Jeffry D Madura

List of Publications by Year in Descending Order

119 papers	35,815 citations	35 h-index	138 g-index
138 ext. papers	40,106 ext. citations	4.2 avg, IF	6.45 L-index

#	Paper	IF	Citations
119	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	2.8	14
118	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	2.9	10
117	A combined computational and experimental approach reveals the structure of a C/EBP Spi1 interaction required for gene transcription. *Journal of Biological Chemistry*, **2018**, 293, 19942-19956	5.4	3
116	Dopamine Transporter Dynamics of -Substituted Benztropine Analogs with Atypical Behavioral Effects. *Journal of Pharmacology and Experimental Therapeutics*, **2018**, 366, 527-540	4.7	5
115	A Python Program for Solving Schrdinger Equation in Undergraduate Physical Chemistry. *Journal of Chemical Education*, **2017**, 94, 813-815	2.4	14
114	Monomeric Polyglutamine Structures That Evolve into Fibrils. *Journal of Physical Chemistry B*, **2017**, 121, 5953-5967	3.4	13
113	Identifying trends in hydration behavior for modifications to the hydrophobicity of poly(n-isopropylacrylamide). *Journal of Molecular Graphics and Modelling*, **2017**, 78, 168-175	2.8	10
112	Molecular dynamics of conformation-specific dopamine transporter-inhibitor complexes. *Journal of Molecular Graphics and Modelling*, **2017**, 76, 143-151	2.8	3
111	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	3.9	10
110	Teaching Reciprocal Space to Undergraduates via Theory and Code Components of an IPython Notebook. *Journal of Chemical Education*, **2016**, 93, 2106-2109	2.4	10
109	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, 8361-8	3.4	3
108	2-Substituted 3Aryltropane Cocaine Analogs Produce Atypical Effects without Inducing Inward-Facing Dopamine Transporter Conformations. *Journal of Pharmacology and Experimental Therapeutics*, **2016**, 356, 624-34	4.7	13
107	Polyglutamine Fibrils: New Insights into Antiparallel Sheet Conformational Preference and Side Chain Structure. *Journal of Physical Chemistry B*, **2016**, 120, 3012-26	3.4	17
106	Photonic crystal protein hydrogel sensor materials enabled by conformationally induced volume phase transition. *Chemical Science*, **2016**, 7, 4557-4562	9.4	55
105	Biological Testing of Organophosphorus-Inactivated Acetylcholinesterase Oxime Reactivators Identified via Virtual Screening. *Chemical Research in Toxicology*, **2016**, 29, 1534-40	4	7
104	Polymorphism and second harmonic generation in a novel diamond-like semiconductor: Li2MnSnS4. *Journal of Solid State Chemistry*, **2015**, 231, 256-266	3.3	20
103	A Role for Fragment-Based Drug Design in Developing Novel Lead Compounds for Central Nervous System Targets. *Frontiers in Neurology*, **2015**, 6, 197	4.1	19

102	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, 253-87	1.4	19
101	Exploring the physicochemical properties of oxime-reactivation therapeutics for cyclosarin, sarin, tabun, and VX inactivated acetylcholinesterase. *Chemical Research in Toxicology*, **2014**, 27, 99-110	4	14
100	Amyloid and neprilysin computational studies identify critical residues implicated in binding specificity. *Journal of Chemical Information and Modeling*, **2014**, 54, 1157-65	6.1	6
99	Discovery of novel-scaffold monoamine transporter ligands via in silico screening with the S1 pocket of the serotonin transporter. *ACS Chemical Neuroscience*, **2014**, 5, 784-92	5.7	8
98	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	0
97	Structural dynamics of the monoamine transporter homolog LeuT from accelerated conformational sampling and channel analysis. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 2289-302	4.2	4
96	New design strategies for antidepressant drugs. *Expert Opinion on Drug Discovery*, **2013**, 8, 1399-414	6.2	17
95	Global transitions of proteins explored by a multiscale hybrid methodology: application to adenylate kinase. *Biophysical Journal*, **2013**, 105, 1643-52	2.9	52
94	A review of monoamine transporter-ligand interactions. *Current Computer-Aided Drug Design*, **2013**, 9, 556-68	1.4	11
93	LeuT conformational sampling utilizing accelerated molecular dynamics and principal component analysis. *Biophysical Journal*, **2012**, 103, L1-3	2.9	27
92	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	2.8	17
91	Solution structural ensembles of substrate-free cytochrome P450(cam). *Biochemistry*, **2012**, 51, 3383-93	3.2	25
90	Conformational free-energy landscapes for a peptide in saline environments. *Biophysical Journal*, **2012**, 103, 2513-20	2.9	5
89	Monoamine transporter structure, function, dynamics, and drug discovery: a computational perspective. *AAPS Journal*, **2012**, 14, 820-31	3.7	36
88	Experimentally restrained molecular dynamics simulations for characterizing the open states of cytochrome P450cam. *Biochemistry*, **2011**, 50, 1664-71	3.2	20
87	Discovery of novel selective serotonin reuptake inhibitors through development of a protein-based pharmacophore. *Journal of Chemical Information and Modeling*, **2011**, 51, 2417-26	6.1	22
86	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	5.7	17
85	Solvation of Metal Cations in Non-aqueous Liquids. *Journal of Solution Chemistry*, **2011**, 40, 1383-1398	1.8	15

84	Design, synthesis, and testing of an 6-O-linked series of benzimidazole based inhibitors of CDK5/p25. *Bioorganic and Medicinal Chemistry*, **2011**, 19, 359-73	3.4	16
83	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	1.8	26
82	Sodium perchlorate effects on the helical stability of a mainly alanine peptide. *Biophysical Journal*, **2010**, 98, 186-96	2.9	22
81	Receptor-Based Discovery of a Plasmalemmal Monoamine Transporter Inhibitor via High Throughput Docking and Pharmacophore Modeling. *ACS Chemical Neuroscience*, **2010**, 1, 223-233	5.7	9
80	Benchmarking docking and scoring protocol for the identification of potential acetylcholinesterase inhibitors. *Journal of Molecular Graphics and Modelling*, **2010**, 28, 870-82	2.8	20
79	Molecular dynamics of leucine and dopamine transporter proteins in a model cell membrane lipid bilayer. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 797-811	4.2	29
78	Investigations of structure and dynamics of water solvation of the type I antifreeze protein. *International Journal of Quantum Chemistry*, **2009**, 109, 73-80	2.1	12
77	Structural and dynamic implications of an effector-induced backbone amide cis-trans isomerization in cytochrome P450cam. *Journal of Molecular Biology*, **2009**, 388, 801-14	6.5	25
76	Salt dependence of an alpha-helical peptide folding energy landscapes. *Biochemistry*, **2009**, 48, 10818-26	3.2	29
75	CO2(aq) Parameterization Through Free Energy Perturbation/Monte Carlo Simulations for Use in CO2 Sequestration **2009**, 337-357		1
74	Free Energy Perturbation Monte Carlo Simulations of Salt Influences on Aqueous Freezing Point Depression **2009**, 359-370		
73	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	3.5	11
72	Computational and experimental determination of the alpha-helix unfolding reaction coordinate. *Biochemistry*, **2008**, 47, 2046-50	3.2	8
71	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, 1092-103	6.1	35
70	Interaction of the phospholipid head group with representative quartz and aluminosilicate structures: an ab initio study. *Journal of Physical Chemistry B*, **2008**, 112, 7095-103	3.4	20
69	Structure of aqueous sodium perchlorate solutions. *Journal of Physical Chemistry B*, **2008**, 112, 15417-25	3.4	18
68	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, 1033-46	4.2	69
67	Antifreeze proteins at the ice/water interface: three calculated discriminating properties for orientation of type I proteins. *Biophysical Journal*, **2007**, 93, 1442-51	2.9	85

66	Computational Chemistry in the Undergraduate Curriculum. *Reviews in Computational Chemistry*, **2007**, 149-228		1
65	Family 18 chitolectins: comparison of MGP40 and HUMGP39. *Biochemical and Biophysical Research Communications*, **2007**, 359, 221-6	3.4	18
64	Biological Applications of Electrostatic Calculations and Brownian Dynamics Simulations. *Reviews in Computational Chemistry*, **2007**, 229-267		54
63	HIV-1 RT nonnucleoside inhibitors and their interaction with RT for antiviral drug development. *Infectious Disorders - Drug Targets*, **2006**, 6, 391-413	1.1	28
62	Comparative Protein Modeling. *Reviews in Computational Chemistry*, **2006**, 57-167		14
61	Solubility of simple, nonpolar compounds in TIP4P-Ew. *Journal of Chemical Physics*, **2006**, 124, 16102	3.9	20
60	A novel hybrid simulation for study of multiscale phenomena. *Molecular Simulation*, **2006**, 32, 825-830	2	
59	An introduction to simulation and visualization of biological systems at multiple scales: a summer training program for interdisciplinary research. *Biotechnology Progress*, **2006**, 22, 179-85	2.8	5
58	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, 580-92	4.2	35
57	MT1 receptor binding pocket insights based on de novo molecular modeling. *FASEB Journal*, **2006**, 20, A1119	0.9	1
56	Chapter 5 A Review of the TIP4P, TIP4P-Ew, TIP5P, and TIP5P-E Water Models. *Annual Reports in Computational Chemistry*, **2005**, 1, 59-74	1.8	12
55	Molecular dynamics simulation studies of the effect of phosphocitrate on crystal-induced membranolysis. *Biophysical Journal*, **2005**, 89, 2251-7	2.9	11
54	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, 17253-60	16.4	71
53	CoMFA 3D-QSAR Analysis of HIV-1 RT Nonnucleoside Inhibitors, TIBO Derivatives Based on Docking Conformation and Alignment.. *ChemInform*, **2005**, 36, no		1
52	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	4.2	32
51	Development of an improved four-site water model for biomolecular simulations: TIP4P-Ew. *Journal of Chemical Physics*, **2004**, 120, 9665-78	3.9	1424
50	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, 2167-78		43
49	Family 18 chitinase-oligosaccharide substrate interaction: subsite preference and anomer selectivity of Serratia marcescens chitinase A. *Biochemical Journal*, **2003**, 376, 87-95	3.8	83

48	Kinetic and docking studies of the interaction of quinones with the quinone reductase active site. *Biochemistry*, **2003**, 42, 1985-94	3.2	27
47	Molecular Dynamics Simulation of Crystal-Induced Membranolysis. *Journal of Physical Chemistry B*, **2003**, 107, 12346-12351	3.4	17
46	Homology models for the tetrameric and dodecameric complexes of Lumbricus terrestris hemoglobin. *Computational and Theoretical Chemistry*, **2002**, 592, 173-181		4
45	Docking of non-nucleoside inhibitors: neotripterifordin and its derivatives to HIV-1 reverse transcriptase. *Proteins: Structure, Function and Bioinformatics*, **2002**, 49, 529-42	4.2	18
44	A cell multipole based domain decomposition algorithm for molecular dynamics simulation of systems of arbitrary shape. *Computer Physics Communications*, **2002**, 144, 141-153	4.2	1
43	Effective computational modeling of constitutional isomerism and aggregation states of explicit solvates of lithiated phenylacetonitrile. *Journal of Organic Chemistry*, **2002**, 67, 3832-40	4.2	17
42	Quantitative Impact of a Cognitive Modeling Intelligent Tutoring System on Student Performance in Balancing Chemical Equations. *The Chemical Educator*, **2002**, 7, 379-383		4
41	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		
40	Molecular dynamics of HIV-1 reverse transcriptase indicates increased flexibility upon DNA binding. *Proteins: Structure, Function and Bioinformatics*, **2001**, 45, 176-82	4.2	28
39	Kinetic and mechanistic studies of prolyl oligopeptidase from the hyperthermophile Pyrococcus furiosus. *Journal of Biological Chemistry*, **2001**, 276, 19310-7	5.4	43
38	Hydrogen bond analysis of Type 1 antifreeze protein in water and the ice/water interface. *PhysChemComm*, **2001**, 4, 32-36		15
37	Molecular recognition and binding of thermal hysteresis proteins to ice. *Journal of Molecular Recognition*, **2000**, 13, 101-13	2.6	78
36	Docking of sulfonamides to carbonic anhydrase II and IV. *Journal of Molecular Graphics and Modelling*, **2000**, 18, 283-9, 307-8	2.8	39
35	Docking Substrates to Metalloenzymes. *Molecular Simulation*, **2000**, 24, 293-306	2	3
34	Peptide-encapsulated CdS nanoclusters from a combinatorial ligand library. *Chemical Communications*, **2000**, 209-210	5.8	19
33	Modeling of Antifreeze Proteins. *Theoretical and Computational Chemistry*, **1999**, 8, 537-568		
32	Homology modeling of glycosyl hydrolase family 18 enzymes and proteins. *Journal of Chemical Information and Computer Sciences*, **1997**, 37, 999-1005		35
31	Modeling studies of binding of sea raven type II antifreeze protein to ice. *Journal of Chemical Information and Computer Sciences*, **1997**, 37, 1006-10		28

30	Physical and structural properties of taurine and taurine analogues. *Amino Acids*, **1997**, 13, 131-139	3.5	11
29	Calculations of the electrostatic free energy contributions to the binding free energy of sulfonamides to carbonic anhydrase. *Structural Chemistry*, **1996**, 7, 131-138	1.8	20
28	The dynamics and binding of a Type III antifreeze protein in water and on ice. *Computational and Theoretical Chemistry*, **1996**, 388, 65-77		13
27	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	3.8	47
26	Synthesis and computational evaluation of a boronium ion analogue of the tropane ring system. *Tetrahedron Letters*, **1996**, 37, 2729-2730	2	12
25	Gibbs free energies of formation of pcdds: Evaluation of estimation methods and application for predicting dehalogenation pathways **1996**, 15, 824		3
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	3.9	51
23	Electrostatics and diffusion of molecules in solution: simulations with the University of Houston Brownian Dynamics program. *Computer Physics Communications*, **1995**, 91, 57-95	4.2	567
22	Molecular dynamics simulation with a continuum electrostatic model of the solvent. *Journal of Computational Chemistry*, **1995**, 16, 1081-1095	3.5	91
21	Simulation of enzyme-substrate encounter with gated active sites. *Nature Structural and Molecular Biology*, **1994**, 1, 65-9	17.6	65
20	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	16.4	59
19	Molecular recognition: effect of rotational isomers on host-guest binding. *Journal of the American Chemical Society*, **1993**, 115, 879-884	16.4	21
18	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		48
17	Electrostatics and diffusion of molecules in solution: simulations with the University of Houston Brownian dynamics program. *Computer Physics Communications*, **1991**, 62, 187-197	4.2	440
16	Diffusion-controlled enzymatic reactions. *Methods in Enzymology*, **1991**, 202, 473-97	1.7	54
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	16.4	62
14	Methods for calculating geometries of transition states in solution. *Chemical Physics*, **1989**, 129, 185-191	2.3	4
13	Brownian dynamics simulation of diffusional encounters between triose phosphate isomerase and D-glyceraldehyde phosphate. *The Journal of Physical Chemistry*, **1989**, 93, 7285-7287		26

12	Effects of truncating long-range interactions in aqueous ionic solution simulations. *Chemical Physics Letters*, **1988**, 150, 105-108	2.5	57
11	Water under high pressure. *Molecular Physics*, **1988**, 64, 325-336	1.7	41
10	Geometric considerations in the calculation of relative free energies of activation. *Chemical Physics Letters*, **1987**, 141, 83-87	2.5	6
9	Computer simulations of organic reactions in solution. *Annals of the New York Academy of Sciences*, **1986**, 482, 198-209	6.5	28
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	16.4	161
7	Temperature and size dependence for Monte Carlo simulations of TIP4P water. *Molecular Physics*, **1985**, 56, 1381-1392	1.7	630
6	Optimized intermolecular potential functions for liquid hydrocarbons. *Journal of the American Chemical Society*, **1984**, 106, 6638-6646	16.4	1815
5	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	16.4	311
4	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	16.4	82
3	Comparison of simple potential functions for simulating liquid water. *Journal of Chemical Physics*, **1983**, 79, 926-935	3.9	27805
2	Development of an improved four-site water model for biomolecular simulations: TIP4P-Ew		1
1	Brownian Dynamics		1