

# Thomas Simonson

## List of Publications by Year in descending order

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119  
papers

5,648  
citations

134610

34  
h-index

97045

71  
g-index

127  
all docs

127  
docs citations

127  
times ranked

4410  
citing authors

#	ARTICLE	IF	CITATIONS
1	How much can physics do for protein design?. <i>Current Opinion in Structural Biology</i> , 2022, 72, 46-54.	2.6	10
2	Knowledge-Based Unfolded State Model for Protein Design. <i>Methods in Molecular Biology</i> , 2022, 2405, 403-424.	0.4	0
3	A Computational Model for the PLP-Dependent Enzyme Methionine Î³-Lyase. <i>Frontiers in Molecular Biosciences</i> , 2022, 9, 886358.	1.6	1
4	Computational Design of PDZ-Peptide Binding. <i>Methods in Molecular Biology</i> , 2021, 2256, 237-255.	0.4	3
5	Physics-Based Computational Protein Design: An Update. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10637-10648.	1.1	16
6	Hybrid MC/MD for protein design. <i>Journal of Chemical Physics</i> , 2020, 153, 054113.	1.2	9
7	Application of Various Molecular Modelling Methods in the Study of Estrogens and Xenoestrogens. <i>International Journal of Molecular Sciences</i> , 2020, 21, 6411.	1.8	6
8	A physics-based energy function allows the computational redesign of a PDZ domain. <i>Scientific Reports</i> , 2020, 10, 11150.	1.6	7
9	Adaptive landscape flattening allows the design of both enzyme: Substrate binding and catalytic power. <i>PLoS Computational Biology</i> , 2020, 16, e1007600.	1.5	13
10	Biochemical and Structural Characterization of De Novo Designed PDZ Domains. <i>Biophysical Journal</i> , 2019, 116, 320a.	0.2	0
11	Variable Neighborhood Search with Cost Function Networks To Solve Large Computational Protein Design Problems. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 127-136.	2.5	9
12	Adaptive landscape flattening in amino acid sequence space for the computational design of protein:peptide binding. <i>Journal of Chemical Physics</i> , 2018, 149, 072302.	1.2	22
13	Accurate PDZ/Peptide Binding Specificity with Additive and Polarizable Free Energy Simulations. <i>Biophysical Journal</i> , 2018, 114, 1091-1102.	0.2	30
14	Protein p <i>K<sub>a</sub></i> ™s from Adaptive Landscape Flattening Instead of Constant-pH Simulations. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6714-6721.	2.3	7
15	Classical Drude Polarizable Force Field Model for Methyl Phosphate and Its Interactions with Mg <sup>2+</sup> . <i>Journal of Physical Chemistry A</i> , 2018, 122, 6147-6155.	1.1	23
16	Equivalence of M- and P-Summation in Calculations of Ionic Solvation Free Energies. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1525-1530.	1.1	15
17	Computational Design of the Tiam1 PDZ Domain and Its Ligand Binding. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2271-2289.	2.3	12
18	Probing the stereospecificity of tyrosyl- and glutaminyI-tRNA synthetase with molecular dynamics. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 71, 192-199.	1.3	2

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19	Full Protein Sequence Redesign with an MMGBSA Energy Function. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4932-4943.	2.3	11
20	Comparing pairwise-additive and many-body generalized Born models for acid/base calculations and protein design. <i>Journal of Computational Chemistry</i> , 2017, 38, 2396-2410.	1.5	19
21	Simple models for nonpolar solvation: Parameterization and testing. <i>Journal of Computational Chemistry</i> , 2017, 38, 2509-2519.	1.5	20
22	Computational design of fully overlapping coding schemes for protein pairs and triplets. <i>Scientific Reports</i> , 2017, 7, 15873.	1.6	22
23	A Simple PB/LIE Free Energy Function Accurately Predicts the Peptide Binding Specificity of the Tiam1 PDZ Domain. <i>Frontiers in Molecular Biosciences</i> , 2017, 4, 65.	1.6	10
24	Comparing three stochastic search algorithms for computational protein design: Monte Carlo, replica exchange Monte Carlo, and a multistart, steepest-descent heuristic. <i>Journal of Computational Chemistry</i> , 2016, 37, 1781-1793.	1.5	25
25	Protein side chain conformation predictions with an MMGBSA energy function. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 803-819.	1.5	21
26	Redesigning the stereospecificity of tyrosyl-tRNA synthetase. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 240-253.	1.5	19
27	Protein:Ligand binding free energies: A stringent test for computational protein design. <i>Journal of Computational Chemistry</i> , 2016, 37, 404-415.	1.5	15
28	Concepts and protocols for electrostatic free energies. <i>Molecular Simulation</i> , 2016, 42, 1090-1101.	0.9	30
29	Protein Sequence Optimization with a Polarizable Force Field: Insights from PDZ Domains. <i>Biophysical Journal</i> , 2016, 110, 345a-346a.	0.2	0
30	Proteus and the Design of Ligand Binding Sites. <i>Methods in Molecular Biology</i> , 2016, 1414, 77-97.	0.4	2
31	A Hybrid Monte Carlo Scheme for Multibackbone Protein Design. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 6035-6048.	2.3	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. <i>ChemPhysChem</i> , 2015, 16, 658-665.	1.0	12
34	Electrostatic free energies in translational GTPases: Classic allostery and the rest. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2015, 1850, 1006-1016.	1.1	5
35	Pairwise decomposition of an MMGBSA energy function for computational protein design. <i>Journal of Computational Chemistry</i> , 2014, 35, 1371-1387.	1.5	40
36	An Overview of Electrostatic Free Energy Computations for Solutions and Proteins. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2690-2709.	2.3	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.	2.3	16
38	Computational protein design: The proteus software and selected applications. Journal of Computational Chemistry, 2013, 34, 2472-2484.	1.5	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.	1.5	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.	1.5	19
41	Protein: Ligand Recognition: Simple Models for Electrostatic Effects. Current Pharmaceutical Design, 2013, 19, 4241-4256.	0.9	18
42	Conformational Selection by the $\alpha$ F2 GTPase: A Molecular Dynamics Study of Functional Pathways. Biochemistry, 2012, 51, 353-361.	1.2	8
43	Nucleotide recognition by the initiation factor $\alpha$ F5B: Free energy simulations of a neoclassical GTPase. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2742-2757.	1.5	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.	1.5	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.	1.2	26
47	Computational protein design with a generalized born solvent model: Application to asparaginyl-tRNA synthetase. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3448-3468.	1.5	20
48	A large decoy set of protein-protein complexes produced by flexible docking. Journal of Computational Chemistry, 2011, 32, 106-120.	1.5	3
49	Computational design of protein-ligand binding: Modifying the specificity of asparaginyl-tRNA synthetase. Journal of Computational Chemistry, 2010, 31, 1273-1286.	1.5	14
50	A molecular mechanics model for imatinib and imatinib:kinase binding. Journal of Computational Chemistry, 2010, 31, 1550-1560.	1.5	16
51	Alchemical free energy simulations for biological complexes: powerful but temperamental. Journal of Molecular Recognition, 2010, 23, 117-127.	1.1	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.	1.6	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.	1.2	29
54	Nonantibiotic Properties of Tetracyclines: Structural Basis for Inhibition of Secretory Phospholipase A2. Journal of Molecular Biology, 2010, 398, 83-96.	2.0	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.	1.1	16
56	Molecular mechanics models for tetracycline analogs. Journal of Computational Chemistry, 2009, 30, 243-255.	1.5	19
57	Computational protein design as a tool for fold recognition. Proteins: Structure, Function and Bioinformatics, 2009, 77, 139-158.	1.5	25
58	Tetracycline-Tet Repressor Binding Specificity: Insights from Experiments and Simulations. Biophysical Journal, 2009, 97, 2829-2838.	0.2	16
59	Probing electrostatic interactions and ligand binding in aspartyl-tRNA synthetase through site-directed mutagenesis and computer simulations. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1450-1460.	1.5	12
60	Dielectric relaxation in proteins: the computational perspective. Photosynthesis Research, 2008, 97, 21-32.	1.6	20
61	Computational protein design: Software implementation, parameter optimization, and performance of a simple model. Journal of Computational Chemistry, 2008, 29, 1092-1102.	1.5	27
62	Testing the Coulomb/Accessible Surface Area solvent model for protein stability, ligand binding, and protein design. BMC Bioinformatics, 2008, 9, 148.	1.2	28
63	Homology modelling of protein-protein complexes: a simple method and its possibilities and limitations. BMC Bioinformatics, 2008, 9, 427.	1.2	33
64	Neutral evolution of proteins: The superfunnel in sequence space and its relation to mutational robustness. Journal of Chemical Physics, 2008, 129, 185104.	1.2	10
65	Tet Repressor Induction by Tetracycline: A Molecular Dynamics, Continuum Electrostatics, and Crystallographic Study. Journal of Molecular Biology, 2008, 378, 898-912.	2.0	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.	1.2	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.	6.6	30
68	Ammonium Scanning in an Enzyme Active Site. Journal of Biological Chemistry, 2007, 282, 30856-30868.	1.6	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.	1.3	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.	1.5	61

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73	Recognizing protein-protein interfaces with empirical potentials and reduced amino acid alphabets. <i>BMC Bioinformatics</i> , 2007, 8, 270.	1.2	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 Mg <sup>2+</sup> Contributes to Amino Acid and Aminoacyl Adenylate Binding Specificity in Aspartyl-tRNA Synthetase through Long Range Electrostatic Interactions. <i>Journal of Biological Chemistry</i> , 2006, 281, 23792-23803.	1.6	34
76	CysxHisy-Zn <sup>2+</sup> interactions: Possibilities and limitations of a simple pairwise force field. <i>Journal of Molecular Graphics and Modelling</i> , 2006, 24, 404-411.	1.3	25
77	Free-Energy Simulations and Experiments Reveal Long-Range Electrostatic Interactions and Substrate-Assisted Specificity in an Aminoacyl-tRNA Synthetase. <i>ChemBioChem</i> , 2006, 7, 337-344.	1.3	37
78	The tetracycline: Mg <sup>2+</sup> complex: A molecular mechanics force field. <i>Journal of Computational Chemistry</i> , 2006, 27, 1517-1533.	1.5	19
79	A Residue-Pairwise Generalized Born Scheme Suitable for Protein Design Calculations. <i>Journal of Physical Chemistry B</i> , 2005, 109, 22667-22673.	1.2	36
80	Proton Binding to Proteins: A Free-Energy Component Analysis Using a Dielectric Continuum Model. <i>Biophysical Journal</i> , 2005, 88, 3888-3904.	0.2	71
81	Theory and simulation: from protons to genomes. <i>Current Opinion in Structural Biology</i> , 2004, 14, 189-191.	2.6	1
82	Proton Binding to Proteins: pKa Calculations with Explicit and Implicit Solvent Models. <i>Journal of the American Chemical Society</i> , 2004, 126, 4167-4180.	6.6	266
83	Reintroducing electrostatics into protein X-ray structure refinement: bulk solvent treated as a dielectric continuum. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2003, 59, 2094-2103.	2.5	32
84	Electrostatics and dynamics of proteins. <i>Reports on Progress in Physics</i> , 2003, 66, 737-787.	8.1	220
85	Gaussian fluctuations and linear response in an electron transfer protein. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 6544-6549.	3.3	92
86	Molecular Dynamics of the tRNA <sup>Ala</sup> Acceptor Stem: Comparison between Continuum Reaction Field and Particle-Mesh Ewald Electrostatic Treatments. <i>Journal of Physical Chemistry B</i> , 2002, 106, 3696-3705.	1.2	42
87	Free Energy Simulations Come of Age: Protein-Ligand Recognition. <i>Accounts of Chemical Research</i> , 2002, 35, 430-437.	7.6	355
88	CysxHisy-Zn <sup>2+</sup> interactions: Thiol vs. thiolate coordination. <i>Proteins: Structure, Function and Bioinformatics</i> , 2002, 49, 37-48.	1.5	62
89	Dielectric Relaxation in an Enzyme Active Site: Molecular Dynamics Simulations Interpreted with a Macroscopic Continuum Model. <i>Journal of the American Chemical Society</i> , 2001, 123, 11047-11056.	6.6	49
90	Binding free energies and free energy components from molecular dynamics and Poisson-Boltzmann calculations. Application to amino acid recognition by aspartyl-tRNA synthetase. Edited by A. R. Fersht. <i>Journal of Molecular Biology</i> , 2001, 306, 307-327.	2.0	107

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91	Protein molecular dynamics with the generalized born/ACE solvent model. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001, 45, 144-158.	1.5	102
92	Dielectric relaxation in proteins: a continuum electrostatics model incorporating dielectric heterogeneity of the protein and time-dependent charges. <i>Journal of Computational Chemistry</i> , 2001, 22, 290-305.	1.5	27
93	Macromolecular electrostatics: continuum models and their growing pains. <i>Current Opinion in Structural Biology</i> , 2001, 11, 243-252.	2.6	246
94	Free Energy Calculations. , 2001, , .		8
95	Electrostatic Free Energy Calculations for Macromolecules: A Hybrid Molecular Dynamics/Continuum Electrostatics Approach. <i>Journal of Physical Chemistry B</i> , 2000, 104, 6509-6513.	1.2	37
96	Implicit solvent models. <i>Biophysical Chemistry</i> , 1999, 78, 1-20.	1.5	793
97	Dielectric relaxation in proteins: Microscopic and macroscopic models. <i>International Journal of Quantum Chemistry</i> , 1999, 73, 45-57.	1.0	36
98	Implicit solvent models: Combining an analytical formulation of continuum electrostatics with simple models of the hydrophobic effect. <i>Journal of Computational Chemistry</i> , 1999, 20, 322-335.	1.5	30
99	Molecular dynamics simulations of the Ras:Raf and Rap:Raf complexes. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999, 35, 89-100.	1.5	17
100	A Poisson-Boltzmann Study of Charge Insertion in an Enzyme Active Site: The Effect of Dielectric Relaxation. <i>Journal of Physical Chemistry B</i> , 1999, 103, 6142-6156.	1.2	86
101	Protein-protein recognition: An experimental and computational study of the R89K mutation in Raf and its effect on Ras binding. <i>Protein Science</i> , 1999, 8, 50-64.	3.1	31
102	Dielectric relaxation in proteins: Microscopic and macroscopic models. , 1999, 73, 45.		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 Mg <sup>2+</sup> 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 Cytochrome c from Simulations in a Water Droplet Including All Electrostatic Interactions. <i>Journal of the American Chemical Society</i> , 1998, 120, 4875-4876.	6.6	51
106	Specific amino acid recognition by aspartyl-tRNA synthetase studied by free energy simulations I. <i>Journal of Molecular Biology</i> , 1998, 275, 823-846.	2.0	75
107	Classical and Quantum Simulations of Tryptophan in Solution. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1935-1945.	1.1	29
108	Continuum Treatment of Long-Range Interactions in Free Energy Calculations. Application to Protein-Ligand Binding. <i>Journal of Physical Chemistry B</i> , 1997, 101, 8349-8362.	1.2	111

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109	Charge Screening and the Dielectric Constant of Proteins: Insights from Molecular Dynamics. Journal of the American Chemical Society, 1996, 118, 8452-8458.	6.6	348
110	Polar fluctuations in proteins: molecular-dynamic studies of cytochrome c in aqueous solution. Faraday Discussions, 1996, 103, 71.	1.6	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.	1.2	47
112	Dielectric properties of proteins from simulations: tools and techniques. Computer Physics Communications, 1995, 91, 291-303.	3.0	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.	6.6	116
114	Proline <i>cis</i> → <i>trans</i> isomerization in staphylococcal nuclease: Multi-substate free energy perturbation calculations. Protein Science, 1995, 4, 636-654.	3.1	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.	0.8	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.	1.2	66
119	Intramolecular dielectric screening in proteins. Journal of Molecular Biology, 1991, 218, 859-886.	2.0	66