

Jeffry D Madura

List of Publications by Year in descending order

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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	Comparison of simple potential functions for simulating liquid water. <i>Journal of Chemical Physics</i> , 1983, 79, 926-935.	1.2	34,333
2	Optimized intermolecular potential functions for liquid hydrocarbons. <i>Journal of the American Chemical Society</i> , 1984, 106, 6638-6646.	6.6	2,069
3	Development of an improved four-site water model for biomolecular simulations: TIP4P-Ew. <i>Journal of Chemical Physics</i> , 2004, 120, 9665-9678.	1.2	1,747
4	Temperature and size dependence for Monte Carlo simulations of TIP4P water. <i>Molecular Physics</i> , 1985, 56, 1381-1392.	0.8	706
5	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.	3.0	622
6	Electrostatics and diffusion of molecules in solution: simulations with the University of Houston Brownian dynamics program. <i>Computer Physics Communications</i> , 1991, 62, 187-197.	3.0	457
7	Quantum and statistical mechanical studies of liquids. 25. Solvation and conformation of methanol in water. <i>Journal of the American Chemical Society</i> , 1983, 105, 1407-1413.	6.6	378
8	Ab initio and Monte Carlo calculations for a nucleophilic addition reaction in the gas phase and in aqueous solution. <i>Journal of the American Chemical Society</i> , 1986, 108, 2517-2527.	6.6	185
9	Electronic origins and consequences of pyramidalization of asymmetric alkenes in ground and triplet excited states. <i>Journal of the American Chemical Society</i> , 1983, 105, 5980-5988.	6.6	97
10	Molecular dynamics simulation with a continuum electrostatic model of the solvent. <i>Journal of Computational Chemistry</i> , 1995, 16, 1081-1095.	1.5	96
11	Family 18 chitinase-oligosaccharide substrate interaction: subsite preference and anomer selectivity of <i>Serratia marcescens</i> chitinase A. <i>Biochemical Journal</i> , 2003, 376, 87-95.	1.7	91
12	Antifreeze Proteins at the Ice/Water Interface: Three Calculated Discriminating Properties for Orientation of Type I Proteins. <i>Biophysical Journal</i> , 2007, 93, 1442-1451.	0.2	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. <i>Journal of the American Chemical Society</i> , 2005, 127, 17253-17260.	6.6	74
15	Fischer route to pyrido[3,2-g]indoles. A novel receptor for urea derivatives. <i>Journal of the American Chemical Society</i> , 1990, 112, 4549-4550.	6.6	73
16	Dopamine transporter comparative molecular modeling and binding site prediction using the LeuT leucine transporter as a template. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 70, 1033-1046.	1.5	72
17	Photonic crystal protein hydrogel sensor materials enabled by conformationally induced volume phase transition. <i>Chemical Science</i> , 2016, 7, 4557-4562.	3.7	72
18	Simulation of enzyme-substrate encounter with gated active sites. <i>Nature Structural and Molecular Biology</i> , 1994, 1, 65-69.	3.6	71

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19	Biological Applications of Electrostatic Calculations and Brownian Dynamics Simulations. <i>Reviews in Computational Chemistry</i> , 2007, , 229-267.	1.5	70
20	[22] Diffusion-controlled enzymatic reactions. <i>Methods in Enzymology</i> , 1991, 202, 473-497.	0.4	63
21	Interactions of the D- and L-Forms of Winter Flounder Antifreeze Peptide with the {201} Planes of Ice. <i>Journal of the American Chemical Society</i> , 1994, 116, 417-418.	6.6	63
22	Global Transitions of Proteins Explored by a Multiscale Hybrid Methodology: Application to Adenylate Kinase. <i>Biophysical Journal</i> , 2013, 105, 1643-1652.	0.2	63
23	Effects of truncating long-range interactions in aqueous ionic solution simulations. <i>Chemical Physics Letters</i> , 1988, 150, 105-108.	1.2	59
24	Scanning electron microscopy and molecular modeling of inhibition of calcium oxalate monohydrate crystal growth by citrate and phosphocitrate. <i>Calcified Tissue International</i> , 1995, 56, 297-304.	1.5	51
25	Gibbs free energies of formation of pcdds: Evaluation of estimation methods and application for predicting dehalogenation pathways. <i>Environmental Toxicology and Chemistry</i> , 1996, 15, 824-836.	2.2	51
26	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
27	Kinetic and Mechanistic Studies of Prolyl Oligopeptidase from the Hyperthermophile <i>Pyrococcus furiosus</i> . <i>Journal of Biological Chemistry</i> , 2001, 276, 19310-19317.	1.6	50
28	Water under high pressure. <i>Molecular Physics</i> , 1988, 64, 325-336.	0.8	46
29	Docking of sulfonamides to carbonic anhydrase II and IV. <i>Journal of Molecular Graphics and Modelling</i> , 2000, 18, 283-289.	1.3	45
30	CoMFA 3D-QSAR Analysis of HIV-1 RT Nonnucleoside Inhibitors, TIBO Derivatives Based on Docking Conformation and Alignment. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 2167-2178.	2.8	45
31	Monoamine Transporter Structure, Function, Dynamics, and Drug Discovery: A Computational Perspective. <i>AAPS Journal</i> , 2012, 14, 820-831.	2.2	39
32	Homology Modeling of Glycosyl Hydrolase Family 18 Enzymes and Proteins. <i>Journal of Chemical Information and Computer Sciences</i> , 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. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 65, 580-592.	1.5	37
34	Receptor-Based Modeling and 3D-QSAR for a Quantitative Prediction of the Butyrylcholinesterase Inhibitors Based on Genetic Algorithm. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 1092-1103.	2.5	37
35	Relative free energy of binding and binding mode calculations of HIV-1 RT inhibitors based on dock-MM-PB/GS. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 57, 493-503.	1.5	35
36	Molecular dynamics of leucine and dopamine transporter proteins in a model cell membrane lipid bilayer. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 797-811.	1.5	33

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37	Computer Simulations of Organic Reactions in Solution. <i>Annals of the New York Academy of Sciences</i> , 1986, 482, 198-209.	1.8	32
38	Salt Dependence of an α -Helical Peptide Folding Energy Landscapes. <i>Biochemistry</i> , 2009, 48, 10818-10826.	1.2	32
39	A Review of Coarse-Grained Molecular Dynamics Techniques to Access Extended Spatial and Temporal Scales in Biomolecular Simulations. <i>Annual Reports in Computational Chemistry</i> , 2011, , 67-87.	0.9	32
40	Modeling Studies of Binding of Sea Raven Type II Antifreeze Protein to Ice. <i>Journal of Chemical Information and Computer Sciences</i> , 1997, 37, 1006-1010.	2.8	30
41	Molecular dynamics of HIV-1 reverse transcriptase indicates increased flexibility upon DNA binding. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001, 45, 176-182.	1.5	30
42	Solution Structural Ensembles of Substrate-Free Cytochrome P450cam. <i>Biochemistry</i> , 2012, 51, 3383-3393.	1.2	30
43	HIV-1 RT Nonnucleoside Inhibitors and Their Interaction with RT for Antiviral Drug Development. <i>Infectious Disorders - Drug Targets</i> , 2006, 6, 391-413.	0.4	29
44	Structural and Dynamic Implications of an Effector-induced Backbone Amide cis \rightleftharpoons trans Isomerization in Cytochrome P450cam. <i>Journal of Molecular Biology</i> , 2009, 388, 801-814.	2.0	28
45	LeuT Conformational Sampling Utilizing Accelerated Molecular Dynamics and Principal Component Analysis. <i>Biophysical Journal</i> , 2012, 103, L1-L3.	0.2	28
46	Brownian dynamics simulation of diffusional encounters between triose phosphate isomerase and D-glyceraldehyde phosphate. <i>The Journal of Physical Chemistry</i> , 1989, 93, 7285-7287.	2.9	27
47	Kinetic and Docking Studies of the Interaction of Quinones with the Quinone Reductase Active Site. <i>Biochemistry</i> , 2003, 42, 1985-1994.	1.2	27
48	Discovery of Novel Selective Serotonin Reuptake Inhibitors through Development of a Protein-Based Pharmacophore. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 2417-2426.	2.5	27
49	Polyglutamine Fibrils: New Insights into Antiparallel β -Sheet Conformational Preference and Side Chain Structure. <i>Journal of Physical Chemistry B</i> , 2016, 120, 3012-3026.	1.2	27
50	A Python Program for Solving Schrödinger's Equation in Undergraduate Physical Chemistry. <i>Journal of Chemical Education</i> , 2017, 94, 813-815.	1.1	27
51	Polymorphism and second harmonic generation in a novel diamond-like semiconductor: Li ₂ MnSnS ₄ . <i>Journal of Solid State Chemistry</i> , 2015, 231, 256-266.	1.4	26
52	Chemical Shift Tensors of Cimetidine Form A Modeled with Density Functional Theory Calculations: Implications for NMR Crystallography. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3109-3119.	1.1	26
53	Solubility of simple, nonpolar compounds in TIP4P-Ew. <i>Journal of Chemical Physics</i> , 2006, 124, 016102.	1.2	25
54	Benchmarking docking and scoring protocol for the identification of potential acetylcholinesterase inhibitors. <i>Journal of Molecular Graphics and Modelling</i> , 2010, 28, 870-882.	1.3	25

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55	Sodium Perchlorate Effects on the Helical Stability of a Mainly Alanine Peptide. <i>Biophysical Journal</i> , 2010, 98, 186-196.	0.2	25
56	Accelerated Molecular Dynamics and Protein Conformational Change: A Theoretical and Practical Guide Using a Membrane Embedded Model Neurotransmitter Transporter. <i>Methods in Molecular Biology</i> , 2015, 1215, 253-287.	0.4	25
57	Molecular recognition: effect of rotational isomers on host-guest binding. <i>Journal of the American Chemical Society</i> , 1993, 115, 879-884.	6.6	24
58	Experimentally Restrained Molecular Dynamics Simulations for Characterizing the Open States of Cytochrome P450 _{cam} . <i>Biochemistry</i> , 2011, 50, 1664-1671.	1.2	24
59	Peptide-encapsulated CdS nanoclusters from a combinatorial ligand library. <i>Chemical Communications</i> , 2000, , 209-210.	2.2	22
60	A Role for Fragment-Based Drug Design in Developing Novel Lead Compounds for Central Nervous System Targets. <i>Frontiers in Neurology</i> , 2015, 6, 197.	1.1	22
61	Calculations of the electrostatic free energy contributions to the binding free energy of sulfonamides to carbonic anhydrase. <i>Structural Chemistry</i> , 1996, 7, 131-138.	1.0	21
62	Interaction of the Phospholipid Head Group with Representative Quartz and Aluminosilicate Structures: An Ab initio Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 7095-7103.	1.2	21
63	Docking of non-nucleoside inhibitors: Neotripterifordin and its derivatives to HIV-1 reverse transcriptase. <i>Proteins: Structure, Function and Bioinformatics</i> , 2002, 49, 529-542.	1.5	20
64	Design, synthesis, and testing of an 6-O-linked series of benzimidazole based inhibitors of CDK5/p25. <i>Bioorganic and Medicinal Chemistry</i> , 2011, 19, 359-373.	1.4	20
65	Effective Computational Modeling of Constitutional Isomerism and Aggregation States of Explicit Solvates of Lithiated Phenylacetonitrile. <i>Journal of Organic Chemistry</i> , 2002, 67, 3832-3840.	1.7	19
66	Comparative Protein Modeling. <i>Reviews in Computational Chemistry</i> , 2006, , 57-167.	1.5	19
67	Family 18 chitolectins: Comparison of MGP40 and HUMGP39. <i>Biochemical and Biophysical Research Communications</i> , 2007, 359, 221-226.	1.0	19
68	Structure of Aqueous Sodium Perchlorate Solutions. <i>Journal of Physical Chemistry B</i> , 2008, 112, 15417-15425.	1.2	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. <i>Journal of Molecular Graphics and Modelling</i> , 2012, 38, 1-12.	1.3	19
70	New design strategies for antidepressant drugs. <i>Expert Opinion on Drug Discovery</i> , 2013, 8, 1399-1414.	2.5	19
71	A Review of Monoamine Transporter-Ligand Interactions. <i>Current Computer-Aided Drug Design</i> , 2013, 9, 556-568.	0.8	19
72	Identification of a Novel Selective Serotonin Reuptake Inhibitor by Coupling Monoamine Transporter-Based Virtual Screening and Rational Molecular Hybridization. <i>ACS Chemical Neuroscience</i> , 2011, 2, 544-552.	1.7	18

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73	Monomeric Polyglutamine Structures That Evolve into Fibrils. <i>Journal of Physical Chemistry B</i> , 2017, 121, 5953-5967.	1.2	18
74	Structure activity relationships of anthranilic acid-based compounds on cellular and in vivo mitogen activated protein kinase-5 signaling pathways. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2018, 28, 2294-2301.	1.0	18
75	Hydrogen bond analysis of Type 1 antifreeze protein in water and the ice/water interface. <i>PhysChemComm</i> , 2001, 4, 32-36.	0.8	17
76	Molecular Dynamics Simulation of Crystal-Induced Membranolysis. <i>Journal of Physical Chemistry B</i> , 2003, 107, 12346-12351.	1.2	17
77	Solvation of Metal Cations in Non-aqueous Liquids. <i>Journal of Solution Chemistry</i> , 2011, 40, 1383-1398.	0.6	16
78	The dynamics and binding of a Type III antifreeze protein in water and on ice. <i>Computational and Theoretical Chemistry</i> , 1996, 388, 65-77.	1.5	15
79	Chapter 5 A Review of the TIP4P, TIP4P-Ew, TIP5P, and TIP5P-E Water Models. <i>Annual Reports in Computational Chemistry</i> , 2005, 1, 59-74.	0.9	15
80	Physical and structural properties of taurine and taurine analogues. <i>Amino Acids</i> , 1997, 13, 131-139.	1.2	14
81	Exploring the Physicochemical Properties of Oxime-Reactivation Therapeutics for Cyclosarin, Sarin, Tabun, and VX Inactivated Acetylcholinesterase. <i>Chemical Research in Toxicology</i> , 2014, 27, 99-110.	1.7	14
82	2-Substituted 3- β -Aryltropane Cocaine Analogs Produce Atypical Effects without Inducing Inward-Facing Dopamine Transporter Conformations. <i>Journal of Pharmacology and Experimental Therapeutics</i> , 2016, 356, 624-634.	1.3	14
83	Teaching Reciprocal Space to Undergraduates via Theory and Code Components of an IPython Notebook. <i>Journal of Chemical Education</i> , 2016, 93, 2106-2109.	1.1	13
84	Synthesis and computational evaluation of a boronium ion analogue of the tropane ring system. <i>Tetrahedron Letters</i> , 1996, 37, 2729-2730.	0.7	12
85	Molecular Dynamics Simulation Studies of the Effect of Phosphocitrate on Crystal-Induced Membranolysis. <i>Biophysical Journal</i> , 2005, 89, 2251-2257.	0.2	12
86	Investigations of structure and dynamics of water solvation of the type I antifreeze protein. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 73-80.	1.0	12
87	Rapid and sustained antidepressant properties of an NMDA antagonist/monoamine reuptake inhibitor identified via transporter-based virtual screening. <i>Pharmacology Biochemistry and Behavior</i> , 2016, 150-151, 22-30.	1.3	12
88	Role of Nonpolar Amino Acid Functional Groups in the Surface Orientation-Dependent Adsorption of Natural and Synthetic Antifreeze Peptides on Ice. <i>Crystal Growth and Design</i> , 2008, 8, 3420-3429.	1.4	11
89	Receptor-Based Discovery of a Plasmalemmal Monoamine Transporter Inhibitor via High-Throughput Docking and Pharmacophore Modeling. <i>ACS Chemical Neuroscience</i> , 2010, 1, 223-233.	1.7	11
90	β -Amyloid and Neprilysin Computational Studies Identify Critical Residues Implicated in Binding Specificity. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1157-1165.	2.5	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. <i>ACS Chemical Neuroscience</i> , 2014, 5, 784-792.	1.7	10
92	Identifying trends in hydration behavior for modifications to the hydrophobicity of poly(n-isopropylacrylamide). <i>Journal of Molecular Graphics and Modelling</i> , 2017, 78, 168-175.	1.3	10
93	Computational and Experimental Determination of the α -Helix Unfolding Reaction Coordinate. <i>Biochemistry</i> , 2008, 47, 2046-2050.	1.2	8
94	Biological Testing of Organophosphorus-Inactivated Acetylcholinesterase Oxime Reactivators Identified via Virtual Screening. <i>Chemical Research in Toxicology</i> , 2016, 29, 1534-1540.	1.7	7
95	Geometric considerations in the calculation of relative free energies of activation. <i>Chemical Physics Letters</i> , 1987, 141, 83-87.	1.2	6
96	An Introduction to Simulation and Visualization of Biological Systems at Multiple Scales: A Summer Training Program for Interdisciplinary Research. <i>Biotechnology Progress</i> , 2006, 22, 179-185.	1.3	6
97	Quantitative Impact of a Cognitive Modeling Intelligent Tutoring System on Student Performance in Balancing Chemical Equations. <i>The Chemical Educator</i> , 2002, 7, 379-383.	0.0	5
98	Homology models for the tetrameric and dodecameric complexes of <i>Lumbricus terrestris</i> hemoglobin. <i>Computational and Theoretical Chemistry</i> , 2002, 592, 173-181.	1.5	5
99	Conformational Free-Energy Landscapes for a Peptide in Saline Environments. <i>Biophysical Journal</i> , 2012, 103, 2513-2520.	0.2	5
100	Molecular dynamics of conformation-specific dopamine transporter-inhibitor complexes. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 76, 143-151.	1.3	5
101	A combined computational and experimental approach reveals the structure of a C/EBP β -Spi1 interaction required for IL1B gene transcription. <i>Journal of Biological Chemistry</i> , 2018, 293, 19942-19956.	1.6	5
102	Dopamine Transporter Dynamics of <i>N</i> -Substituted Bztrapine Analogs with Atypical Behavioral Effects. <i>Journal of Pharmacology and Experimental Therapeutics</i> , 2018, 366, 527-540.	1.3	5
103	Methods for calculating geometries of transition states in solution. <i>Chemical Physics</i> , 1989, 129, 185-191.	0.9	4
104	Docking Substrates to Metalloenzymes. <i>Molecular Simulation</i> , 2000, 24, 293-306.	0.9	4
105	Computational Chemistry in the Undergraduate Curriculum. <i>Reviews in Computational Chemistry</i> , 2007, , 149-228.	1.5	4
106	Structural dynamics of the monoamine transporter homolog LeuT from accelerated conformational sampling and channel analysis. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 2289-2302.	1.5	4
107	Structure and Dynamics Study of LeuT Using the Markov State Model and Perturbation Response Scanning Reveals Distinct Ion Induced Conformational States. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8361-8368.	1.2	3
108	Gibbs free energies of formation of pcdds: Evaluation of estimation methods and application for predicting dehalogenation pathways. , 1996, 15, 824.		3

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109	A cell multipole based domain decomposition algorithm for molecular dynamics simulation of systems of arbitrary shape. <i>Computer Physics Communications</i> , 2002, 144, 141-153.	3.0	1
110	CoMFA 3D-QSAR Analysis of HIV-1 RT Nonnucleoside Inhibitors, TIBO Derivatives Based on Docking Conformation and Alignment.. <i>ChemInform</i> , 2005, 36, no.	0.1	1
111	Sodium versus potassium effects on the glutamic acid side-chains interaction on a heptapeptide. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1440004.	1.8	1
112	CO ₂ (aq) Parameterization Through Free Energy Perturbation/Monte Carlo Simulations for Use in CO ₂ 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 <i>de novo</i> molecular modeling. <i>FASEB Journal</i> , 2006, 20, A1119.	0.2	1
115	Modeling of Antifreeze Proteins. <i>Theoretical and Computational Chemistry</i> , 1999, 8, 537-568.	0.2	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. <i>The Chemical Educator</i> , 2001, 6, 70-71.	0.0	0
117	A novel hybrid simulation for study of multiscale phenomena. <i>Molecular Simulation</i> , 2006, 32, 825-830.	0.9	0
118	Topical perspectives. <i>Journal of Molecular Graphics and Modelling</i> , 2010, 29, 115.	1.3	0
119	The JMGM/MGMS graphics prize. <i>Journal of Molecular Graphics and Modelling</i> , 2010, 29, 1.	1.3	0
120	Circular Dichroism and UV Resonance Raman Study of the Impact of Salts and Alcohols on the Gibbs Free Energy Landscape of an α -helical Peptide. , 2010, , .		0
121	Computational Investigation of the Effect of Ions on the Secondary Structure of Small Peptides. <i>Biophysical Journal</i> , 2011, 100, 378a.	0.2	0
122	Ligand Exit and Entry Pathways for Monoamine Transporters. <i>Biophysical Journal</i> , 2011, 100, 245a.	0.2	0
123	Global Transitions of Proteins Explored by a Multiscale Hybrid Methodology: Application to Dopamine Transporter. <i>Biophysical Journal</i> , 2013, 104, 226a-227a.	0.2	0
124	Analyzing a Conformational Sampling of LeuT from Accelerated Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2014, 106, 364a.	0.2	0
125	Editorial: In silico Modeling of Brain Receptors for Antidepressants, Psychostimulants, and Other CNS-Active Drugs. <i>Frontiers in Pharmacology</i> , 2015, 6, 302.	1.6	0
126	Tribute to J. Andrew McCammon. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8055-8056.	1.2	0

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127	Evaluating Free Energies of Dimerization of Short Polyglutamine Peptides with Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2016, 110, 400a.	0.2	0
128	Crosslinking-Mass Spectrometry of Targeted Single Cys Mutants to Refine Allostery and Model Building in the Glycine Receptor. <i>Biophysical Journal</i> , 2017, 112, 321a-322a.	0.2	0
129	Free Energy Perturbation Monte Carlo Simulations of Salt Influences on Aqueous Freezing Point Depression. , 2009, , 359-370.		0