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	How much can physics do for protein design?. Current Opinion in Structural Biology, 2022, 72, 46-54.	5.7	10
2	Knowledge-Based Unfolded State Model for Protein Design. Methods in Molecular Biology, 2022, 2405, 403-424.	0.9	0
3	A Computational Model for the PLP-Dependent Enzyme Methionine Î³-Lyase. Frontiers in Molecular Biosciences, 2022, 9, 886358.	3.5	1
4	Computational Design of PDZ-Peptide Binding. Methods in Molecular Biology, 2021, 2256, 237-255.	0.9	3
5	Physics-Based Computational Protein Design: An Update. Journal of Physical Chemistry A, 2020, 124, 10637-10648.	2.5	16
6	Hybrid MC/MD for protein design. Journal of Chemical Physics, 2020, 153, 054113.	3.0	9
7	Application of Various Molecular Modelling Methods in the Study of Estrogens and Xenoestrogens. International Journal of Molecular Sciences, 2020, 21, 6411.	4.1	6
8	A physics-based energy function allows the computational redesign of a PDZ domain. Scientific Reports, 2020, 10, 11150.	3.3	7
9	Adaptive landscape flattening allows the design of both enzyme: Substrate binding and catalytic power. PLoS Computational Biology, 2020, 16, e1007600.	3.2	13
10	Biochemical and Structural Characterization of De Novo Designed PDZ Domains. Biophysical Journal, 2019, 116, 320a.	0.5	0
11	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
12	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
13	Accurate PDZ/Peptide Binding Specificity with Additive and Polarizable Free Energy Simulations. Biophysical Journal, 2018, 114, 1091-1102.	0.5	30
14	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
15	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
16	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
17	Computational Design of the Tiam1 PDZ Domain and Its Ligand Binding. Journal of Chemical Theory and Computation, 2017, 13, 2271-2289.	5.3	12
18	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

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19	Full Protein Sequence Redesign with an MMGBSA Energy Function. Journal of Chemical Theory and Computation, 2017, 13, 4932-4943.	5.3	11
20	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
21	Simple models for nonpolar solvation: Parameterization and testing. Journal of Computational Chemistry, 2017, 38, 2509-2519.	3.3	20
22	Computational design of fully overlapping coding schemes for protein pairs and triplets. Scientific Reports, 2017, 7, 15873.	3.3	22
23	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
24	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
25	Protein side chain conformation predictions with an <scp>MMGBSA</scp> energy function. Proteins: Structure, Function and Bioinformatics, 2016, 84, 803-819.	2.6	21
26	Redesigning the stereospecificity of tyrosyl-tRNA synthetase. Proteins: Structure, Function and Bioinformatics, 2016, 84, 240-253.	2.6	19
27	Protein:Ligand binding free energies: A stringent test for computational protein design. Journal of Computational Chemistry, 2016, 37, 404-415.	3.3	15
28	Concepts and protocols for electrostatic free energies. Molecular Simulation, 2016, 42, 1090-1101.	2.0	30
29	Protein Sequence Optimization with a Polarizable Force Field: Insights from PDZ Domains. Biophysical Journal, 2016, 110, 345a-346a.	0.5	0
30	Proteus and the Design of Ligand Binding Sites. Methods in Molecular Biology, 2016, 1414, 77-97.	0.9	2
31	A Hybrid Monte Carlo Scheme for Multibackbone Protein Design. Journal of Chemical Theory and Computation, 2016, 12, 6035-6048.	5.3	14
32	The Physical Basis of Ligand Binding. , 2015, , 3-43.		4
33	Structure and Thermodynamics of Mg:Phosphate Interactions in Water: A Simulation Study. ChemPhysChem, 2015, 16, 658-665.	2.1	12
34	Electrostatic free energies in translational GTPases: Classic allostery and the rest. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 1006-1016.	2.4	5
35	Pairwise decomposition of an MMGBSA energy function for computational protein design. Journal of Computational Chemistry, 2014, 35, 1371-1387.	3.3	40
36	An Overview of Electrostatic Free Energy Computations for Solutions and Proteins. Journal of Chemical Theory and Computation, 2014, 10, 2690-2709.	5.3	118

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37	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
38	Computational protein design: The proteus software and selected applications. Journal of Computational Chemistry, 2013, 34, 2472-2484.	3.3	44
39	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
40	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
41	Protein: Ligand Recognition: Simple Models for Electrostatic Effects. Current Pharmaceutical Design, 2013, 19, 4241-4256.	1.9	18
42	Conformational Selection by the aIF2 GTPase: A Molecular Dynamics Study of Functional Pathways. Biochemistry, 2012, 51, 353-361.	2.5	8
43	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
44	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
45	The Inverse Protein Folding Problem: Protein Design and Structure Prediction in the Genomic Era. , 2012, , 121-140.		1
46	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
47	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
48	A large decoy set of proteinâ€“protein complexes produced by flexible docking. Journal of Computational Chemistry, 2011, 32, 106-120.	3.3	3
49	Computational design of proteinâ€“ligand binding: Modifying the specificity of asparaginylâ€tRNA synthetase. Journal of Computational Chemistry, 2010, 31, 1273-1286.	3.3	14
50	A molecular mechanics model for imatinib and imatinib:kinase binding. Journal of Computational Chemistry, 2010, 31, 1550-1560.	3.3	16
51	Alchemical free energy simulations for biological complexes: powerful but temperamentalâ€‰â€¦. Journal of Molecular Recognition, 2010, 23, 117-127.	2.1	54
52	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
53	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
54	Nonantibiotic Properties of Tetracyclines: Structural Basis for Inhibition of Secretory Phospholipase A2. Journal of Molecular Biology, 2010, 398, 83-96.	4.2	27

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55	Computational Protein Design: Validation and Possible Relevance as a Tool for Homology Searching and Fold Recognition. PLoS ONE, 2010, 5, e10410.	2.5	16
56	Molecular mechanics models for tetracycline analogs. Journal of Computational Chemistry, 2009, 30, 243-255.	3.3	19
57	Computational protein design as a tool for fold recognition. Proteins: Structure, Function and Bioinformatics, 2009, 77, 139-158.	2.6	25
58	Tetracycline-Tet Repressor Binding Specificity: Insights from Experiments and Simulations. Biophysical Journal, 2009, 97, 2829-2838.	0.5	16
59	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
60	Dielectric relaxation in proteins: the computational perspective. Photosynthesis Research, 2008, 97, 21-32.	2.9	20
61	Computational protein design: Software implementation, parameter optimization, and performance of a simple model. Journal of Computational Chemistry, 2008, 29, 1092-1102.	3.3	27
62	Testing the Coulomb/Accessible Surface Area solvent model for protein stability, ligand binding, and protein design. BMC Bioinformatics, 2008, 9, 148.	2.6	28
63	Homology modelling of protein-protein complexes: a simple method and its possibilities and limitations. BMC Bioinformatics, 2008, 9, 427.	2.6	33
64	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
65	Tet Repressor Induction by Tetracycline: A Molecular Dynamics, Continuum Electrostatics, and Crystallographic Study. Journal of Molecular Biology, 2008, 378, 898-912.	4.2	34
66	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
67	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
68	Ammonium Scanning in an Enzyme Active Site. Journal of Biological Chemistry, 2007, 282, 30856-30868.	3.4	23
69	Free Energy Calculations: Approximate Methods for Biological Macromolecules. Springer Series in Chemical Physics, 2007, , 423-461.	0.2	5
70	Protonation Patterns in Tetracycline:Tet Repressor Recognition: Simulations and Experiments. ChemBioChem, 2007, 8, 675-685.	2.6	40
71	Neutral evolution of protein-protein interactions: a computational study using simple models. BMC Structural Biology, 2007, 7, 79.	2.3	2
72	Computational sidechain placement and protein mutagenesis with implicit solvent models. Proteins: Structure, Function and Bioinformatics, 2007, 67, 853-867.	2.6	61

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73	Recognizing proteinâ€“protein interfaces with empirical potentials and reduced amino acid alphabets. BMC Bioinformatics, 2007, 8, 270.	2.6	17
74	Applications of Free Energy Calculations to Chemistry and Biology. Springer Series in Chemical Physics, 2007, , 463-501.	0.2	11
75	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
76	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
77	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
78	The tetracycline: Mg2+ complex: A molecular mechanics force field. Journal of Computational Chemistry, 2006, 27, 1517-1533.	3.3	19
79	A Residue-Pairwise Generalized Born Scheme Suitable for Protein Design Calculations. Journal of Physical Chemistry B, 2005, 109, 22667-22673.	2.6	36
80	Proton Binding to Proteins: A Free-Energy Component Analysis Using a Dielectric Continuum Model. Biophysical Journal, 2005, 88, 3888-3904.	0.5	71
81	Theory and simulation: from protons to genomes. Current Opinion in Structural Biology, 2004, 14, 189-191.	5.7	1
82	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
83	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
84	Electrostatics and dynamics of proteins. Reports on Progress in Physics, 2003, 66, 737-787.	20.1	220
85	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
86	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
87	Free Energy Simulations Come of Age:â€‰ Proteinâ€“Ligand Recognition. Accounts of Chemical Research, 2002, 35, 430-437.	15.6	355
88	CysxHisy?Zn2+ interactions: Thiol vs. thiolate coordination. Proteins: Structure, Function and Bioinformatics, 2002, 49, 37-48.	2.6	62
89	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
90	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

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91	Protein molecular dynamics with the generalized born/ACE solvent model. Proteins: Structure, Function and Bioinformatics, 2001, 45, 144-158.	2.6	102
92	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
93	Macromolecular electrostatics: continuum models and their growing pains. Current Opinion in Structural Biology, 2001, 11, 243-252.	5.7	246
94	Free Energy Calculations. , 2001, , .		8
95	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
96	Implicit solvent models. Biophysical Chemistry, 1999, 78, 1-20.	2.8	793
97	Dielectric relaxation in proteins: Microscopic and macroscopic models. International Journal of Quantum Chemistry, 1999, 73, 45-57.	2.0	36
98	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
99	Molecular dynamics simulations of the Ras:Raf and Rap:Raf complexes. Proteins: Structure, Function and Bioinformatics, 1999, 35, 89-100.	2.6	17
100	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
101	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
102	Dielectric relaxation in proteins: Microscopic and macroscopic models. International Journal of Quantum Chemistry, 1999, 73, 45-57.	2.0	1
103	Conformation of the Ras-binding domain of Raf studied by molecular dynamics and free energy simulations. , 1998, 31, 186-200.		9
104	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
105	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
106	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
107	Classical and Quantum Simulations of Tryptophan in Solution. Journal of Physical Chemistry A, 1997, 101, 1935-1945.	2.5	29
108	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

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109	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
110	Polar fluctuations in proteins: molecular-dynamic studies of cytochrome c in aqueous solution. Faraday Discussions, 1996, 103, 71.	3.2	33
111	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
112	Dielectric properties of proteins from simulations: tools and techniques. Computer Physics Communications, 1995, 91, 291-303.	7.5	15
113	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
114	Proline cisâ€trans isomerization in staphylococcal nuclease: Multiâ€substate free energy perturbation calculations. Protein Science, 1995, 4, 636-654.	7.6	21
115	Solvation Free Energies Estimated from Macroscopic Continuum Theory: An Accuracy Assessment. The Journal of Physical Chemistry, 1994, 98, 4683-4694.	2.9	188
116	Conformational substrates and uncertainty in macromolecular free energy calculations. The Journal of Physical Chemistry, 1993, 97, 3409-3417.	2.9	52
117	Free energy of particle insertion. Molecular Physics, 1993, 80, 441-447.	1.7	114
118	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
119	Intramolecular dielectric screening in proteins. Journal of Molecular Biology, 1991, 218, 859-886.	4.2	66