor-Based Modeling and 3D-QSAR for a Quantitative Production of the Butyrylcholinesterase Inhibitors Based on Genetic Algorithm. Journal of Chemical Information and Modeling, 2008, 48, 1092-1103.	5.4	37
35	Relative free energy of binding and binding mode calculations of HIV-1 RT inhibitors based on dock-MM-PB/GS. Proteins: Structure, Function and Bioinformatics, 2004, 57, 493-503.	2.6	35
36	Molecular dynamics of leucine and dopamine transporter proteins in a model cell membrane lipid bilayer. Proteins: Structure, Function and Bioinformatics, 2010, 78, 797-811.	2.6	33

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37	Computer Simulations of Organic Reactions in Solution. Annals of the New York Academy of Sciences, 1986, 482, 198-209.	3.8	32
38	Salt Dependence of an Î±-Helical Peptide Folding Energy Landscapes. Biochemistry, 2009, 48, 10818-10826.	2.5	32
39	A Review of Coarse-Grained Molecular Dynamics Techniques to Access Extended Spatial and Temporal Scales in Biomolecular Simulations. Annual Reports in Computational Chemistry, 2011, , 67-87.	1.7	32
40	Modeling Studies of Binding of Sea Raven Type II Antifreeze Protein to Ice. Journal of Chemical Information and Computer Sciences, 1997, 37, 1006-1010.	2.8	30
41	Molecular dynamics of HIV-1 reverse transcriptase indicates increased flexibility upon DNA binding. Proteins: Structure, Function and Bioinformatics, 2001, 45, 176-182.	2.6	30
42	Solution Structural Ensembles of Substrate-Free Cytochrome P450_{cam}. Biochemistry, 2012, 51, 3383-3393.	2.5	30
43	HIV-1 RT Nonnucleoside Inhibitors and Their Interaction with RT for Antiviral Drug Development. Infectious Disorders - Drug Targets, 2006, 6, 391-413.	0.8	29
44	Structural and Dynamic Implications of an Effector-induced Backbone Amide cisâ€“trans Isomerization in Cytochrome P450cam. Journal of Molecular Biology, 2009, 388, 801-814.	4.2	28
45	LeuT Conformational Sampling Utilizing Accelerated Molecular Dynamics and Principal Component Analysis. Biophysical Journal, 2012, 103, L1-L3.	0.5	28
46	Brownian dynamics simulation of diffusional encounters between triose phosphate isomerase and D-glyceraldehyde phosphate. The Journal of Physical Chemistry, 1989, 93, 7285-7287.	2.9	27
47	Kinetic and Docking Studies of the Interaction of Quinones with the Quinone Reductase Active Siteâ€. Biochemistry, 2003, 42, 1985-1994.	2.5	27
48	Discovery of Novel Selective Serotonin Reuptake Inhibitors through Development of a Protein-Based Pharmacophore. Journal of Chemical Information and Modeling, 2011, 51, 2417-2426.	5.4	27
49	Polyglutamine Fibrils: New Insights into Antiparallel Î²-Sheet Conformational Preference and Side Chain Structure. Journal of Physical Chemistry B, 2016, 120, 3012-3026.	2.6	27
50	A Python Program for Solving SchrÃ¶dingerâ€™s Equation in Undergraduate Physical Chemistry. Journal of Chemical Education, 2017, 94, 813-815.	2.3	27
51	Polymorphism and second harmonic generation in a novel diamond-like semiconductor: Li2MnSnS4. Journal of Solid State Chemistry, 2015, 231, 256-266.	2.9	26
52	Chemical Shift Tensors of Cimetidine Form A Modeled with Density Functional Theory Calculations: Implications for NMR Crystallography. Journal of Physical Chemistry A, 2020, 124, 3109-3119.	2.5	26
53	Solubility of simple, nonpolar compounds in TIP4P-Ew. Journal of Chemical Physics, 2006, 124, 016102.	3.0	25
54	Benchmarking docking and scoring protocol for the identification of potential acetylcholinesterase inhibitors. Journal of Molecular Graphics and Modelling, 2010, 28, 870-882.	2.4	25

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55	Sodium Perchlorate Effects on the Helical Stability of a Mainly Alanine Peptide. Biophysical Journal, 2010, 98, 186-196.	0.5	25
56	Accelerated Molecular Dynamics and Protein Conformational Change: A Theoretical and Practical Guide Using a Membrane Embedded Model Neurotransmitter Transporter. Methods in Molecular Biology, 2015, 1215, 253-287.	0.9	25
57	Molecular recognition: effect of rotational isomers on host-guest binding. Journal of the American Chemical Society, 1993, 115, 879-884.	13.7	24
58	Experimentally Restrained Molecular Dynamics Simulations for Characterizing the Open States of Cytochrome P450_{cam}. Biochemistry, 2011, 50, 1664-1671.	2.5	24
59	Peptide-encapsulated CdS nanoclusters from a combinatorial ligand library. Chemical Communications, 2000, , 209-210.	4.1	22
60	A Role for Fragment-Based Drug Design in Developing Novel Lead Compounds for Central Nervous System Targets. Frontiers in Neurology, 2015, 6, 197.	2.4	22
61	Calculations of the electrostatic free energy contributions to the binding free energy of sulfonamides to carbonic anhydrase. Structural Chemistry, 1996, 7, 131-138.	2.0	21
62	Interaction of the Phospholipid Head Group with Representative Quartz and Aluminosilicate Structures: An Ab initio Study. Journal of Physical Chemistry B, 2008, 112, 7095-7103.	2.6	21
63	Docking of non-nucleoside inhibitors: Neotripterifordin and its derivatives to HIV-1 reverse transcriptase. Proteins: Structure, Function and Bioinformatics, 2002, 49, 529-542.	2.6	20
64	Design, synthesis, and testing of an 6-O-linked series of benzimidazole based inhibitors of CDK5/p25. Bioorganic and Medicinal Chemistry, 2011, 19, 359-373.	3.0	20
65	Effective Computational Modeling of Constitutional Isomerism and Aggregation States of Explicit Solvates of Lithiated Phenylacetonitrile. Journal of Organic Chemistry, 2002, 67, 3832-3840.	3.2	19
66	Comparative Protein Modeling. Reviews in Computational Chemistry, 2006, , 57-167.	1.5	19
67	Family 18 chitolectins: Comparison of MGP40 and HUMGP39. Biochemical and Biophysical Research Communications, 2007, 359, 221-226.	2.1	19
68	Structure of Aqueous Sodium Perchlorate Solutions. Journal of Physical Chemistry B, 2008, 112, 15417-15425.	2.6	19
69	Insights from molecular dynamics: The binding site of cocaine in the dopamine transporter and permeation pathways of substrates in the leucine and dopamine transporters. Journal of Molecular Graphics and Modelling, 2012, 38, 1-12.	2.4	19
70	New design strategies for antidepressant drugs. Expert Opinion on Drug Discovery, 2013, 8, 1399-1414.	5.0	19
71	A Review of Monoamine Transporter-Ligand Interactions. Current Computer-Aided Drug Design, 2013, 9, 556-568.	1.2	19
72	Identification of a Novel Selective Serotonin Reuptake Inhibitor by Coupling Monoamine Transporter-Based Virtual Screening and Rational Molecular Hybridization. ACS Chemical Neuroscience, 2011, 2, 544-552.	3.5	18

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73	Monomeric Polyglutamine Structures That Evolve into Fibrils. Journal of Physical Chemistry B, 2017, 121, 5953-5967.	2.6	18
74	Structure activity relationships of anthranilic acid-based compounds on cellular and in vivo mitogen activated protein kinase-5 signaling pathways. Bioorganic and Medicinal Chemistry Letters, 2018, 28, 2294-2301.	2.2	18
75	Hydrogen bond analysis of Type 1 antifreeze protein in water and the ice/water interface. PhysChemComm, 2001, 4, 32-36.	0.8	17
76	Molecular Dynamics Simulation of Crystal-Induced Membranolysis. Journal of Physical Chemistry B, 2003, 107, 12346-12351.	2.6	17
77	Solvation of Metal Cations in Non-aqueous Liquids. Journal of Solution Chemistry, 2011, 40, 1383-1398.	1.2	16
78	The dynamics and binding of a Type III antifreeze protein in water and on ice. Computational and Theoretical Chemistry, 1996, 388, 65-77.	1.5	15
79	Chapter 5 A Review of the TIP4P, TIP4P-Ew, TIP5P, and TIP5P-E Water Models. Annual Reports in Computational Chemistry, 2005, 1, 59-74.	1.7	15
80	Physical and structural properties of taurine and taurine analogues. Amino Acids, 1997, 13, 131-139.	2.7	14
81	Exploring the Physicochemical Properties of Oxime-Reactivation Therapeutics for Cyclosarin, Sarin, Tabun, and VX Inactivated Acetylcholinesterase. Chemical Research in Toxicology, 2014, 27, 99-110.	3.3	14
82	2-Substituted 3Â-Aryltropane Cocaine Analogs Produce Atypical Effects without Inducing Inward-Facing Dopamine Transporter Conformations. Journal of Pharmacology and Experimental Therapeutics, 2016, 356, 624-634.	2.5	14
83	Teaching Reciprocal Space to Undergraduates via Theory and Code Components of an IPython Notebook. Journal of Chemical Education, 2016, 93, 2106-2109.	2.3	13
84	Synthesis and computational evaluation of a boronium ion analogue of the tropane ring system. Tetrahedron Letters, 1996, 37, 2729-2730.	1.4	12
85	Molecular Dynamics Simulation Studies of the Effect of Phosphocitrate on Crystal-Induced Membranolysis. Biophysical Journal, 2005, 89, 2251-2257.	0.5	12
86	Investigations of structure and dynamics of water solvation of the type I antifreeze protein. International Journal of Quantum Chemistry, 2009, 109, 73-80.	2.0	12
87	Rapid and sustained antidepressant properties of an NMDA antagonist/monoamine reuptake inhibitor identified via transporter-based virtual screening. Pharmacology Biochemistry and Behavior, 2016, 150-151, 22-30.	2.9	12
88	Role of Nonpolar Amino Acid Functional Groups in the Surface Orientation-Dependent Adsorption of Natural and Synthetic Antifreeze Peptides on Ice. Crystal Growth and Design, 2008, 8, 3420-3429.	3.0	11
89	Receptor-Based Discovery of a Plasmalemmal Monoamine Transporter Inhibitor via High-Throughput Docking and Pharmacophore Modeling. ACS Chemical Neuroscience, 2010, 1, 223-233.	3.5	11
90	Î²-Amyloid and Neprilysin Computational Studies Identify Critical Residues Implicated in Binding Specificity. Journal of Chemical Information and Modeling, 2014, 54, 1157-1165.	5.4	10

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91	Discovery of Novel-Scaffold Monoamine Transporter Ligands via in Silico Screening with the S1 Pocket of the Serotonin Transporter. ACS Chemical Neuroscience, 2014, 5, 784-792.	3.5	10
92	Identifying trends in hydration behavior for modifications to the hydrophobicity of poly(n-isopropylacrylamide). Journal of Molecular Graphics and Modelling, 2017, 78, 168-175.	2.4	10
93	Computational and Experimental Determination of the Î±-Helix Unfolding Reaction Coordinate. Biochemistry, 2008, 47, 2046-2050.	2.5	8
94	Biological Testing of Organophosphorus-Inactivated Acetylcholinesterase Oxime Reactivators Identified via Virtual Screening. Chemical Research in Toxicology, 2016, 29, 1534-1540.	3.3	7
95	Geometric considerations in the calculation of relative free energies of activation. Chemical Physics Letters, 1987, 141, 83-87.	2.6	6
96	An Introduction to Simulation and Visualization of Biological Systems at Multiple Scales: A Summer Training Program for Interdisciplinary Research. Biotechnology Progress, 2006, 22, 179-185.	2.6	6
97	Quantitative Impact of a Cognitive Modeling Intelligent Tutoring System on Student Performance in Balancing Chemical Equations. The Chemical Educator, 2002, 7, 379-383.	0.0	5
98	Homology models for the tetrameric and dodecameric complexes of Lumbricus terrestris hemoglobin. Computational and Theoretical Chemistry, 2002, 592, 173-181.	1.5	5
99	Conformational Free-Energy Landscapes for a Peptide in Saline Environments. Biophysical Journal, 2012, 103, 2513-2520.	0.5	5
100	Molecular dynamics of conformation-specific dopamine transporter-inhibitor complexes. Journal of Molecular Graphics and Modelling, 2017, 76, 143-151.	2.4	5
101	A combined computational and experimental approach reveals the structure of a C/EBPÎ²â€“Spi1 interaction required for IL1B gene transcription. Journal of Biological Chemistry, 2018, 293, 19942-19956.	3.4	5
102	Dopamine Transporter Dynamics of N-Substituted Benztropine Analogs with Atypical Behavioral Effects. Journal of Pharmacology and Experimental Therapeutics, 2018, 366, 527-540.	2.5	5
103	Methods for calculating geometries of transition states in solution. Chemical Physics, 1989, 129, 185-191.	1.9	4
104	Docking Substrates to Metalloenzymes. Molecular Simulation, 2000, 24, 293-306.	2.0	4
105	Computational Chemistry in the Undergraduate Curriculum. Reviews in Computational Chemistry, 2007, , 149-228.	1.5	4
106	Structural dynamics of the monoamine transporter homolog LeuT from accelerated conformational sampling and channel analysis. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2289-2302.	2.6	4
107	Structure and Dynamics Study of LeuT Using the Markov State Model and Perturbation Response Scanning Reveals Distinct Ion Induced Conformational States. Journal of Physical Chemistry B, 2016, 120, 8361-8368.	2.6	3
108	GIBBS FREE ENERGIES OF FORMATION OF PCDDS: EVALUATION OF ESTIMATION METHODS AND APPLICATION FOR PREDICTING DEHALOGENATION PATHWAYS. Environmental Toxicology and Chemistry, 1996, 15, 824.	4.3	3

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109	A cell multipole based domain decomposition algorithm for molecular dynamics simulation of systems of arbitrary shape. Computer Physics Communications, 2002, 144, 141-153.	7.5	1
110	CoMFA 3D-QSAR Analysis of HIV-1 RT Nonnucleoside Inhibitors, TIBO Derivatives Based on Docking Conformation and Alignment.. ChemInform, 2005, 36, no.	0.0	1
111	Sodium versus potassium effects on the glutamic acid side-chains interaction on a heptapeptide. Journal of Theoretical and Computational Chemistry, 2014, 13, 1440004.	1.8	1
112	CO2(aq) Parameterization Through Free Energy Perturbation/Monte Carlo Simulations for Use in CO2 Sequestration. , 2009, , 337-357.		1
113	Development of an improved four-site water model for biomolecular simulations: TIP4P-Ew. , 0, .		1
114	MT ₁ receptor binding pocket insights based on de novo molecular modeling. FASEB Journal, 2006, 20, A1119.	0.5	1
115	Modeling of Antifreeze Proteins. Theoretical and Computational Chemistry, 1999, 8, 537-568.	0.4	0
116	Nucleic Acids: Structures, Properties, and Function. By Victor A. Bloomfield, Donald M. Crothers, and Ignacio Tinoco, Jr. University Science Books: Sausalito, CA; 2000. Clothbound, 800 pp, $88.00, ISBN 0-935702-49-0. The Chemical Educator, 2001, 6, 70-71.	0.0	0
117	A novel hybrid simulation for study of multiscale phenomena. Molecular Simulation, 2006, 32, 825-830.	2.0	0
118	Topical perspectives. Journal of Molecular Graphics and Modelling, 2010, 29, 115.	2.4	0
119	The JMGM/MGMS graphics prize. Journal of Molecular Graphics and Modelling, 2010, 29, 1.	2.4	0
120	Circular Dichroism and UV Resonance Raman Study of the Impact of Salts and Alcohols on the Gibbs Free Energy Landscape of an Î±-helical Peptide. , 2010, , .		0
121	Computational Investigation of the Effect of Ions on the Secondary Structure of Small Peptides. Biophysical Journal, 2011, 100, 378a.	0.5	0
122	Ligand Exit and Entry Pathways for Monoamine Transporters. Biophysical Journal, 2011, 100, 245a.	0.5	0
123	Global Transitions or Proteins Explored by a Multiscale Hybrid Methodology: Application to Dopamine Transporter. Biophysical Journal, 2013, 104, 226a-227a.	0.5	0
124	Analyzing a Conformational Sampling of LeuT from Accelerated Molecular Dynamics Simulations. Biophysical Journal, 2014, 106, 364a.	0.5	0
125	Editorial: In silico Modeling of Brain Receptors for Antidepressants, Psychostimulants, and Other CNS-Active Drugs. Frontiers in Pharmacology, 2015, 6, 302.	3.5	0
126	Tribute to J. Andrew McCammon. Journal of Physical Chemistry B, 2016, 120, 8055-8056.	2.6	0

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127	Evaluating Free Energies of Dimerization of Short Polyglutamine Peptides with Molecular Dynamics Simulations. Biophysical Journal, 2016, 110, 400a.	0.5	0
128	Crosslinking-Mass Spectrometry of Targeted Single Cys Mutants to Refine Allostery and Model Building in the Glycine Receptor. Biophysical Journal, 2017, 112, 321a-322a.	0.5	0
129	Free Energy Perturbation Monte Carlo Simulations of Salt Influences on Aqueous Freezing Point Depression. , 2009, , 359-370.		0