Jeffry D Madura

List of Publications by Year
in descending order

129 papers	43,436 citations	126858 33 h-index	24232 110 g-index
138 all docs	138 docs citations	138 times ranked	37496 citing authors

#	Article	IF	Citations
1	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.	1.1	26
2	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.	1.6	5
3	Dopamine Transporter Dynamics of N-Substituted Benztropine Analogs with Atypical Behavioral Effects. Journal of Pharmacology and Experimental Therapeutics, 2018, 366, 527-540.	1.3	5
4	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.	1.0	18
5	A Python Program for Solving SchrÃ¶dingerâ€™s Equation in Undergraduate Physical Chemistry. Journal of Chemical Education, 2017, 94, 813-815.	1.1	27
6	Monomeric Polyglutamine Structures That Evolve into Fibrils. Journal of Physical Chemistry B, 2017, 121, 5953-5967.	1.2	18
7	Crosslinking-Mass Spectrometry of Targeted Single Cys Mutants to Refine Allostery and Model Building in the Glycine Receptor. Biophysical Journal, 2017, 112, 321a-322a.	0.2	0
8	Identifying trends in hydration behavior for modifications to the hydrophobicity of poly(n-isopropylacrylamide). Journal of Molecular Graphics and Modelling, 2017, 78, 168-175.	1.3	10
9	Molecular dynamics of conformation-specific dopamine transporter-inhibitor complexes. Journal of Molecular Graphics and Modelling, 2017, 76, 143-151.	1.3	5
10	Photonic crystal protein hydrogel sensor materials enabled by conformationally induced volume phase transition. Chemical Science, 2016, 7, 4557-4562.	3.7	72
11	Biological Testing of Organophosphorus-Inactivated Acetylcholinesterase Oxime Reactivators Identified via Virtual Screening. Chemical Research in Toxicology, 2016, 29, 1534-1540.	1.7	7
12	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.	1.3	12
13	Tribute to J. Andrew McCammon. Journal of Physical Chemistry B, 2016, 120, 8055-8056.	1.2	0
14	Teaching Reciprocal Space to Undergraduates via Theory and Code Components of an IPython Notebook. Journal of Chemical Education, 2016, 93, 2106-2109.	1.1	13
15	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.	1.2	3
16	Evaluating Free Energies of Dimerization of Short Polyglutamine Peptides with Molecular Dynamics Simulations. Biophysical Journal, 2016, 110, 400a.	0.2	0
17	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.	1.3	14
18	Polyglutamine Fibrils: New Insights into Antiparallel Î²-Sheet Conformational Preference and Side Chain Structure. Journal of Physical Chemistry B, 2016, 120, 3012-3026.	1.2	27

#	Article	IF	Citations
19	A Role for Fragment-Based Drug Design in Developing Novel Lead Compounds for Central Nervous System Targets. Frontiers in Neurology, 2015, 6, 197.	1.1	22
20	Polymorphism and second harmonic generation in a novel diamond-like semiconductor: Li2MnSnS4. Journal of Solid State Chemistry, 2015, 231, 256-266.	1.4	26
21	Editorial: In silico Modeling of Brain Receptors for Antidepressants, Psychostimulants, and Other CNS-Active Drugs. Frontiers in Pharmacology, 2015, 6, 302.	1.6	0
22	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.	0.4	25
23	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
24	Structural dynamics of the monoamine transporter homolog LeuT from accelerated conformational sampling and channel analysis. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2289-2302.	1.5	4
25	Exploring the Physicochemical Properties of Oxime-Reactivation Therapeutics for Cyclosarin, Sarin, Tabun, and VX Inactivated Acetylcholinesterase. Chemical Research in Toxicology, 2014, 27, 99-110.	1.7	14
26	Î²-Amyloid and Neprilysin Computational Studies Identify Critical Residues Implicated in Binding Specificity. Journal of Chemical Information and Modeling, 2014, 54, 1157-1165.	2.5	10
27	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.	1.7	10
28	Analyzing a Conformational Sampling of LeuT from Accelerated Molecular Dynamics Simulations. Biophysical Journal, 2014, 106, 364a.	0.2	0
29	New design strategies for antidepressant drugs. Expert Opinion on Drug Discovery, 2013, 8, 1399-1414.	2.5	19
30	Global Transitions of Proteins Explored by a Multiscale Hybrid Methodology: Application to Adenylate Kinase. Biophysical Journal, 2013, 105, 1643-1652.	0.2	63
31	Global Transitions or Proteins Explored by a Multiscale Hybrid Methodology: Application to Dopamine Transporter. Biophysical Journal, 2013, 104, 226a-227a.	0.2	0
32	A Review of Monoamine Transporter-Ligand Interactions. Current Computer-Aided Drug Design, 2013, 9, 556-568.	0.8	19
33	LeuT Conformational Sampling Utilizing Accelerated Molecular Dynamics and Principal Component Analysis. Biophysical Journal, 2012, 103, L1-L3.	0.2	28
34	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.	1.3	19
35	Solution Structural Ensembles of Substrate-Free Cytochrome P450_{cam}. Biochemistry, 2012, 51, 3383-3393.	1.2	30
36	Conformational Free-Energy Landscapes for a Peptide in Saline Environments. Biophysical Journal, 2012, 103, 2513-2520.	0.2	5

#	Article	IF	Citations
37	Monoamine Transporter Structure, Function, Dynamics, and Drug Discovery: A Computational Perspective. AAPS Journal, 2012, 14, 820-831.	2.2	39
38	Experimentally Restrained Molecular Dynamics Simulations for Characterizing the Open States of Cytochrome P450_{cam}. Biochemistry, 2011, 50, 1664-1671.	1.2	24
39	Discovery of Novel Selective Serotonin Reuptake Inhibitors through Development of a Protein-Based Pharmacophore. Journal of Chemical Information and Modeling, 2011, 51, 2417-2426.	2.5	27
40	Computational Investigation of the Effect of Ions on the Secondary Structure of Small Peptides. Biophysical Journal, 2011, 100, 378a.	0.2	0
41	Ligand Exit and Entry Pathways for Monoamine Transporters. Biophysical Journal, 2011, 100, 245a.	0.2	0
42	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.	1.7	18
43	Solvation of Metal Cations in Non-aqueous Liquids. Journal of Solution Chemistry, 2011, 40, 1383-1398.	0.6	16
44	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.	1.4	20
45	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.	0.9	32
46	Topical perspectives. Journal of Molecular Graphics and Modelling, 2010, 29, 115.	1.3	0
47	Benchmarking docking and scoring protocol for the identification of potential acetylcholinesterase inhibitors. Journal of Molecular Graphics and Modelling, 2010, 28, 870-882.	1.3	25
48	The JMGM/MGMS graphics prize. Journal of Molecular Graphics and Modelling, 2010, 29, 1.	1.3	0
49	Molecular dynamics of leucine and dopamine transporter proteins in a model cell membrane lipid bilayer. Proteins: Structure, Function and Bioinformatics, 2010, 78, 797-811.	1.5	33
50	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
51	Sodium Perchlorate Effects on the Helical Stability of a Mainly Alanine Peptide. Biophysical Journal, 2010, 98, 186-196.	0.2	25
52	Receptor-Based Discovery of a Plasmalemmal Monoamine Transporter Inhibitor via High-Throughput Docking and Pharmacophore Modeling. ACS Chemical Neuroscience, 2010, 1, 223-233.	1.7	11
53	Investigations of structure and dynamics of water solvation of the type I antifreeze protein. International Journal of Quantum Chemistry, 2009, 109, 73-80.	1.0	12
54	Structural and Dynamic Implications of an Effector-induced Backbone Amide cisâ€“trans Isomerization in Cytochrome P450cam. Journal of Molecular Biology, 2009, 388, 801-814.	2.0	28

#	Article	IF	Citations
55	Salt Dependence of an Î±-Helical Peptide Folding Energy Landscapes. Biochemistry, 2009, 48, 10818-10826.	1.2	32
56	CO2(aq) Parameterization Through Free Energy Perturbation/Monte Carlo Simulations for Use in CO2 Sequestration. , 2009, , 337-357.		1
57	Free Energy Perturbation Monte Carlo Simulations of Salt Influences on Aqueous Freezing Point Depression. , 2009, , 359-370.		0
58	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.	1.5	72
59	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.	1.4	11
60	Computational and Experimental Determination of the Î±-Helix Unfolding Reaction Coordinate. Biochemistry, 2008, 47, 2046-2050.	1.2	8
61	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.	2.5	37
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.	1.2	21
63	Structure of Aqueous Sodium Perchlorate Solutions. Journal of Physical Chemistry B, 2008, 112, 15417-15425.	1.2	19
64	Computational Chemistry in the Undergraduate Curriculum. Reviews in Computational Chemistry, 2007, , 149-228.	1.5	4
65	Family 18 chitolectins: Comparison of MGP40 and HUMGP39. Biochemical and Biophysical Research Communications, 2007, 359, 221-226.	1.0	19
66	Biological Applications of Electrostatic Calculations and Brownian Dynamics Simulations. Reviews in Computational Chemistry, 2007, , 229-267.	1.5	70
67	Antifreeze Proteins at the Ice/Water Interface: Three Calculated Discriminating Properties for Orientation of Type I Proteins. Biophysical Journal, 2007, 93, 1442-1451.	0.2	90
68	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.	1.3	6
69	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.	1.5	37
70	HIV-1 RT Nonnucleoside Inhibitors and Their Interaction with RT for Antiviral Drug Development. Infectious Disorders - Drug Targets, 2006, 6, 391-413.	0.4	29
71	Comparative Protein Modeling. Reviews in Computational Chemistry, 2006, , 57-167.	1.5	19
72	Solubility of simple, nonpolar compounds in TIP4P-Ew. Journal of Chemical Physics, 2006, 124, 016102.	1.2	25

#	Article	IF	Citations
73	A novel hybrid simulation for study of multiscale phenomena. Molecular Simulation, 2006, 32, 825-830.	0.9	0
74	MT ₁ receptor binding pocket insights based on de novo molecular modeling. FASEB Journal, 2006, 20, A1119.	0.2	1
75	CoMFA 3D-QSAR Analysis of HIV-1 RT Nonnucleoside Inhibitors, TIBO Derivatives Based on Docking Conformation and Alignment.. ChemInform, 2005, 36, no.	0.1	1
76	Chapter 5 A Review of the TIP4P, TIP4P-Ew, TIP5P, and TIP5P-E Water Models. Annual Reports in Computational Chemistry, 2005, 1, 59-74.	0.9	15
77	Molecular Dynamics Simulation Studies of the Effect of Phosphocitrate on Crystal-Induced Membranolysis. Biophysical Journal, 2005, 89, 2251-2257.	0.2	12
78	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.	6.6	74
79	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.	1.5	35
80	Development of an improved four-site water model for biomolecular simulations: TIP4P-Ew. Journal of Chemical Physics, 2004, 120, 9665-9678.	1.2	1,747
81	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
82	Kinetic and Docking Studies of the Interaction of Quinones with the Quinone Reductase Active Siteâ€. Biochemistry, 2003, 42, 1985-1994.	1.2	27
83	Molecular Dynamics Simulation of Crystal-Induced Membranolysis. Journal of Physical Chemistry B, 2003, 107, 12346-12351.	1.2	17
84	Family 18 chitinaseâ€“oligosaccharide substrate interaction: subsite preference and anomer selectivity of Serratia marcescens chitinase A. Biochemical Journal, 2003, 376, 87-95.	1.7	91
85	Effective Computational Modeling of Constitutional Isomerism and Aggregation States of Explicit Solvates of Lithiated Phenylacetonitrile. Journal of Organic Chemistry, 2002, 67, 3832-3840.	1.7	19
86	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
87	Homology models for the tetrameric and dodecameric complexes of Lumbricus terrestris hemoglobin. Computational and Theoretical Chemistry, 2002, 592, 173-181.	1.5	5
88	Docking of non-nucleoside inhibitors: Neotripterifordin and its derivatives to HIV-1 reverse transcriptase. Proteins: Structure, Function and Bioinformatics, 2002, 49, 529-542.	1.5	20
89	A cell multipole based domain decomposition algorithm for molecular dynamics simulation of systems of arbitrary shape. Computer Physics Communications, 2002, 144, 141-153.	3.0	1
90	Hydrogen bond analysis of Type 1 antifreeze protein in water and the ice/water interface. PhysChemComm, 2001, 4, 32-36.	0.8	17

#	Article	IF	Citations
91	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
92	Molecular dynamics of HIV-1 reverse transcriptase indicates increased flexibility upon DNA binding. Proteins: Structure, Function and Bioinformatics, 2001, 45, 176-182.	1.5	30
93	Kinetic and Mechanistic Studies of Prolyl Oligopeptidase from the Hyperthermophile Pyrococcus furiosus. Journal of Biological Chemistry, 2001, 276, 19310-19317.	1.6	50
94	Molecular recognition and binding of thermal hysteresis proteins to ice. , 2000, 13, 101-113.		88
95	Docking of sulfonamides to carbonic anhydrase II and IV. Journal of Molecular Graphics and Modelling, 2000, 18, 283-289.	1.3	45
96	Docking Substrates to Metalloenzymes. Molecular Simulation, 2000, 24, 293-306.	0.9	4
97	Peptide-encapsulated CdS nanoclusters from a combinatorial ligand library. Chemical Communications, 2000, , 209-210.	2.2	22
98	Modeling of Antifreeze Proteins. Theoretical and Computational Chemistry, 1999, 8, 537-568.	0.2	0
99	Homology Modeling of Glycosyl Hydrolase Family 18 Enzymes and Proteins. Journal of Chemical Information and Computer Sciences, 1997, 37, 999-1005.	2.8	38
100	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
101	Physical and structural properties of taurine and taurine analogues. Amino Acids, 1997, 13, 131-139.	1.2	14
102	Calculations of the electrostatic free energy contributions to the binding free energy of sulfonamides to carbonic anhydrase. Structural Chemistry, 1996, 7, 131-138.	1.0	21
103	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
104	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.	2.2	51
105	Synthesis and computational evaluation of a boronium ion analogue of the tropane ring system. Tetrahedron Letters, 1996, 37, 2729-2730.	0.7	12
106	Gibbs free energies of formation of pcdds: Evaluation of estimation methods and application for predicting dehalogenation pathways. , 1996, 15, 824.		3
107	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
108	Molecular dynamics simulation with a continuum electrostatic model of the solvent. Journal of Computational Chemistry, 1995, 16, 1081-1095.	1.5	96

#	Article	IF	Citations
109	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.	1.5	51
110	Simulation of enzymeâ€"substrate encounter with gated active sites. Nature Structural and Molecular Biology, 1994, 1, 65-69.	3.6	71
111	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.	6.6	63
112	Molecular recognition: effect of rotational isomers on host-guest binding. Journal of the American Chemical Society, 1993, 115, 879-884.	6.6	24
113	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
114	Electrostatics and diffusion of molecules in solution: simulations with the University of Houston Brownian dynamics program. Computer Physics Communications, 1991, 62, 187-197.	3.0	457
115	[22] Diffusion-controlled enzymatic reactions. Methods in Enzymology, 1991, 202, 473-497.	0.4	63
116	Fischer route to pyrido[3,2-g]indoles. A novel receptor for urea derivatives. Journal of the American Chemical Society, 1990, 112, 4549-4550.	6.6	73
117	Methods for calculating geometries of transition states in solution. Chemical Physics, 1989, 129, 185-191.	0.9	4
118	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
119	Effects of truncating long-range interactions in aqueous ionic solution simulations. Chemical Physics Letters, 1988, 150, 105-108.	1.2	59
120	Water under high pressure. Molecular Physics, 1988, 64, 325-336.	0.8	46
121	Geometric considerations in the calculation of relative free energies of activation. Chemical Physics Letters, 1987, 141, 83-87.	1.2	6
122	Computer Simulations of Organic Reactions in Solution. Annals of the New York Academy of Sciences, 1986, 482, 198-209.	1.8	32
123	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.	6.6	185
124	Temperature and size dependence for Monte Carlo simulations of TIP4P water. Molecular Physics, 1985, 56, 1381-1392.	0.8	706
125	Optimized intermolecular potential functions for liquid hydrocarbons. Journal of the American Chemical Society, 1984, 106, 6638-6646.	6.6	2,069
126	Comparison of simple potential functions for simulating liquid water. Journal of Chemical Physics, 1983, 79, 926-935.	1.2	34,333

#	Article	IF	Citations
127	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.	6.6	378
128	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.	6.6	97
129	Development of an improved four-site water model for biomolecular simulations: TIP4P-Ew. , 0, .		1