Thomas Simonson

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

119 papers	5,102 citations	33 h-index	68 g-index
127 ext. papers	5,342 ext. citations	4.8 avg, IF	5.96 L-index

#	Paper	IF	Citations
119	Knowledge-Based Unfolded State Model for Protein Design.. *Methods in Molecular Biology*, **2022**, 2405, 403-424	1.4	
118	A Computational Model for the PLP-Dependent Enzyme Methionine -Lyase.. *Frontiers in Molecular Biosciences*, **2022**, 9, 886358	5.6	
117	Computational Design of PDZ-Peptide Binding. *Methods in Molecular Biology*, **2021**, 2256, 237-255	1.4	1
116	How much can physics do for protein design?. *Current Opinion in Structural Biology*, **2021**, 72, 46-54	8.1	1
115	A physics-based energy function allows the computational redesign of a PDZ domain. *Scientific Reports*, **2020**, 10, 11150	4.9	3
114	Adaptive landscape flattening allows the design of both enzyme: Substrate binding and catalytic power. *PLoS Computational Biology*, **2020**, 16, e1007600	5	9
113	Physics-Based Computational Protein Design: An Update. *Journal of Physical Chemistry A*, **2020**, 124, 10637-10648	2.8	7
112	Hybrid MC/MD for protein design. *Journal of Chemical Physics*, **2020**, 153, 054113	3.9	2
111	Application of Various Molecular Modelling Methods in the Study of Estrogens and Xenoestrogens. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	3
110	Variable Neighborhood Search with Cost Function Networks To Solve Large Computational Protein Design Problems. *Journal of Chemical Information and Modeling*, **2019**, 59, 127-136	6.1	5
109	Adaptive landscape flattening in amino acid sequence space for the computational design of protein:peptide binding. *Journal of Chemical Physics*, **2018**, 149, 072302	3.9	18
108	Accurate PDZ/Peptide Binding Specificity with Additive and Polarizable Free Energy Simulations. *Biophysical Journal*, **2018**, 114, 1091-1102	2.9	16
107	Classical Drude Polarizable Force Field Model for Methyl Phosphate and Its Interactions with Mg. *Journal of Physical Chemistry A*, **2018**, 122, 6147-6155	2.8	15
106	Protein p K_as from Adaptive Landscape Flattening Instead of Constant-pH Simulations. *Journal of Chemical Theory and Computation*, **2018**, 14, 6714-6721	6.4	7
105	Equivalence of M- and P-Summation in Calculations of Ionic Solvation Free Energies. *Journal of Physical Chemistry A*, **2017**, 121, 1525-1530	2.8	12
104	Computational Design of the Tiam1 PDZ Domain and Its Ligand Binding. *Journal of Chemical Theory and Computation*, **2017**, 13, 2271-2289	6.4	10
103	Probing the stereospecificity of tyrosyl- and glutaminyl-tRNA synthetase with molecular dynamics. *Journal of Molecular Graphics and Modelling*, **2017**, 71, 192-199	2.8	2

102	Full Protein Sequence Redesign with an MMGBSA Energy Function. *Journal of Chemical Theory and Computation*, **2017**, 13, 4932-4943	6.4	8
101	Comparing pairwise-additive and many-body generalized Born models for acid/base calculations and protein design. *Journal of Computational Chemistry*, **2017**, 38, 2396-2410	3.5	16
100	Simple models for nonpolar solvation: Parameterization and testing. *Journal of Computational Chemistry*, **2017**, 38, 2509-2519	3.5	16
99	Computational design of fully overlapping coding schemes for protein pairs and triplets. *Scientific Reports*, **2017**, 7, 15873	4.9	18
98	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	5.6	9
97	A Hybrid Monte Carlo Scheme for Multibackbone Protein Design. *Journal of Chemical Theory and Computation*, **2016**, 12, 6035-6048	6.4	12
96	Comparing three stochastic search algorithms for computational protein design: Monte Carlo, replica exchange Monte Carlo, and a multistart, steepest-descent heuristic. *Journal of Computational Chemistry*, **2016**, 37, 1781-93	3.5	23
95	Protein side chain conformation predictions with an MMGBSA energy function. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 803-19	4.2	17
94	Redesigning the stereospecificity of tyrosyl-tRNA synthetase. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 240-53	4.2	15
93	Protein:Ligand binding free energies: A stringent test for computational protein design. *Journal of Computational Chemistry*, **2016**, 37, 404-15	3.5	13
92	Concepts and protocols for electrostatic free energies. *Molecular Simulation*, **2016**, 42, 1090-1101	2	25
91	Proteus and the Design of Ligand Binding Sites. *Methods in Molecular Biology*, **2016**, 1414, 77-97	1.4	2
90	Structure and thermodynamics of Mg:phosphate interactions in water: a simulation study. *ChemPhysChem*, **2015**, 16, 658-65	3.2	11
89	Electrostatic free energies in translational GTPases: Classic allostery and the rest. *Biochimica Et Biophysica Acta - General Subjects*, **2015**, 1850, 1006-1016	4	4
88	The Physical Basis of Ligand Binding **2015**, 3-43		4
87	An Overview of Electrostatic Free Energy Computations for Solutions and Proteins. *Journal of Chemical Theory and Computation*, **2014**, 10, 2690-709	6.4	103
86	Pairwise decomposition of an MMGBSA energy function for computational protein design. *Journal of Computational Chemistry*, **2014**, 35, 1371-87	3.5	32
85	What Is the Dielectric Constant of a Protein When Its Backbone Is Fixed?. *Journal of Chemical Theory and Computation*, **2013**, 9, 4603-8	6.4	14

84	Computational protein design: the Proteus software and selected applications. *Journal of Computational Chemistry*, **2013**, 34, 2472-84	3.5	38
83	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, 2742-56	3.5	28
82	Simulating GTP:Mg and GDP:Mg with a simple force field: a structural and thermodynamic analysis. *Journal of Computational Chemistry*, **2013**, 34, 836-46	3.5	14
81	Protein: ligand recognition: simple models for electrostatic effects. *Current Pharmaceutical Design*, **2013**, 19, 4241-56	3.3	15
80	Conformational selection by the aIF2 GTPase: a molecular dynamics study of functional pathways. *Biochemistry*, **2012**, 51, 353-61	3.2	8
79	Nucleotide recognition by the initiation factor aIF5B: free energy simulations of a neoclassical GTPase. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 2742-57	4.2	5
78	Conformational selection through electrostatics: Free energy simulations of GTP and GDP binding to archaeal initiation factor 2. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 1264-82	4.2	8
77	The Inverse Protein Folding Problem: Protein Design and Structure Prediction in the Genomic Era **2012**, 121-140		1
76	Computational protein design with a generalized Born solvent model: application to Asparaginyl-tRNA synthetase. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 3448-68	4.2	19
75	A large decoy set of protein-protein complexes produced by flexible docking. *Journal of Computational Chemistry*, **2011**, 32, 106-20	3.5	3
74	Free energy simulations of a GTPase: GTP and GDP binding to archaeal initiation factor 2. *Journal of Physical Chemistry B*, **2011**, 115, 6749-63	3.4	26
73	Molecular dynamics simulations show that conformational selection governs the binding preferences of imatinib for several tyrosine kinases. *Journal of Biological Chemistry*, **2010**, 285, 13807-15	5.4	65
72	Predicting the acid/base behavior of proteins: a constant-pH Monte Carlo approach with generalized born solvent. *Journal of Physical Chemistry B*, **2010**, 114, 10634-48	3.4	28
71	Nonantibiotic properties of tetracyclines: structural basis for inhibition of secretory phospholipase A2. *Journal of Molecular Biology*, **2010**, 398, 83-96	6.5	27
70	Computational design of protein-ligand binding: modifying the specificity of asparaginyl-tRNA synthetase. *Journal of Computational Chemistry*, **2010**, 31, 1273-86	3.5	10
69	A molecular mechanics model for imatinib and imatinib:kinase binding. *Journal of Computational Chemistry*, **2010**, 31, 1550-60	3.5	13
68	Alchemical free energy simulations for biological complexes: powerful but temperamental. *Journal of Molecular Recognition*, **2010**, 23, 117-27	2.6	46
67	Computational protein design: validation and possible relevance as a tool for homology searching and fold recognition. *PLoS ONE*, **2010**, 5, e10410	3.7	16

66	Molecular mechanics models for tetracycline analogs. *Journal of Computational Chemistry*, **2009**, 30, 243-55	3.5	16
65	Computational protein design as a tool for fold recognition. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77, 139-58	4.2	24
64	Tetracycline-tet repressor binding specificity: insights from experiments and simulations. *Biophysical Journal*, **2009**, 97, 2829-38	2.9	13
63	Testing the Coulomb/Accessible Surface Area solvent model for protein stability, ligand binding, and protein design. *BMC Bioinformatics*, **2008**, 9, 148	3.6	25
62	Homology modelling of protein-protein complexes: a simple method and its possibilities and limitations. *BMC Bioinformatics*, **2008**, 9, 427	3.6	28
61	Neutral evolution of proteins: The superfunnel in sequence space and its relation to mutational robustness. *Journal of Chemical Physics*, **2008**, 129, 185104	3.9	7
60	Tet repressor induction by tetracycline: a molecular dynamics, continuum electrostatics, and crystallographic study. *Journal of Molecular Biology*, **2008**, 378, 898-912	6.5	29
59	Binding of tetracyclines to elongation factor Tu, the Tet repressor, and the ribosome: a molecular dynamics simulation study. *Biochemistry*, **2008**, 47, 13594-603	3.2	19
58	Molecular dynamics simulations of the 30S ribosomal subunit reveal a preferred tetracycline binding site. *Journal of the American Chemical Society*, **2008**, 130, 1114-5	16.4	24
57	Probing electrostatic interactions and ligand binding in aspartyl-tRNA synthetase through site-directed mutagenesis and computer simulations. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 1450-60	4.2	12
56	Dielectric relaxation in proteins: the computational perspective. *Photosynthesis Research*, **2008**, 97, 21-32	3.7	18
55	Computational protein design: software implementation, parameter optimization, and performance of a simple model. *Journal of Computational Chemistry*, **2008**, 29, 1092-102	3.5	26
54	Protonation patterns in tetracycline:tet repressor recognition: simulations and experiments. *ChemBioChem*, **2007**, 8, 675-85	3.8	32
53	Neutral evolution of protein-protein interactions: a computational study using simple models. *BMC Structural Biology*, **2007**, 7, 79	2.7	2
52	Computational sidechain placement and protein mutagenesis with implicit solvent models. *Proteins: Structure, Function and Bioinformatics*, **2007**, 67, 853-67	4.2	57
51	Recognizing protein-protein interfaces with empirical potentials and reduced amino acid alphabets. *BMC Bioinformatics*, **2007**, 8, 270	3.6	17
50	Applications of Free Energy Calculations to Chemistry and Biology. *Springer Series in Chemical Physics*, **2007**, 463-501	0.3	11
49	Ammonium scanning in an enzyme active site. The chiral specificity of aspartyl-tRNA synthetase. *Journal of Biological Chemistry*, **2007**, 282, 30856-68	5.4	22

48	Free Energy Calculations: Approximate Methods for Biological Macromolecules. *Springer Series in Chemical Physics*, **2007**, 423-461	0.3	5
47	Free-energy simulations and experiments reveal long-range electrostatic interactions and substrate-assisted specificity in an aminoacyl-tRNA synthetase. *ChemBioChem*, **2006**, 7, 337-44	3.8	34
46	The tetracycline: Mg2+ complex: a molecular mechanics force field. *Journal of Computational Chemistry*, **2006**, 27, 1517-33	3.5	15
45	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, 23792-803	5.4	33
44	Cys(x)His(y)-Zn2+ interactions: possibilities and limitations of a simple pairwise force field. *Journal of Molecular Graphics and Modelling*, **2006**, 24, 404-11	2.8	20
43	A residue-pairwise generalized born scheme suitable for protein design calculations. *Journal of Physical Chemistry B*, **2005**, 109, 22667-73	3.4	36
42	Proton binding to proteins: a free-energy component analysis using a dielectric continuum model. *Biophysical Journal*, **2005**, 88, 3888-904	2.9	66
41	Proton binding to proteins: pK(a) calculations with explicit and implicit solvent models. *Journal of the American Chemical Society*, **2004**, 126, 4167-80	16.4	239
40	Electrostatics and dynamics of proteins. *Reports on Progress in Physics*, **2003**, 66, 737-787	14.4	198
39	Reintroducing electrostatics into protein X-ray structure refinement: bulk solvent treated as a dielectric continuum. *Acta Crystallographica Section D: Biological Crystallography*, **2003**, 59, 2094-103		29
38	Cys(x)His(y)-Zn2+ interactions: thiol vs. thiolate coordination. *Proteins: Structure, Function and Bioinformatics*, **2002**, 49, 37-48	4.2	60
37	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, 6544-9	11.5	87
36	Molecular Dynamics of the tRNAAla Acceptor Stem: Comparison between Continuum Reaction Field and Particle-Mesh Ewald Electrostatic Treatments. *Journal of Physical Chemistry B*, **2002**, 106, 3696-3705	3.4	40
35	Free energy simulations come of age: protein-ligand recognition. *Accounts of Chemical Research*, **2002**, 35, 430-7	24.3	328
34	Protein molecular dynamics with the generalized Born/ACE solvent model. *Proteins: Structure, Function and Bioinformatics*, **2001**, 45, 144-58	4.2	94
33	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	3.5	27
32	Macromolecular electrostatics: continuum models and their growing pains. *Current Opinion in Structural Biology*, **2001**, 11, 243-52	8.1	228
31	Dielectric relaxation in an enzyme active site: molecular dynamics simulations interpreted with a macroscopic continuum model. *Journal of the American Chemical Society*, **2001**, 123, 11047-56	16.4	49

30	Binding free energies and free energy components from molecular dynamics and Poisson-Boltzmann calculations. Application to amino acid recognition by aspartyl-tRNA synthetase. *Journal of Molecular Biology*, **2001**, 306, 307-27	6.5	103
29	Free Energy Calculations **2001**,		6
28	Electrostatic Free Energy Calculations for Macromolecules: A Hybrid Molecular Dynamics/Continuum Electrostatics Approach. *Journal of Physical Chemistry B*, **2000**, 104, 6509-6513	3.4	36
27	Protein-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	6.3	29
26	Implicit solvent models. *Biophysical Chemistry*, **1999**, 78, 1-20	3.5	708
25	Dielectric relaxation in proteins: Microscopic and macroscopic models. *International Journal of Quantum Chemistry*, **1999**, 73, 45-57	2.1	36
24	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	3.5	30
23	Molecular dynamics simulations of the Ras:Raf and Rap:Raf complexes. *Proteins: Structure, Function and Bioinformatics*, **1999**, 35, 89-100	4.2	17
22	A PoissonBoltzmann Study of Charge Insertion in an Enzyme Active Site: The Effect of Dielectric Relaxation. *Journal of Physical Chemistry B*, **1999**, 103, 6142-6156	3.4	82
21	Dielectric relaxation in proteins: Microscopic and macroscopic models **1999**, 73, 45		1
20	Conformation of the Ras-binding domain of Raf studied by molecular dynamics and free energy simulations. *Proteins: Structure, Function and Bioinformatics*, **1998**, 31, 186-200	4.2	9
19	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		11
18	Dielectric Constant of Cytochrome c from Simulations in a Water Droplet Including All Electrostatic Interactions. *Journal of the American Chemical Society*, **1998**, 120, 4875-4876	16.4	50
17	Specific amino acid recognition by aspartyl-tRNA synthetase studied by free energy simulations. *Journal of Molecular Biology*, **1998**, 275, 823-46	6.5	75
16	Classical and Quantum Simulations of Tryptophan in Solution. *Journal of Physical Chemistry A*, **1997**, 101, 1935-1945	2.8	29
15	Continuum Treatment of Long-Range Interactions in Free Energy Calculations. Application to Protein Ligand Binding.. *Journal of Physical Chemistry B*, **1997**, 101, 8349-8362	3.4	107
14	Charge Screening and the Dielectric Constant of Proteins: Insights from Molecular Dynamics. *Journal of the American Chemical Society*, **1996**, 118, 8452-8458	16.4	320
13	Polar fluctuations in proteins: molecular-dynamic studies of cytochrome c in aqueous solution. *Faraday Discussions*, **1996**, 71-90	3.6	28

12	Accurate calculation of the dielectric constant of water from simulations of a microscopic droplet in vacuum. *Chemical Physics Letters*, **1996**, 250, 450-454	2.5	45
11	Proline cis-trans isomerization in staphylococcal nuclease: multi-substrate free energy perturbation calculations. *Protein Science*, **1995**, 4, 636-54	6.3	18
10	Microscopic Dielectric Properties of Cytochrome c from Molecular Dynamics Simulations in Aqueous Solution. *Journal of the American Chemical Society*, **1995**, 117, 7987-8000	16.4	106
9	Dielectric properties of proteins from simulations: tools and techniques. *Computer Physics Communications*, **1995**, 91, 291-303	4.2	13
8	Solvation Free Energies Estimated from Macroscopic Continuum Theory: An Accuracy Assessment. *The Journal of Physical Chemistry*, **1994**, 98, 4683-4694		178
7	Conformational substrates and uncertainty in macromolecular free energy calculations. *The Journal of Physical Chemistry*, **1993**, 97, 3409-3417		49
6	Free energy of particle insertion. *Molecular Physics*, **1993**, 80, 441-447	1.7	102
5	Thermodynamics of protein-peptide interactions in the ribonuclease-S system studied by molecular dynamics and free energy calculations. *Biochemistry*, **1992**, 31, 8661-74	3.2	60
4	Intramolecular dielectric screening in proteins. *Journal of Molecular Biology*, **1991**, 218, 859-86	6.5	58
3	Proteus software for physics-based protein design		1
2	Adaptive landscape flattening allows the design of both enzyme:substrate binding and catalytic power		1
1	A physics-based energy function allows the computational redesign of a PDZ domain		1