

Heather A Carlson

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.

90
papers

5,008
citations

39
h-index

70
g-index

96
ext. papers

5,627
ext. citations

6.4
avg, IF

5.94
L-index

#	Paper	IF	Citations
90	Computational Identification of Possible Allosteric Sites and Modulators of the SARS-CoV-2 Main Protease.. <i>Journal of Chemical Information and Modeling</i> , 2022 , 62, 618-626	6.1	1
89	Randomized Trial of a Palliative Care Intervention to Improve End-of-Life Care Discussions in Patients With Metastatic Breast Cancer.. <i>Journal of the National Comprehensive Cancer Network: JNCCN</i> , 2022 , 20, 136-143	7.3	3
88	In silico analysis of SARS-CoV-2 proteins as targets for clinically available drugs.. <i>Scientific Reports</i> , 2022 , 12, 5320	4.9	2
87	Chemical validation of a druggable site on Hsp27/HSPB1 using in silico solvent mapping and biophysical methods. <i>Bioorganic and Medicinal Chemistry</i> , 2021 , 34, 115990	3.4	
86	A Virtual Docking Screen at 23 SARS-CoV-2 Proteins Identifies Drug Repurposing Candidates at New Sites and Targets. <i>FASEB Journal</i> , 2021 , 35,	0.9	78
85	Identification of Cryptic Binding Sites Using MixMD with Standard and Accelerated Molecular Dynamics. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 1287-1299	6.1	7
84	Mixed-solvent molecular dynamics simulation-based discovery of a putative allosteric site on regulator of G protein signaling 4. <i>Journal of Computational Chemistry</i> , 2021 , 42, 2170-2180	3.5	2
83	Crowdsourced identification of multi-target kinase inhibitors for RET- and TAU- based disease: The Multi-Targeting Drug DREAM Challenge. <i>PLoS Computational Biology</i> , 2021 , 17, e1009302	5	4
82	Predicting binding sites from unbound versus bound protein structures. <i>Scientific Reports</i> , 2020 , 10, 15856	4.9	8
81	Updates to Binding MOAD (Mother of All Databases): Polypharmacology Tools and Their Utility in Drug Repurposing. <i>Journal of Molecular Biology</i> , 2019 , 431, 2423-2433	6.5	23
80	Free Energies and Entropies of Binding Sites Identified by MixMD Cosolvent Simulations. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 2035-2045	6.1	14
79	Inherent versus induced protein flexibility: Comparisons within and between apo and holo structures. <i>PLoS Computational Biology</i> , 2019 , 15, e1006705	5	24
78	Predicting Displaceable Water Sites Using Mixed-Solvent Molecular Dynamics. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 305-314	6.1	12
77	MixMD Probeview: Robust Binding Site Prediction from Cosolvent Simulations. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 1426-1433	6.1	19
76	Comparing pharmacophore models derived from crystallography and NMR ensembles. <i>Journal of Computer-Aided Molecular Design</i> , 2017 , 31, 979-993	4.2	2
75	Are there physicochemical differences between allosteric and competitive ligands?. <i>PLoS Computational Biology</i> , 2017 , 13, e1005813	5	16
74	Multi-targeting Drug Community Challenge. <i>Cell Chemical Biology</i> , 2017 , 24, 1434-1435	8.2	9

73	CSAR Benchmark Exercise 2013: Evaluation of Results from a Combined Computational Protein Design, Docking, and Scoring/Ranking Challenge. <i>Journal of Chemical Information and Modeling</i> , 2016 , 56, 1022-31	6.1	36
72	ChemTreeMap: an interactive map of biochemical similarity in molecular datasets. <i>Bioinformatics</i> , 2016 , 32, 3584-3592	7.2	10
71	Moving Beyond Active-Site Detection: MixMD Applied to Allosteric Systems. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 8685-95	3.4	58
70	Dynamic behavior of the post-SET loop region of NSD1: Implications for histone binding and drug development. <i>Protein Science</i> , 2016 , 25, 1021-9	6.3	12
69	CSAR 2014: A Benchmark Exercise Using Unpublished Data from Pharma. <i>Journal of Chemical Information and Modeling</i> , 2016 , 56, 1063-77	6.1	72
68	Prevalence of CTX-M extended-spectrum beta-lactamases and sequence type 131 in Korean blood, urine, and rectal <i>Escherichia coli</i> isolates. <i>Infection, Genetics and Evolution</i> , 2016 , 41, 292-295	4.5	6
67	D3R grand challenge 2015: Evaluation of protein-ligand pose and affinity predictions. <i>Journal of Computer-Aided Molecular Design</i> , 2016 , 30, 651-668	4.2	141
66	Driving Structure-Based Drug Discovery through Cosolvent Molecular Dynamics. <i>Journal of Medicinal Chemistry</i> , 2016 , 59, 10383-10399	8.3	48
65	Identifying binding hot spots on protein surfaces by mixed-solvent molecular dynamics: HIV-1 protease as a test case. <i>Biopolymers</i> , 2016 , 105, 21-34	2.2	29
64	Recent improvements to Binding MOAD: a resource for protein-ligand binding affinities and structures. <i>Nucleic Acids Research</i> , 2015 , 43, D465-9	20.1	59
63	Substrate-Competitive Activity-Based Profiling of Ester Prodrug Activating Enzymes. <i>Molecular Pharmaceutics</i> , 2015 , 12, 3399-407	5.6	17
62	Parameter choice matters: validating probe parameters for use in mixed-solvent simulations. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 2190-9	6.1	28
61	An allosteric modulator of HIV-1 protease shows equipotent inhibition of wild-type and drug-resistant proteases. <i>Journal of Medicinal Chemistry</i> , 2014 , 57, 6468-78	8.3	17
60	Check your confidence: size really does matter. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 1837-41	6.1	10
59	Improving protocols for protein mapping through proper comparison to crystallography data. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 391-402	6.1	29
58	CSAR data set release 2012: ligands, affinities, complexes, and docking decoys. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 1842-52	6.1	74
57	CSAR benchmark exercise 2011-2012: evaluation of results from docking and relative ranking of blinded congeneric series. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 1853-70	6.1	107
56	Novel deletion of lysine 7 expands the clinical, histopathological and genetic spectrum of TPM2-related myopathies. <i>Brain</i> , 2013 , 136, 508-21	11.2	43

55	Identification of key hinge residues important for nucleotide-dependent allostery in E. coli Hsp70/DnaK. <i>PLoS Computational Biology</i> , 2013 , 9, e1003279	5	13
54	Exploring the composition of protein-ligand binding sites on a large scale. <i>PLoS Computational Biology</i> , 2013 , 9, e1003321	5	37
53	Overcoming sequence misalignments with weighted structural superposition. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012 , 80, 2523-35	4.2	3
52	Protein flexibility in docking and surface mapping. <i>Quarterly Reviews of Biophysics</i> , 2012 , 45, 301-43	7	90
51	Biophysical limits of protein-ligand binding. <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 2098-1106	31	
50	Full protein flexibility is essential for proper hot-spot mapping. <i>Journal of the American Chemical Society</i> , 2011 , 133, 200-2	16.4	91
49	Computational methods for identifying a layered allosteric regulatory mechanism for ALS-causing mutations of Cu-Zn superoxide dismutase 1. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011 , 79, 417-27	4.2	6
48	The role of tyrosine 71 in modulating the flap conformations of BACE1. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011 , 79, 2247-59	4.2	18
47	Binding to the open conformation of HIV-1 protease. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011 , 79, 2282-90	4.2	12
46	Chemical screens against a reconstituted multiprotein complex: myricetin blocks DnaJ regulation of DnaK through an allosteric mechanism. <i>Chemistry and Biology</i> , 2011 , 18, 210-21		80
45	CSAR benchmark exercise of 2010: selection of the protein-ligand complexes. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 2036-46	6.1	102
44	Correction to CSAR Benchmark Exercise of 2010: Selection of the Protein-Ligand Complexes. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 2146-2146	6.1	4
43	CSAR benchmark exercise of 2010: combined evaluation across all submitted scoring functions. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 2115-31	6.1	117
42	Mutagenesis reveals the complex relationships between ATPase rate and the chaperone activities of Escherichia coli heat shock protein 70 (Hsp70/DnaK). <i>Journal of Biological Chemistry</i> , 2010 , 285, 21282-21291	54	
41	UPDATING BINDING MOAD DATA MANAGEMENT AND INFORMATION WORKFLOW. <i>New Mathematics and Natural Computation</i> , 2010 , 06, 49-56	0.6	0
40	Chemical probes that selectively recognize the earliest AB oligomers in complex mixtures. <i>Journal of the American Chemical Society</i> , 2010 , 132, 17655-7	16.4	27
39	Binding of a small molecule at a protein-protein interface regulates the chaperone activity of hsp70-hsp40. <i>ACS Chemical Biology</i> , 2010 , 5, 611-22	4.9	116
38	Clarifying allosteric control of flap conformations in the 1TW7 crystal structure of HIV-1 protease. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009 , 74, 872-80	4.2	8

37	Computational methods for predicting sites of functionally important dynamics. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 6613-22	3.4	11
36	Differences between high- and low-affinity complexes of enzymes and nonenzymes. <i>Journal of Medicinal Chemistry</i> , 2008 , 51, 6432-41	8.3	23
35	Automated clustering of probe molecules from solvent mapping of protein surfaces: new algorithms applied to hot-spot mapping and structure-based drug design. <i>Journal of Computer-Aided Molecular Design</i> , 2008 , 22, 727-36	4.2	10
34	A poke in the eye: inhibiting HIV-1 protease through its flap-recognition pocket. <i>Biopolymers</i> , 2008 , 89, 643-52	2.2	34
33	Binding MOAD, a high-quality protein-ligand database. <i>Nucleic Acids Research</i> , 2008 , 36, D674-8	20.1	115
32	Exploring experimental sources of multiple protein conformations in structure-based drug design. <i>Journal of the American Chemical Society</i> , 2007 , 129, 8225-35	16.4	126
31	Incorporating dynamics in E. coli dihydrofolate reductase enhances structure-based drug discovery. <i>Journal of Chemical Information and Modeling</i> , 2007 , 47, 2358-65	6.1	31
30	Protein flexibility and species specificity in structure-based drug discovery: dihydrofolate reductase as a test system. <i>Journal of the American Chemical Society</i> , 2007 , 129, 3634-40	16.4	48
29	Small molecule inhibitors of the MDM2-p53 interaction discovered by ensemble-based receptor models. <i>Journal of the American Chemical Society</i> , 2007 , 129, 12809-14	16.4	119
28	Refining the multiple protein structure pharmacophore method: consistency across three independent HIV-1 protease models. <i>Journal of Medicinal Chemistry</i> , 2006 , 49, 3478-84	8.3	27
27	Gaussian-weighted RMSD superposition of proteins: a structural comparison for flexible proteins and predicted protein structures. <i>Biophysical Journal</i> , 2006 , 90, 4558-73	2.9	89
26	Conformational Studies of Polyprolines. <i>Journal of Chemical Theory and Computation</i> , 2006 , 2, 342-53	6.4	27
25	Exploring protein-ligand recognition with Binding MOAD. <i>Journal of Molecular Graphics and Modelling</i> , 2006 , 24, 414-25	2.8	53
24	Quantum Mechanics/Molecular Mechanics Calculations of the Vanadium Dependent Chloroperoxidase. <i>Journal of Chemical Theory and Computation</i> , 2005 , 1, 1265-74	6.4	43
23	Docking studies and ligand recognition in folylpolyglutamate synthetase. <i>Journal of Medicinal Chemistry</i> , 2005 , 48, 7764-72	8.3	7
22	The role of aspartic acid 143 in E. coli tRNA-guanine transglycosylase: insights from mutagenesis studies and computational modeling. <i>Biophysical Journal</i> , 2005 , 89, 1965-77	2.9	4
21	Computational studies and peptidomimetic design for the human p53-MDM2 complex. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005 , 58, 222-34	4.2	70
20	Solvation influences flap collapse in HIV-1 protease. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005 , 58, 119-25	4.2	67

19	Binding MOAD (Mother Of All Databases). <i>Proteins: Structure, Function and Bioinformatics</i> , 2005 , 60, 333-40	4.0	187
18	Quantum mechanical models of the resting state of the vanadium-dependent haloperoxidase. <i>Inorganic Chemistry</i> , 2004 , 43, 4127-36	5.1	54
17	Incorporating protein flexibility in structure-based drug discovery: using HIV-1 protease as a test case. <i>Journal of the American Chemical Society</i> , 2004 , 126, 13276-81	16.4	105
16	Development of polyphosphate parameters for use with the AMBER force field. <i>Journal of Computational Chemistry</i> , 2003 , 24, 1016-25	3.5	440
15	Secondary structural preferences of 2,2-disubstituted pyrrolidine-4-carboxylic acid oligomers: beta-peptide foldamers that cannot form internal hydrogen bonds. <i>Journal of the American Chemical Society</i> , 2003 , 125, 9035-7	16.4	58
14	Conformational behavior of beta-proline oligomers. <i>Journal of the American Chemical Society</i> , 2003 , 125, 15855-62	16.4	32
13	Protein flexibility and drug design: how to hit a moving target. <i>Current Opinion in Chemical Biology</i> , 2002 , 6, 447-52	9.7	278
12	Protein flexibility is an important component of structure-based drug discovery. <i>Current Pharmaceutical Design</i> , 2002 , 8, 1571-8	3.3	107
11	Developing a dynamic pharmacophore model for HIV-1 integrase. <i>Journal of Medicinal Chemistry</i> , 2000 , 43, 2100-14	8.3	248
10	Method for Including the Dynamic Fluctuations of a Protein in Computer-Aided Drug Design. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 10213-10219	2.8	91
9	Molecular dynamics of cryptophane and its complexes with tetramethylammonium and neopentane using a continuum solvent model. <i>Journal of Computational Chemistry</i> , 1999 , 20, 956-970	3.5	9
8	Molecular dynamics studies on the HIV-1 integrase catalytic domain. <i>Biophysical Journal</i> , 1999 , 76, 2999-3011	10.1	73
7	Calculation of the pKa values for the ligands and side chains of Escherichia coli D-alanine:D-alanine ligase. <i>Journal of Medicinal Chemistry</i> , 1999 , 42, 109-17	8.3	28
6	Free energies of solvation in chloroform and water from a linear response approach. <i>Journal of Physical Organic Chemistry</i> , 1997 , 10, 563-576	2.1	92
5	Monte Carlo Investigations of Solvent Effects on the Chorismate to Prephenate Rearrangement. <i>Journal of the American Chemical Society</i> , 1996 , 118, 8475-8484	16.4	48
4	Investigations into the stereochemistry of cyclophane-steroid complexes via Monte Carlo simulations. <i>Tetrahedron</i> , 1995 , 51, 449-472	2.4	7
3	An Extended Linear Response Method for Determining Free Energies of Hydration. <i>The Journal of Physical Chemistry</i> , 1995 , 99, 10667-10673		226
2	Accuracy of free energies of hydration for organic molecules from 6-31g*-derived partial charges. <i>Journal of Computational Chemistry</i> , 1993 , 14, 1240-1249	3.5	142

- 1 How stable is cyclobutynes? The activation energy for the unimolecular rearrangement to butatriene. *Journal of the American Chemical Society*, **1992**, 114, 5344-5348 16.4 21