

# Carlos L Simmerling

## List of Publications by Year in descending order

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89  
papers

27,938  
citations

76031

42  
h-index

51423

90  
g-index

102  
all docs

102  
docs citations

102  
times ranked

31440  
citing authors

#	ARTICLE	IF	CITATIONS
1	<i>GlycoGrip</i>: Cell Surface-Inspired Universal Sensor for Betacoronaviruses. ACS Central Science, 2022, 8, 22-42.	5.3	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.	2.3	5
3	The flexibility of ACE2 in the context of SARS-CoV-2 infection. Biophysical Journal, 2021, 120, 1072-1084.	0.2	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.	1.2	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.	2.3	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.	6.6	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.	2.3	843
8	Protein storytelling through physics. Science, 2020, 370, .	6.0	49
9	Exploring Protocols to Build Reservoirs to Accelerate Temperature Replica Exchange MD Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7776-7799.	2.3	9
10	Unraveling the Mechanism of a LOV Domain Optogenetic Sensor: A Glutamine Lever Induces Unfolding of the J± Helix. ACS Chemical Biology, 2020, 15, 2752-2765.	1.6	29
11	Copper stabilizes antiparallel $\beta$ -sheet fibrils of the amyloid $\beta$ 40 (A $\beta$ 40)-Iowa variant. Journal of Biological Chemistry, 2020, 295, 8914-8927.	1.6	7
12	Fast Implementation of the Nudged Elastic Band Method in AMBER. Journal of Chemical Theory and Computation, 2019, 15, 4699-4707.	2.3	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.	1.2	9
14	Blinded prediction of protein-ligand binding affinity using Amber thermodynamic integration for the 2018 D3R grand challenge 4. Journal of Computer-Aided Molecular Design, 2019, 33, 1021-1029.	1.3	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.	2.3	28
16	Laguerre-Intersection Method for Implicit Solvation. International Journal of Computational Geometry and Applications, 2018, 28, 1-38.	0.3	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.	6.6	25
18	Characterization of Biomolecular Helices and Their Complementarity Using Geometric Analysis. Journal of Chemical Information and Modeling, 2017, 57, 864-874.	2.5	9

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19	A human transcription factor in search mode. <i>Nucleic Acids Research</i> , 2016, 44, 63-74.	6.5	52
20	Selectivity of Pyridone- and Diphenyl Ether-Based Inhibitors for the <i>Yersinia pestis</i> FabV Enoyl-ACP Reductase. <i>Biochemistry</i> , 2016, 55, 2992-3006.	1.2	6
21	Experimental and Computational Analysis of Protein Stabilization by Gly-to-Ala Substitution: A Convolution of Native State and Unfolded State Effects. <i>Journal of the American Chemical Society</i> , 2016, 138, 15682-15689.	6.6	20
22	Base Flipping by MTERF1 Can Accommodate Multiple Conformations and Occurs in a Stepwise Fashion. <i>Journal of Molecular Biology</i> , 2016, 428, 2542-2556.	2.0	3
23	Advances in free-energy-based simulations of protein folding and ligand binding. <i>Current Opinion in Structural Biology</i> , 2016, 36, 25-31.	2.6	121
24	A dynamic checkpoint in oxidative lesion discrimination by formamidopyrimidine-DNA glycosylase. <i>Nucleic Acids Research</i> , 2016, 44, 683-694.	6.5	19
25	Rational Modulation of the Induced-Fit Conformational Change for Slow-Onset Inhibition in <i>Mycobacterium tuberculosis</i> InhA. <i>Biochemistry</i> , 2015, 54, 4683-4691.	1.2	30
26	ff14SB: Improving the Accuracy of Protein Side Chain and Backbone Parameters from ff99SB. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3696-3713.	2.3	7,322
27	Refinement of Generalized Born Implicit Solvation Parameters for Nucleic Acids and Their Complexes with Proteins. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3714-3728.	2.3	58
28	Active destabilization of base pairs by a DNA glycosylase wedge initiates damage recognition. <i>Nucleic Acids Research</i> , 2015, 43, 272-281.	6.5	49
29	Grid-Based Backbone Correction to the ff12SB Protein Force Field for Implicit-Solvent Simulations. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4770-4779.	2.3	76
30	Time-Dependent Diaryl Ether Inhibitors of InhA: Structure-Activity Relationship Studies of Enzyme Inhibition, Antibacterial Activity, and <i>in vivo</i> Efficacy. <i>ChemMedChem</i> , 2014, 9, 776-791.	1.6	48
31	A Structural and Energetic Model for the Slow-Onset Inhibition of the <i>Mycobacterium tuberculosis</i> Enoyl-ACP Reductase InhA. <i>ACS Chemical Biology</i> , 2014, 9, 986-993.	1.6	63
32	Ultrafast Structural Dynamics of BlsA, a Photoreceptor from the Pathogenic Bacterium <i>Acinetobacter baumannii</i> . <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 220-224.	2.1	25
33	Folding Simulations for Proteins with Diverse Topologies Are Accessible in Days with a Physics-Based Force Field and Implicit Solvent. <i>Journal of the American Chemical Society</i> , 2014, 136, 13959-13962.	6.6	199
34	The Role of Select Subtype Polymorphisms on HIV-1 Protease Conformational Sampling and Dynamics. <i>Journal of Biological Chemistry</i> , 2014, 289, 17203-17214.	1.6	43
35	Thiolactomycin-based $\beta^2$ -Ketoacyl-AcpM Synthase A (KasA) Inhibitors. <i>Journal of Biological Chemistry</i> , 2013, 288, 6045-6052.	1.6	32
36	Improved Generalized Born Solvent Model Parameters for Protein Simulations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2020-2034.	2.3	387

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37	Molecular Dynamics Applied in Drug Discovery: The Case of HIV-1 Protease. <i>Methods in Molecular Biology</i> , 2012, 819, 527-549.	0.4	9
38	CoA Adducts of 4-Oxo-4-phenylbut-2-enoates: Inhibitors of MenB from the <i>M. tuberculosis</i> Menaquinone Biosynthesis Pathway. <i>ACS Medicinal Chemistry Letters</i> , 2011, 2, 818-823.	1.3	40
39	Energetic Preference of 8-oxoG Eversion Pathways in a DNA Glycosylase. <i>Journal of the American Chemical Society</i> , 2011, 133, 14504-14506.	6.6	30
40	Improving the description of salt bridge strength and geometry in a Generalized Born model. <i>Journal of Molecular Graphics and Modelling</i> , 2011, 29, 676-684.	1.3	18
41	An Overview of String-Based Path Sampling Methods. <i>Annual Reports in Computational Chemistry</i> , 2011, 7, 89-97.	0.9	3
42	Synthesis and Molecular Modeling of a Nitrogen Mustard DNA Interstrand Crosslink. <i>Chemistry - A European Journal</i> , 2010, 16, 12100-12103.	1.7	30
43	Slow Onset Inhibition of Bacterial $\beta$ -Ketoacyl-acyl Carrier Protein Synthases by Thiolactomycin. <i>Journal of Biological Chemistry</i> , 2010, 285, 6161-6169.	1.6	42
44	Three-Dimensional Molecular Theory of Solvation Coupled with Molecular Dynamics in Amber. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 607-624.	2.3	232
45	Recent Advances in the Study of the Bioactive Conformation of Taxol. <i>ChemMedChem</i> , 2009, 4, 719-731.	1.6	36
46	A partial nudged elastic band implementation for use with large or explicitly solvated systems. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 3781-3790.	1.0	40
47	Evaluating the Performance of the ff99SB Force Field Based on NMR Scalar Coupling Data. <i>Biophysical Journal</i> , 2009, 97, 853-856.	0.2	201
48	Drug Pressure Selected Mutations in HIV-1 Protease Alter Flap Conformations. <i>Journal of the American Chemical Society</i> , 2009, 131, 430-431.	6.6	70
49	An Improved Reaction Coordinate for Nucleic Acid Base Flipping Studies. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 3105-3113.	2.3	55
50	Molecular mechanics parameters for the FapydG DNA lesion. <i>Journal of Computational Chemistry</i> , 2008, 29, 17-23.	1.5	11
51	Structural insights for designed alanine-rich helices: Comparing NMR helicity measures and conformational ensembles from molecular dynamics simulation. <i>Biopolymers</i> , 2008, 89, 747-760.	1.2	25
52	Evaluation of Salt Bridge Structure and Energetics in Peptides Using Explicit, Implicit, and Hybrid Solvation Models. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 488-498.	2.3	35
53	Solution Structure of HIV-1 Protease Flaps Probed by Comparison of Molecular Dynamics Simulation Ensembles and EPR Experiments. <i>Journal of the American Chemical Society</i> , 2008, 130, 7184-7185.	6.6	63
54	Design, Synthesis, and Biological Evaluation of Novel C14 $\sim$ C3 $\beta$ -BzN-Linked Macrocyclic Taxoids. <i>Journal of Organic Chemistry</i> , 2008, 73, 9584-9593.	1.7	26

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55	Improving Convergence of Replica-Exchange Simulations through Coupling to a High-Temperature Structure Reservoir. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 557-568.	2.3	70
56	Coupling of Replica Exchange Simulations to a Non-Boltzmann Structure Reservoir. <i>Journal of Physical Chemistry B</i> , 2007, 111, 2415-2418.	1.2	80
57	Generalized Born Model with a Simple, Robust Molecular Volume Correction. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 156-169.	2.3	334
58	Molecular Simulations Reveal a Common Binding Mode for Glycosylase Binding of Oxidatively Damaged DNA Lesions. <i>Journal of the American Chemical Society</i> , 2007, 129, 14536-14537.	6.6	14
59	Reconciling the Solution and X-ray Structures of the Villin Headpiece Helical Subdomain: A Molecular Dynamics Simulations and Double Mutant Cycles Reveal a Stabilizing Cation- $\pi$ Interaction. <i>Biochemistry</i> , 2007, 46, 3624-3634.	1.2	23
60	Secondary Structure Bias in Generalized Born Solvent Models: A Comparison of Conformational Ensembles and Free Energy of Solvent Polarization from Explicit and Implicit Solvation. <i>Journal of Physical Chemistry B</i> , 2007, 111, 1846-1857.	1.2	121
61	Targeting structural flexibility in HIV-1 protease inhibitor binding. <i>Drug Discovery Today</i> , 2007, 12, 132-138.	3.2	120
62	The Open Structure of a Multi-Drug-Resistant HIV-1 Protease is Stabilized by Crystal Packing Contacts. <i>Journal of the American Chemical Society</i> , 2006, 128, 13360-13361.	6.6	39
63	Chapter 6 Hybrid Explicit/Implicit Solvation Methods. <i>Annual Reports in Computational Chemistry</i> , 2006, 2, 97-109.	0.9	23
64	Insight through Molecular Mechanics Poisson-Boltzmann Surface Area Calculations into the Binding Affinity of Triclosan and Three Analogues for FabI, the E. coli Enoyl Reductase. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 4574-4580.	2.9	32
65	Investigation of Salt Bridge Stability in a Generalized Born Solvent Model. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 115-127.	2.3	110
66	HIV-1 Protease Flaps Spontaneously Close to the Correct Structure in Simulations Following Manual Placement of an Inhibitor into the Open State. <i>Journal of the American Chemical Society</i> , 2006, 128, 2812-2813.	6.6	103
67	HIV-1 protease flaps spontaneously open and reclose in molecular dynamics simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 915-920.	3.3	344
68	Improved Efficiency of Replica Exchange Simulations through Use of a Hybrid Explicit/Implicit Solvation Model. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 420-433.	2.3	126
69	Computational Analysis of the Mode of Binding of 8-Oxoguanine to Formamidopyrimidine-DNA Glycosylase. <i>Biochemistry</i> , 2006, 45, 10886-10894.	1.2	27
70	The Unfolded State of the Villin Headpiece Helical Subdomain: Computational Studies of the Role of Locally Stabilized Structure. <i>Journal of Molecular Biology</i> , 2006, 360, 1094-1107.	2.0	46
71	Comparison of multiple Amber force fields and development of improved protein backbone parameters. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 65, 712-725.	1.5	6,049
72	Structure of Acyl Carrier Protein Bound to FabI, the FASII Enoyl Reductase from Escherichia coli. <i>Journal of Biological Chemistry</i> , 2006, 281, 39285-39293.	1.6	101

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73	Use of the Tubulin Bound Paclitaxel Conformation for Structure-Based Rational Drug Design. <i>Chemistry and Biology</i> , 2005, 12, 339-348.	6.2	73
74	The Amber biomolecular simulation programs. <i>Journal of Computational Chemistry</i> , 2005, 26, 1668-1688.	1.5	7,742
75	Structural Requirements of the Extracellular to Transmembrane Domain Junction for Erythropoietin Receptor Function. <i>Journal of Biological Chemistry</i> , 2005, 280, 14844-14854.	1.6	40
76	Dynamic Behavior of DNA Base Pairs Containing 8-Oxoguanine. <i>Journal of the American Chemical Society</i> , 2005, 127, 13906-13918.	6.6	73
77	Folding Cooperativity in a Three-stranded $\beta^2$ -Sheet Model. <i>Journal of Molecular Biology</i> , 2005, 352, 370-381.	2.0	45
78	Modified Replica Exchange Simulation Methods for Local Structure Refinement. <i>Journal of Physical Chemistry B</i> , 2005, 109, 8220-8230.	1.2	105
79	Inhibition of the Bacterial Enoyl Reductase FabI by Triclosan: A Structure-Reactivity Analysis of FabI Inhibition by Triclosan Analogues. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 509-518.	2.9	101
80	Development of softcore potential functions for overcoming steric barriers in molecular dynamics simulations. <i>Journal of Molecular Graphics and Modelling</i> , 2004, 22, 405-413.	1.3	30
81	Using PC clusters to evaluate the transferability of molecular mechanics force fields for proteins. <i>Journal of Computational Chemistry</i> , 2003, 24, 21-31.	1.5	94
82	Generation of accurate protein loop conformations through low-barrier molecular dynamics. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003, 51, 577-590.	1.5	47
83	All-Atom Structure Prediction and Folding Simulations of a Stable Protein. <i>Journal of the American Chemical Society</i> , 2002, 124, 11258-11259.	6.6	564
84	The Disordered Mobile Loop of GroES Folds into a Defined $\beta^2$ -Hairpin upon Binding GroEL. <i>Journal of Biological Chemistry</i> , 2001, 276, 31257-31264.	1.6	33
85	Combining MONSSTER and LES/PME to Predict Protein Structure from Amino Acid Sequence: Application to the Small Protein CMTI-1. <i>Journal of the American Chemical Society</i> , 2000, 122, 8392-8402.	6.6	36
86	Use of Locally Enhanced Sampling in Free Energy Calculations: Testing and Application to the $\beta^2$ Anomerization of Glucose. <i>Journal of the American Chemical Society</i> , 1998, 120, 5771-5782.	6.6	88
87	Combined Locally Enhanced Sampling and Particle Mesh Ewald as a Strategy To Locate the Experimental Structure of a Nonhelical Nucleic Acid. <i>Journal of the American Chemical Society</i> , 1998, 120, 7149-7155.	6.6	67
88	MOIL: A program for simulations of macromolecules. <i>Computer Physics Communications</i> , 1995, 91, 159-189.	3.0	154
89	Hydrophobic "Collapse" in a Cyclic Hexapeptide: Computer Simulations of CHDLFC and CAAAAC in Water. <i>Journal of the American Chemical Society</i> , 1994, 116, 2534-2547.	6.6	46