Thomas Simonson

List of Publications by Year
in descending order

119 papers	5,648 citations	117625 34 h-index	85541 71 g-index
127 all docs	127 docs citations	127 times ranked	3809 citing authors

#	Article	IF	Citations
1	Implicit solvent models. Biophysical Chemistry, 1999, 78, 1-20.	2.8	793
2	Free Energy Simulations Come of Age:â€‰ Proteinâ^'Ligand Recognition. Accounts of Chemical Research, 2002, 35, 430-437.	15.6	355
3	Charge Screening and the Dielectric Constant of Proteins:â€‰ Insights from Molecular Dynamics. Journal of the American Chemical Society, 1996, 118, 8452-8458.	13.7	348
4	Proton Binding to Proteins:Â pKaCalculations with Explicit and Implicit Solvent Models. Journal of the American Chemical Society, 2004, 126, 4167-4180.	13.7	266
5	Macromolecular electrostatics: continuum models and their growing pains. Current Opinion in Structural Biology, 2001, 11, 243-252.	5.7	246
6	Electrostatics and dynamics of proteins. Reports on Progress in Physics, 2003, 66, 737-787.	20.1	220
7	Solvation Free Energies Estimated from Macroscopic Continuum Theory: An Accuracy Assessment. The Journal of Physical Chemistry, 1994, 98, 4683-4694.	2.9	188
8	An Overview of Electrostatic Free Energy Computations for Solutions and Proteins. Journal of Chemical Theory and Computation, 2014, 10, 2690-2709.	5.3	118
9	Microscopic Dielectric Properties of Cytochrome c from Molecular Dynamics Simulations in Aqueous Solution. Journal of the American Chemical Society, 1995, 117, 7987-8000.	13.7	116
10	Free energy of particle insertion. Molecular Physics, 1993, 80, 441-447.	1.7	114
11	Continuum Treatment of Long-Range Interactions in Free Energy Calculations. Application to Proteinâ^'Ligand Binding.. Journal of Physical Chemistry B, 1997, 101, 8349-8362.	2.6	111
12	Binding free energies and free energy components from molecular dynamics and Poisson-Boltzmann calculations. Application to amino acid recognition by aspartyl-tRNA synthetase11Edited by A. R. Fersht. Journal of Molecular Biology, 2001, 306, 307-327.	4.2	107
13	Protein molecular dynamics with the generalized born/ACE solvent model. Proteins: Structure, Function and Bioinformatics, 2001, 45, 144-158.	2.6	102
14	Gaussian fluctuations and linear response in an electron transfer protein. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 6544-6549.	7.1	92
15	A Poissonâ^'Boltzmann Study of Charge Insertion in an Enzyme Active Site:â€‰ The Effect of Dielectric Relaxation. Journal of Physical Chemistry B, 1999, 103, 6142-6156.	2.6	86
16	Specific amino acid recognition by aspartyl-tRNA synthetase studied by free energy simulations 1 1A. R. Fersht. Journal of Molecular Biology, 1998, 275, 823-846.	4.2	75
17	Proton Binding to Proteins: A Free-Energy Component Analysis Using a Dielectric Continuum Model. Biophysical Journal, 2005, 88, 3888-3904.	0.5	71
18	Molecular Dynamics Simulations Show That Conformational Selection Governs the Binding Preferences of Imatinib for Several Tyrosine Kinases. Journal of Biological Chemistry, 2010, 285, 13807-13815.	3.4	70

#	Article	IF	Citations
19	Intramolecular dielectric screening in proteins. Journal of Molecular Biology, 1991, 218, 859-886.	4.2	66
20	Thermodynamics of protein-peptide interactions in the ribonuclease-S system studied by molecular dynamics and free energy calculations. Biochemistry, 1992, 31, 8661-8674.	2.5	66
21	CysxHisy?Zn2+ interactions: Thiol vs. thiolate coordination. Proteins: Structure, Function and Bioinformatics, 2002, 49, 37-48.	2.6	62
22	Computational sidechain placement and protein mutagenesis with implicit solvent models. Proteins: Structure, Function and Bioinformatics, 2007, 67, 853-867.	2.6	61
23	Alchemical free energy simulations for biological complexes: powerful but temperamentalâ€‰â€¦. Journal of Molecular Recognition, 2010, 23, 117-127.	2.1	54
24	Conformational substrates and uncertainty in macromolecular free energy calculations. The Journal of Physical Chemistry, 1993, 97, 3409-3417.	2.9	52
25	Dielectric Constant of Cytochromecfrom Simulations in a Water Droplet Including All Electrostatic Interactions. Journal of the American Chemical Society, 1998, 120, 4875-4876.	13.7	51
26	Dielectric Relaxation in an Enzyme Active Site:Â Molecular Dynamics Simulations Interpreted with a Macroscopic Continuum Model. Journal of the American Chemical Society, 2001, 123, 11047-11056.	13.7	49
27	Accurate calculation of the dielectric constant of water from simulations of a microscopic droplet in vacuum. Chemical Physics Letters, 1996, 250, 450-454.	2.6	47
28	Computational protein design: The proteus software and selected applications. Journal of Computational Chemistry, 2013, 34, 2472-2484.	3.3	44
29	Molecular Dynamics of the tRNAAla Acceptor Stem:â€‰ Comparison between Continuum Reaction Field and Particle-Mesh Ewald Electrostatic Treatments. Journal of Physical Chemistry B, 2002, 106, 3696-3705.	2.6	42
30	Protonation Patterns in Tetracycline:Tet Repressor Recognition: Simulations and Experiments. ChemBioChem, 2007, 8, 675-685.	2.6	40
31	Pairwise decomposition of an MMGBSA energy function for computational protein design. Journal of Computational Chemistry, 2014, 35, 1371-1387.	3.3	40
32	Electrostatic Free Energy Calculations for Macromolecules:â€‰ A Hybrid Molecular Dynamics/Continuum Electrostatics Approach. Journal of Physical Chemistry B, 2000, 104, 6509-6513.	2.6	37
33	Free-Energy Simulations and Experiments Reveal Long-Range Electrostatic Interactions and Substrate-Assisted Specificity in an Aminoacyl-tRNA Synthetase. ChemBioChem, 2006, 7, 337-344.	2.6	37
34	Dielectric relaxation in proteins: Microscopic and macroscopic models. International Journal of Quantum Chemistry, 1999, 73, 45-57.	2.0	36
35	A Residue-Pairwise Generalized Born Scheme Suitable for Protein Design Calculations. Journal of Physical Chemistry B, 2005, 109, 22667-22673.	2.6	36
36	Molecular Dynamics Simulations Show That Bound Mg2+ Contributes to Amino Acid and Aminoacyl Adenylate Binding Specificity in Aspartyl-tRNA Synthetase through Long Range Electrostatic Interactions. Journal of Biological Chemistry, 2006, 281, 23792-23803.	3.4	34

#	Article	IF	Citations
37	Tet Repressor Induction by Tetracycline: A Molecular Dynamics, Continuum Electrostatics, and Crystallographic Study. Journal of Molecular Biology, 2008, 378, 898-912.	4.2	34
38	Polar fluctuations in proteins: molecular-dynamic studies of cytochrome c in aqueous solution. Faraday Discussions, 1996, 103, 71.	3.2	33
39	Homology modelling of protein-protein complexes: a simple method and its possibilities and limitations. BMC Bioinformatics, 2008, 9, 427.	2.6	33
40	Reintroducing electrostatics into protein X-ray structure refinement: bulk solvent treated as a dielectric continuum. Acta Crystallographica Section D: Biological Crystallography, 2003, 59, 2094-2103.	2.5	32
41	Proteinâ€protein recognition: An experimental and computational study of the R89K mutation in Raf and its effect on Ras binding. Protein Science, 1999, 8, 50-64.	7.6	31
42	Implicit solvent models: Combining an analytical formulation of continuum electrostatics with simple models of the hydrophobic effect. Journal of Computational Chemistry, 1999, 20, 322-335.	3.3	30
43	Molecular Dynamics Simulations of the 30S Ribosomal Subunit Reveal a Preferred Tetracycline Binding Site. Journal of the American Chemical Society, 2008, 130, 1114-1115.	13.7	30
44	Monte carlo simulations of proteins at constant pH with generalized born solvent, flexible sidechains, and an effective dielectric boundary. Journal of Computational Chemistry, 2013, 34, 2742-2756.	3.3	30
45	Concepts and protocols for electrostatic free energies. Molecular Simulation, 2016, 42, 1090-1101.	2.0	30
46	Accurate PDZ/Peptide Binding Specificity with Additive and Polarizable Free Energy Simulations. Biophysical Journal, 2018, 114, 1091-1102.	0.5	30
47	Classical and Quantum Simulations of Tryptophan in Solution. Journal of Physical Chemistry A, 1997, 101, 1935-1945.	2.5	29
48	Predicting the Acid/Base Behavior of Proteins: A Constant-pH Monte Carlo Approach with Generalized Born Solvent. Journal of Physical Chemistry B, 2010, 114, 10634-10648.	2.6	29
49	Testing the Coulomb/Accessible Surface Area solvent model for protein stability, ligand binding, and protein design. BMC Bioinformatics, 2008, 9, 148.	2.6	28
50	Dielectric relaxation in proteins: a continuum electrostatics model incorporating dielectric heterogeneity of the protein and time-dependent charges. Journal of Computational Chemistry, 2001, 22, 290-305.	3.3	27
51	Computational protein design: Software implementation, parameter optimization, and performance of a simple model. Journal of Computational Chemistry, 2008, 29, 1092-1102.	3.3	27
52	Nonantibiotic Properties of Tetracyclines: Structural Basis for Inhibition of Secretory Phospholipase A2. Journal of Molecular Biology, 2010, 398, 83-96.	4.2	27
53	Free Energy Simulations of a GTPase: GTP and GDP Binding to Archaeal Initiation Factor 2. Journal of Physical Chemistry B, 2011, 115, 6749-6763.	2.6	26
54	CysxHisyâ€“Zn2+ interactions: Possibilities and limitations of a simple pairwise force field. Journal of Molecular Graphics and Modelling, 2006, 24, 404-411.	2.4	25

#	Article	IF	Citations
55	Computational protein design as a tool for fold recognition. Proteins: Structure, Function and Bioinformatics, 2009, 77, 139-158.	2.6	25
56	Comparing three stochastic search algorithms for computational protein design: Monte Carlo, replica exchange Monte Carlo, and a multistart, steepestâ€descent heuristic. Journal of Computational Chemistry, 2016, 37, 1781-1793.	3.3	25
57	Ammonium Scanning in an Enzyme Active Site. Journal of Biological Chemistry, 2007, 282, 30856-30868.	3.4	23
58	Classical Drude Polarizable Force Field Model for Methyl Phosphate and Its Interactions with Mg²⁺. Journal of Physical Chemistry A, 2018, 122, 6147-6155.	2.5	23
59	Computational design of fully overlapping coding schemes for protein pairs and triplets. Scientific Reports, 2017, 7, 15873.	3.3	22
60	Adaptive landscape flattening in amino acid sequence space for the computational design of protein:peptide binding. Journal of Chemical Physics, 2018, 149, 072302.	3.0	22
61	Proline cisâ€trans isomerization in staphylococcal nuclease: Multiâ€substate free energy perturbation calculations. Protein Science, 1995, 4, 636-654.	7.6	21
62	Protein side chain conformation predictions with an <scp>MMGBSA</scp> energy function. Proteins: Structure, Function and Bioinformatics, 2016, 84, 803-819.	2.6	21
63	Dielectric relaxation in proteins: the computational perspective. Photosynthesis Research, 2008, 97, 21-32.	2.9	20
64	Binding of Tetracyclines to Elongation Factor Tu, the Tet Repressor, and the Ribosome: A Molecular Dynamics Simulation Study. Biochemistry, 2008, 47, 13594-13603.	2.5	20
65	Computational protein design with a generalized born solvent model: Application to asparaginylâ€tRNA synthetase. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3448-3468.	2.6	20
66	Simple models for nonpolar solvation: Parameterization and testing. Journal of Computational Chemistry, 2017, 38, 2509-2519.	3.3	20
67	The tetracycline: Mg2+ complex: A molecular mechanics force field. Journal of Computational Chemistry, 2006, 27, 1517-1533.	3.3	19
68	Molecular mechanics models for tetracycline analogs. Journal of Computational Chemistry, 2009, 30, 243-255.	3.3	19
69	Simulating GTP:Mg and GDP:Mg with a simple force field: A structural and thermodynamic analysis. Journal of Computational Chemistry, 2013, 34, 836-846.	3.3	19
70	Redesigning the stereospecificity of tyrosyl-tRNA synthetase. Proteins: Structure, Function and Bioinformatics, 2016, 84, 240-253.	2.6	19
71	Comparing pairwiseâ€additive and manyâ€body generalized Born models for acid/base calculations and protein design. Journal of Computational Chemistry, 2017, 38, 2396-2410.	3.3	19
72	Protein: Ligand Recognition: Simple Models for Electrostatic Effects. Current Pharmaceutical Design, 2013, 19, 4241-4256.	1.9	18

#	Article	IF	Citations
73	Molecular dynamics simulations of the Ras:Raf and Rap:Raf complexes. Proteins: Structure, Function and Bioinformatics, 1999, 35, 89-100.	2.6	17
74	Recognizing proteinâ€“protein interfaces with empirical potentials and reduced amino acid alphabets. BMC Bioinformatics, 2007, 8, 270.	2.6	17
75	A molecular mechanics model for imatinib and imatinib:kinase binding. Journal of Computational Chemistry, 2010, 31, 1550-1560.	3.3	16
76	Tetracycline-Tet Repressor Binding Specificity: Insights from Experiments and Simulations. Biophysical Journal, 2009, 97, 2829-2838.	0.5	16
77	What Is the Dielectric Constant of a Protein When Its Backbone Is Fixed?. Journal of Chemical Theory and Computation, 2013, 9, 4603-4608.	5.3	16
78	Physics-Based Computational Protein Design: An Update. Journal of Physical Chemistry A, 2020, 124, 10637-10648.	2.5	16
79	Computational Protein Design: Validation and Possible Relevance as a Tool for Homology Searching and Fold Recognition. PLoS ONE, 2010, 5, e10410.	2.5	16
80	Dielectric properties of proteins from simulations: tools and techniques. Computer Physics Communications, 1995, 91, 291-303.	7.5	15
81	Protein:Ligand binding free energies: A stringent test for computational protein design. Journal of Computational Chemistry, 2016, 37, 404-415.	3.3	15
82	Equivalence of M- and P-Summation in Calculations of Ionic Solvation Free Energies. Journal of Physical Chemistry A, 2017, 121, 1525-1530.	2.5	15
83	Computational design of proteinâ€“ligand binding: Modifying the specificity of asparaginylâ€tRNA synthetase. Journal of Computational Chemistry, 2010, 31, 1273-1286.	3.3	14
84	A Hybrid Monte Carlo Scheme for Multibackbone Protein Design. Journal of Chemical Theory and Computation, 2016, 12, 6035-6048.	5.3	14
85	Adaptive landscape flattening allows the design of both enzyme: Substrate binding and catalytic power. PLoS Computational Biology, 2020, 16, e1007600.	3.2	13
86	Engineering an Mg2+ site to replace a structurally conserved arginine in the catalytic center of histidyl-tRNA synthetase by computer experiments. , 1998, 32, 362-380.		12
87	Probing electrostatic interactions and ligand binding in aspartylâ€tRNA synthetase through siteâ€directed mutagenesis and computer simulations. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1450-1460.	2.6	12
88	Structure and Thermodynamics of Mg:Phosphate Interactions in Water: A Simulation Study. ChemPhysChem, 2015, 16, 658-665.	2.1	12
89	Computational Design of the Tiam1 PDZ Domain and Its Ligand Binding. Journal of Chemical Theory and Computation, 2017, 13, 2271-2289.	5.3	12
90	Applications of Free Energy Calculations to Chemistry and Biology. Springer Series in Chemical Physics, 2007, , 463-501.	0.2	11

#	Article	IF	Citations
91	Full Protein Sequence Redesign with an MMGBSA Energy Function. Journal of Chemical Theory and Computation, 2017, 13, 4932-4943.	5.3	11
92	Neutral evolution of proteins: The superfunnel in sequence space and its relation to mutational robustness. Journal of Chemical Physics, 2008, 129, 185104.	3.0	10
93	A Simple PB/LIE Free Energy Function Accurately Predicts the Peptide Binding Specificity of the Tiam1 PDZ Domain. Frontiers in Molecular Biosciences, 2017, 4, 65.	3.5	10
94	How much can physics do for protein design?. Current Opinion in Structural Biology, 2022, 72, 46-54.	5.7	10
95	Conformation of the Ras-binding domain of Raf studied by molecular dynamics and free energy simulations. , 1998, 31, 186-200.		9
96	Variable Neighborhood Search with Cost Function Networks To Solve Large Computational Protein Design Problems. Journal of Chemical Information and Modeling, 2019, 59, 127-136.	5.4	9
97	Hybrid MC/MD for protein design. Journal of Chemical Physics, 2020, 153, 054113.	3.0	9
98	Conformational Selection by the aIF2 GTPase: A Molecular Dynamics Study of Functional Pathways. Biochemistry, 2012, 51, 353-361.	2.5	8
99	Conformational selection through electrostatics: Free energy simulations of gtp and gdp binding to archaeal initiation factor 2. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1264-1282.	2.6	8
100	Free Energy Calculations. , 2001, , .		8
101	Protein pK_aâ€™s from Adaptive Landscape Flattening Instead of Constant-pH Simulations. Journal of Chemical Theory and Computation, 2018, 14, 6714-6721.	5.3	7
102	A physics-based energy function allows the computational redesign of a PDZ domain. Scientific Reports, 2020, 10, 11150.	3.3	7
103	Nucleotide recognition by the initiation factor aIF5B: Free energy simulations of a neoclassical GTPase. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2742-2757.	2.6	6
104	Application of Various Molecular Modelling Methods in the Study of Estrogens and Xenoestrogens. International Journal of Molecular Sciences, 2020, 21, 6411.	4.1	6
105	Free Energy Calculations: Approximate Methods for Biological Macromolecules. Springer Series in Chemical Physics, 2007, , 423-461.	0.2	5
106	Electrostatic free energies in translational GTPases: Classic allostery and the rest. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 1006-1016.	2.4	5
107	The Physical Basis of Ligand Binding. , 2015, , 3-43.		4
108	A large decoy set of proteinâ€“protein complexes produced by flexible docking. Journal of Computational Chemistry, 2011, 32, 106-120.	3.3	3

#	Article	IF	Citations
109	Computational Design of PDZ-Peptide Binding. Methods in Molecular Biology, 2021, 2256, 237-255.	0.9	3
110	Neutral evolution of protein-protein interactions: a computational study using simple models. BMC Structural Biology, 2007, 7, 79.	2.3	2
111	Proteus and the Design of Ligand Binding Sites. Methods in Molecular Biology, 2016, 1414, 77-97.	0.9	2
112	Probing the stereospecificity of tyrosyl- and glutaminyl-tRNA synthetase with molecular dynamics. Journal of Molecular Graphics and Modelling, 2017, 71, 192-199.	2.4	2
113	Theory and simulation: from protons to genomes. Current Opinion in Structural Biology, 2004, 14, 189-191.	5.7	1
114	Dielectric relaxation in proteins: Microscopic and macroscopic models. International Journal of Quantum Chemistry, 1999, 73, 45-57.	2.0	1
115	The Inverse Protein Folding Problem: Protein Design and Structure Prediction in the Genomic Era. , 2012, , 121-140.		1
116	A Computational Model for the PLP-Dependent Enzyme Methionine Î³-Lyase. Frontiers in Molecular Biosciences, 2022, 9, 886358.	3.5	1
117	Protein Sequence Optimization with a Polarizable Force Field: Insights from PDZ Domains. Biophysical Journal, 2016, 110, 345a-346a.	0.5	0
118	Biochemical and Structural Characterization of De Novo Designed PDZ Domains. Biophysical Journal, 2019, 116, 320a.	0.5	0
119	Knowledge-Based Unfolded State Model for Protein Design. Methods in Molecular Biology, 2022, 2405, 403-424.	0.9	0