Carlos L Simmerling

List of Publications by Year
in descending order

89 papers	27,938 citations	66343 42 h-index	45317 90 g-index
102 all docs	102 docs citations	102 times ranked	28231 citing authors

#	Article	IF	Citations
1	GlycoGrip: Cell Surface-Inspired Universal Sensor for Betacoronaviruses. ACS Central Science, 2022, 8, 22-42.	11.3	31
2	Accelerating the Ensemble Convergence of RNA Hairpin Simulations with a Replica Exchange Structure Reservoir. Journal of Chemical Theory and Computation, 2022, 18, 3930-3947.	5.3	5
3	The flexibility of ACE2 in the context of SARS-CoV-2 infection. Biophysical Journal, 2021, 120, 1072-1084.	0.5	102
4	Quantitative Analysis of Protein Unfolded State Energetics: Experimental and Computational Studies Demonstrate That Non-Native Side-Chain Interactions Stabilize Local Native Backbone Structure. Journal of Physical Chemistry B, 2021, 125, 3269-3277.	2.6	3
5	Scaffold Hopping Transformations Using Auxiliary Restraints for Calculating Accurate Relative Binding Free Energies. Journal of Chemical Theory and Computation, 2021, 17, 3710-3726.	5.3	12
6	Free Energy Landscapes from SARS-CoV-2 Spike Glycoprotein Simulations Suggest that RBD Opening Can Be Modulated via Interactions in an Allosteric Pocket. Journal of the American Chemical Society, 2021, 143, 11349-11360.	13.7	54
7	ff19SB: Amino-Acid-Specific Protein Backbone Parameters Trained against Quantum Mechanics Energy Surfaces in Solution. Journal of Chemical Theory and Computation, 2020, 16, 528-552.	5.3	843
8	Protein storytelling through physics. Science, 2020, 370, .	12.6	49
9	Exploring Protocols to Build Reservoirs to Accelerate Temperature Replica Exchange MD Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7776-7799.	5.3	9
10	Unraveling the Mechanism of a LOV Domain Optogenetic Sensor: A Glutamine Lever Induces Unfolding of the JÎ± Helix. ACS Chemical Biology, 2020, 15, 2752-2765.	3.4	29
11	Copper stabilizes antiparallel Î²-sheet fibrils of the amyloid Î²40 (AÎ²40)-Iowa variant. Journal of Biological Chemistry, 2020, 295, 8914-8927.	3.4	7
12	Fast Implementation of the Nudged Elastic Band Method in AMBER. Journal of Chemical Theory and Computation, 2019, 15, 4699-4707.	5.3	12
13	Dissecting the Energetics of Intrinsically Disordered Proteins via a Hybrid Experimental and Computational Approach. Journal of Physical Chemistry B, 2019, 123, 10394-10402.	2.6	9
14	Blinded prediction of proteinâ€“ligand binding affinity using Amber thermodynamic integration for the 2018 D3R grand challenge 4. Journal of Computer-Aided Molecular Design, 2019, 33, 1021-1029.	2.9	35
15	Fast Pairwise Approximation of Solvent Accessible Surface Area for Implicit Solvent Simulations of Proteins on CPUs and GPUs. Journal of Chemical Theory and Computation, 2018, 14, 5797-5814.	5.3	28
16	Laguerre-Intersection Method for Implicit Solvation. International Journal of Computational Geometry and Applications, 2018, 28, 1-38.	0.5	1
17	DNA Deformation-Coupled Recognition of 8-Oxoguanine: Conformational Kinetic Gating in Human DNA Glycosylase. Journal of the American Chemical Society, 2017, 139, 2682-2692.	13.7	25
18	Characterization of Biomolecular Helices and Their Complementarity Using Geometric Analysis. Journal of Chemical Information and Modeling, 2017, 57, 864-874.	5.4	9

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19	A human transcription factor in search mode. Nucleic Acids Research, 2016, 44, 63-74.	14.5	52
20	Selectivity of Pyridone- and Diphenyl Ether-Based Inhibitors for the Yersinia pestis FabV Enoyl-ACP Reductase. Biochemistry, 2016, 55, 2992-3006.	2.5	6
21	Experimental and Computational Analysis of Protein Stabilization by Gly-to-<scp>d</scp>-Ala Substitution: A Convolution of Native State and Unfolded State Effects. Journal of the American Chemical Society, 2016, 138, 15682-15689.	13.7	20
22	Base Flipping by MTERF1 Can Accommodate Multiple Conformations and Occurs in a Stepwise Fashion. Journal of Molecular Biology, 2016, 428, 2542-2556.	4.2	3
23	Advances in free-energy-based simulations of protein folding and ligand binding. Current Opinion in Structural Biology, 2016, 36, 25-31.	5.7	121
24	A dynamic checkpoint in oxidative lesion discrimination by formamidopyrimidineâ€"DNA glycosylase. Nucleic Acids Research, 2016, 44, 683-694.	14.5	19
25	Rational Modulation of the Induced-Fit Conformational Change for Slow-Onset Inhibition in Mycobacterium tuberculosis InhA. Biochemistry, 2015, 54, 4683-4691.	2.5	30
26	ff14SB: Improving the Accuracy of Protein Side Chain and Backbone Parameters from ff99SB. Journal of Chemical Theory and Computation, 2015, 11, 3696-3713.	5.3	7,322
27	Refinement of Generalized Born Implicit Solvation Parameters for Nucleic Acids and Their Complexes with Proteins. Journal of Chemical Theory and Computation, 2015, 11, 3714-3728.	5.3	58
28	Active destabilization of base pairs by a DNA glycosylase wedge initiates damage recognition. Nucleic Acids Research, 2015, 43, 272-281.	14.5	49
29	Grid-Based Backbone Correction to the ff12SB Protein Force Field for Implicit-Solvent Simulations. Journal of Chemical Theory and Computation, 2015, 11, 4770-4779.	5.3	76
30	Timeâ€Dependent Diaryl Ether Inhibitors of InhA: Structureâ€"Activity Relationship Studies of Enzyme Inhibition, Antibacterial Activity, and inâ€…vivo Efficacy. ChemMedChem, 2014, 9, 776-791.	3.2	48
31	A Structural and Energetic Model for the Slow-Onset Inhibition of the Mycobacterium tuberculosis Enoyl-ACP Reductase InhA. ACS Chemical Biology, 2014, 9, 986-993.	3.4	63
32	Ultrafast Structural Dynamics of BlsA, a Photoreceptor from the Pathogenic Bacterium Acinetobacter baumannii. Journal of Physical Chemistry Letters, 2014, 5, 220-224.	4.6	25
33	Folding Simulations for Proteins with Diverse Topologies Are Accessible in Days with a Physics-Based Force Field and Implicit Solvent. Journal of the American Chemical Society, 2014, 136, 13959-13962.	13.7	199
34	The Role of Select Subtype Polymorphisms on HIV-1 Protease Conformational Sampling and Dynamics. Journal of Biological Chemistry, 2014, 289, 17203-17214.	3.4	43
35	Thiolactomycin-based Î²-Ketoacyl-AcpM Synthase A (KasA) Inhibitors. Journal of Biological Chemistry, 2013, 288, 6045-6052.	3.4	32
36	Improved Generalized Born Solvent Model Parameters for Protein Simulations. Journal of Chemical Theory and Computation, 2013, 9, 2020-2034.	5.3	387

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37	Molecular Dynamics Applied in Drug Discovery: The Case of HIV-1 Protease. Methods in Molecular Biology, 2012, 819, 527-549.	0.9	9
38	CoA Adducts of 4-Oxo-4-phenylbut-2-enoates: Inhibitors of MenB from the M. tuberculosis Menaquinone Biosynthesis Pathway. ACS Medicinal Chemistry Letters, 2011, 2, 818-823.	2.8	40
39	Energetic Preference of 8-oxoG Eversion Pathways in a DNA Glycosylase. Journal of the American Chemical Society, 2011, 133, 14504-14506.	13.7	30
40	Improving the description of salt bridge strength and geometry in a Generalized Born model. Journal of Molecular Graphics and Modelling, 2011, 29, 676-684.	2.4	18
41	An Overview of String-Based Path Sampling Methods. Annual Reports in Computational Chemistry, 2011, 7, 89-97.	1.7	3
42	Synthesis and Molecular Modeling of a Nitrogen Mustard DNA Interstrand Crosslink. Chemistry - A European Journal, 2010, 16, 12100-12103.	3.3	30
43	Slow Onset Inhibition of Bacterial Î²-Ketoacyl-acyl Carrier Protein Synthases by Thiolactomycin. Journal of Biological Chemistry, 2010, 285, 6161-6169.	3.4	42
44	Three-Dimensional Molecular Theory of Solvation Coupled with Molecular Dynamics in Amber. Journal of Chemical Theory and Computation, 2010, 6, 607-624.	5.3	232
45	Recent Advances in the Study of the Bioactive Conformation of Taxol. ChemMedChem, 2009, 4, 719-731.	3.2	36
46	A partial nudged elastic band implementation for use with large or explicitly solvated systems. International Journal of Quantum Chemistry, 2009, 109, 3781-3790.	2.0	40
47	Evaluating the Performance of the ff99SB Force Field Based on NMR ScalarÂCoupling Data. Biophysical Journal, 2009, 97, 853-856.	0.5	201
48	Drug Pressure Selected Mutations in HIV-1 Protease Alter Flap Conformations. Journal of the American Chemical Society, 2009, 131, 430-431.	13.7	70
49	An Improved Reaction Coordinate for Nucleic Acid Base Flipping Studies. Journal of Chemical Theory and Computation, 2009, 5, 3105-3113.	5.3	55
50	Molecular mechanics parameters for the FapydG DNA lesion. Journal of Computational Chemistry, 2008, 29, 17-23.	3.3	11
51	Structural insights for designed alanineâ€rich helices: Comparing NMR helicity measures and conformational ensembles from molecular dynamics simulation. Biopolymers, 2008, 89, 747-760.	2.4	25
52	Evaluation of Salt Bridge Structure and Energetics in Peptides Using Explicit, Implicit, and Hybrid Solvation Models. Journal of Chemical Theory and Computation, 2008, 4, 488-498.	5.3	35
53	Solution Structure of HIV-1 Protease Flaps Probed by Comparison of Molecular Dynamics Simulation Ensembles and EPR Experiments. Journal of the American Chemical Society, 2008, 130, 7184-7185.	13.7	63
54	Design, Synthesis, and Biological Evaluation of Novel C14â^'C3â€²BzN-Linked Macrocyclic Taxoids. Journal of Organic Chemistry, 2008, 73, 9584-9593.	3.2	26

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55	Improving Convergence of Replica-Exchange Simulations through Coupling to a High-Temperature Structure Reservoir. Journal of Chemical Theory and Computation, 2007, 3, 557-568.	5.3	70
56	Coupling of Replica Exchange Simulations to a Non-Boltzmann Structure Reservoir. Journal of Physical Chemistry B, 2007, 111, 2415-2418.	2.6	80
57	Generalized Born Model with a Simple, Robust Molecular Volume Correction. Journal of Chemical Theory and Computation, 2007, 3, 156-169.	5.3	334
58	Molecular Simulations Reveal a Common Binding Mode for Glycosylase Binding of Oxidatively Damaged DNA Lesions. Journal of the American Chemical Society, 2007, 129, 14536-14537.	13.7	14
59	Reconciling the Solution and X-ray Structures of the Villin Headpiece Helical Subdomain:Â Molecular Dynamics Simulations and Double Mutant Cycles Reveal a Stabilizing Cationâ^'Ï€ Interactionâ€. Biochemistry, 2007, 46, 3624-3634.	2.5	23
60	Secondary Structure Bias in Generalized Born Solvent Models:Â Comparison of Conformational Ensembles and Free Energy of Solvent Polarization from Explicit and Implicit Solvation. Journal of Physical Chemistry B, 2007, 111, 1846-1857.	2.6	121
61	Targeting structural flexibility in HIV-1 protease inhibitor binding. Drug Discovery Today, 2007, 12, 132-138.	6.4	120
62	The Open Structure of a Multi-Drug-Resistant HIV-1 Protease is Stabilized by Crystal Packing Contacts. Journal of the American Chemical Society, 2006, 128, 13360-13361.	13.7	39
63	Chapter 6 Hybrid Explicit/Implicit Solvation Methods. Annual Reports in Computational Chemistry, 2006, 2, 97-109.	1.7	23
64	Insight through Molecular Mechanics Poissonâ^'Boltzmann Surface Area Calculations into the Binding Affinity of Triclosan and Three Analogues for FabI, the E. coli Enoyl Reductase. Journal of Medicinal Chemistry, 2006, 49, 4574-4580.	6.4	32
65	Investigation of Salt Bridge Stability in a Generalized Born Solvent Model. Journal of Chemical Theory and Computation, 2006, 2, 115-127.	5.3	110
66	HIV-1 Protease Flaps Spontaneously Close to the Correct Structure in Simulations Following Manual Placement of an Inhibitor into the Open State. Journal of the American Chemical Society, 2006, 128, 2812-2813.	13.7	103
67	HIV-1 protease flaps spontaneously open and reclose in molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 915-920.	7.1	344
68	Improved Efficiency of Replica Exchange Simulations through Use of a Hybrid Explicit/Implicit Solvation Model. Journal of Chemical Theory and Computation, 2006, 2, 420-433.	5.3	126
69	Computational Analysis of the Mode of Binding of 8-Oxoguanine to Formamidopyrimidine-DNA Glycosylaseâ€. Biochemistry, 2006, 45, 10886-10894.	2.5	27
70	The Unfolded State of the Villin Headpiece Helical Subdomain: Computational Studies of the Role of Locally Stabilized Structure. Journal of Molecular Biology, 2006, 360, 1094-1107.	4.2	46
71	Comparison of multiple Amber force fields and development of improved protein backbone parameters. Proteins: Structure, Function and Bioinformatics, 2006, 65, 712-725.	2.6	6,049
72	Structure of Acyl Carrier Protein Bound to FabI, the FASII Enoyl Reductase from Escherichia coli. Journal of Biological Chemistry, 2006, 281, 39285-39293.	3.4	101

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73	Use of the Tubulin Bound Paclitaxel Conformation for Structure-Based Rational Drug Design. Chemistry and Biology, 2005, 12, 339-348.	6.0	73
74	The Amber biomolecular simulation programs. Journal of Computational Chemistry, 2005, 26, 1668-1688.	3.3	7,742
75	Structural Requirements of the Extracellular to Transmembrane Domain Junction for Erythropoietin Receptor Function. Journal of Biological Chemistry, 2005, 280, 14844-14854.	3.4	40
76	Dynamic Behavior of DNA Base Pairs Containing 8-Oxoguanine. Journal of the American Chemical Society, 2005, 127, 13906-13918.	13.7	73
77	Folding Cooperativity in a Three-stranded Î²-Sheet Model. Journal of Molecular Biology, 2005, 352, 370-381.	4.2	45
78	Modified Replica Exchange Simulation Methods for Local Structure Refinement. Journal of Physical Chemistry B, 2005, 109, 8220-8230.	2.6	105
79	Inhibition of the Bacterial Enoyl Reductase FabI by Triclosan:â€‰ A Structureâˆ'Reactivity Analysis of FabI Inhibition by Triclosan Analogues. Journal of Medicinal Chemistry, 2004, 47, 509-518.	6.4	101
80	Development of softcore potential functions for overcoming steric barriers in molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2004, 22, 405-413.	2.4	30
81	Using PC clusters to evaluate the transferability of molecular mechanics force fields for proteins. Journal of Computational Chemistry, 2003, 24, 21-31.	3.3	94
82	Generation of accurate protein loop conformations through low-barrier molecular dynamics. Proteins: Structure, Function and Bioinformatics, 2003, 51, 577-590.	2.6	47
83	All-Atom Structure Prediction and Folding Simulations of a Stable Protein. Journal of the American Chemical Society, 2002, 124, 11258-11259.	13.7	564
84	The Disordered Mobile Loop of GroES Folds into a Defined Î²-Hairpin upon Binding GroEL. Journal of Biological Chemistry, 2001, 276, 31257-31264.	3.4	33
85	Combining MONSSTER and LES/PME to Predict Protein Structure from Amino Acid Sequence:â€‰ Application to the Small Protein CMTI-1. Journal of the American Chemical Society, 2000, 122, 8392-8402.	13.7	36
86	Use of Locally Enhanced Sampling in Free Energy Calculations:â€‰ Testing and Application to the Î± â†' Î² Anomerization of Glucose. Journal of the American Chemical Society, 1998, 120, 5771-5782.	13.7	88
87	Combined Locally Enhanced Sampling and Particle Mesh Ewald as a Strategy To Locate the Experimental Structure of a Nonhelical Nucleic Acid. Journal of the American Chemical Society, 1998, 120, 7149-7155.	13.7	67
88	MOIL: A program for simulations of macromolecules. Computer Physics Communications, 1995, 91, 159-189.	7.5	154
89	Hydrophobic "Collapse" in a Cyclic Hexapeptide: Computer Simulations of CHDLFC and CAAAAC in Water. Journal of the American Chemical Society, 1994, 116, 2534-2547.	13.7	46