Heather A Carlson

List of Publications by Citations

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	Development of polyphosphate parameters for use with the AMBER force field. *Journal of Computational Chemistry*, **2003**, 24, 1016-25	3.5	440
89	Protein flexibility and drug design: how to hit a moving target. *Current Opinion in Chemical Biology*, **2002**, 6, 447-52	9.7	278
88	Developing a dynamic pharmacophore model for HIV-1 integrase. *Journal of Medicinal Chemistry*, **2000**, 43, 2100-14	8.3	248
87	An Extended Linear Response Method for Determining Free Energies of Hydration. *The Journal of Physical Chemistry*, **1995**, 99, 10667-10673		226
86	Binding MOAD (Mother Of All Databases). *Proteins: Structure, Function and Bioinformatics*, **2005**, 60, 333-40	4.2	187
85	Accuracy of free energies of hydration for organic molecules from 6-31g*-derived partial charges. *Journal of Computational Chemistry*, **1993**, 14, 1240-1249	3.5	142
84	D3R grand challenge 2015: Evaluation of protein-ligand pose and affinity predictions. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 651-668	4.2	141
83	Exploring experimental sources of multiple protein conformations in structure-based drug design. *Journal of the American Chemical Society*, **2007**, 129, 8225-35	16.4	126
82	Small molecule inhibitors of the MDM2-p53 interaction discovered by ensemble-based receptor models. *Journal of the American Chemical Society*, **2007**, 129, 12809-14	16.4	119
81	CSAR benchmark exercise of 2010: combined evaluation across all submitted scoring functions. *Journal of Chemical Information and Modeling*, **2011**, 51, 2115-31	6.1	117
80	Binding of a small molecule at a protein-protein interface regulates the chaperone activity of hsp70-hsp40. *ACS Chemical Biology*, **2010**, 5, 611-22	4.9	116
79	Binding MOAD, a high-quality protein-ligand database. *Nucleic Acids Research*, **2008**, 36, D674-8	20.1	115
78	CSAR benchmark exercise 2011-2012: evaluation of results from docking and relative ranking of blinded congeneric series. *Journal of Chemical Information and Modeling*, **2013**, 53, 1853-70	6.1	107
77	Protein flexibility is an important component of structure-based drug discovery. *Current Pharmaceutical Design*, **2002**, 8, 1571-8	3.3	107
76	Incorporating protein flexibility in structure-based drug discovery: using HIV-1 protease as a test case. *Journal of the American Chemical Society*, **2004**, 126, 13276-81	16.4	105
75	CSAR benchmark exercise of 2010: selection of the protein-ligand complexes. *Journal of Chemical Information and Modeling*, **2011**, 51, 2036-46	6.1	102
74	Free energies of solvation in chloroform and water from a linear response approach. *Journal of Physical Organic Chemistry*, **1997**, 10, 563-576	2.1	92

73	Full protein flexibility is essential for proper hot-spot mapping. *Journal of the American Chemical Society*, **2011**, 133, 200-2	16.4	91
72	Method for Including the Dynamic Fluctuations of a Protein in Computer-Aided Drug Design. *Journal of Physical Chemistry A*, **1999**, 103, 10213-10219	2.8	91
71	Protein flexibility in docking and surface mapping. *Quarterly Reviews of Biophysics*, **2012**, 45, 301-43	7	90
70	Gaussian-weighted RMSD superposition of proteins: a structural comparison for flexible proteins and predicted protein structures. *Biophysical Journal*, **2006**, 90, 4558-73	2.9	89
69	Chemical screens against a reconstituted multiprotein complex: myricetin blocks DnaJ regulation of DnaK through an allosteric mechanism. *Chemistry and Biology*, **2011**, 18, 210-21		80
68	A Virtual Docking Screen at 23 SARS-CoV-2 Proteins Identifies Drug Repurposing Candidates at New Sites and Targets. *FASEB Journal*, **2021**, 35,	0.9	78
67	CSAR data set release 2012: ligands, affinities, complexes, and docking decoys. *Journal of Chemical Information and Modeling*, **2013**, 53, 1842-52	6.1	74
66	Molecular dynamics studies on the HIV-1 integrase catalytic domain. *Biophysical Journal*, **1999**, 76, 2999-3011	2.9	73
65	CSAR 2014: A Benchmark Exercise Using Unpublished Data from Pharma. *Journal of Chemical Information and Modeling*, **2016**, 56, 1063-77	6.1	72
64	Computational studies and peptidomimetic design for the human p53-MDM2 complex. *Proteins: Structure, Function and Bioinformatics*, **2005**, 58, 222-34	4.2	70
63	Solvation influences flap collapse in HIV-1 protease. *Proteins: Structure, Function and Bioinformatics*, **2005**, 58, 119-25	4.2	67
62	Recent improvements to Binding MOAD: a resource for protein-ligand binding affinities and structures. *Nucleic Acids Research*, **2015**, 43, D465-9	20.1	59
61	Moving Beyond Active-Site Detection: MixMD Applied to Allosteric Systems. *Journal of Physical Chemistry B*, **2016**, 120, 8685-95	3.4	58
60	Secondary structural preferences of 2,2-disubstituted pyrrolidine-4-carboxylic acid oligomers: beta-peptide foldamers that cannot form internal hydrogen bonds. *Journal of the American Chemical Society*, **2003**, 125, 9035-7	16.4	58
59	Mutagenesis reveals the complex relationships between ATPase rate and the chaperone activities of Escherichia coli heat shock protein 70 (Hsp70/DnaK). *Journal of Biological Chemistry*, **2010**, 285, 21282-91	5.4	54
58	Quantum mechanical models of the resting state of the vanadium-dependent haloperoxidase. *Inorganic Chemistry*, **2004**, 43, 4127-36	5.1	54
57	Exploring protein-ligand recognition with Binding MOAD. *Journal of Molecular Graphics and Modelling*, **2006**, 24, 414-25	2.8	53
56	Protein flexibility and species specificity in structure-based drug discovery: dihydrofolate reductase as a test system. *Journal of the American Chemical Society*, **2007**, 129, 3634-40	16.4	48

55	Monte Carlo Investigations of Solvent Effects on the Chorismate to Prephenate Rearrangement. *Journal of the American Chemical Society*, **1996**, 118, 8475-8484	16.4	48
54	Driving Structure-Based Drug Discovery through Cosolvent Molecular Dynamics. *Journal of Medicinal Chemistry*, **2016**, 59, 10383-10399	8.3	48
53	Novel deletion of lysine 7 expands the clinical, histopathological and genetic spectrum of TPM2-related myopathies. *Brain*, **2013**, 136, 508-21	11.2	43
52	Quantum Mechanics/Molecular Mechanics Calculations of the Vanadium Dependent Chloroperoxidase. *Journal of Chemical Theory and Computation*, **2005**, 1, 1265-74	6.4	43
51	Exploring the composition of protein-ligand binding sites on a large scale. *PLoS Computational Biology*, **2013**, 9, e1003321	5	37
50	CSAR Benchmark Exercise 2013: Evaluation of Results from a Combined Computational Protein Design, Docking, and Scoring/Ranking Challenge. *Journal of Chemical Information and Modeling*, **2016**, 56, 1022-31	6.1	36
49	A poke in the eye: inhibiting HIV-1 protease through its flap-recognition pocket. *Biopolymers*, **2008**, 89, 643-52	2.2	34
48	Conformational behavior of beta-proline oligomers. *Journal of the American Chemical Society*, **2003**, 125, 15855-62	16.4	32
47	Biophysical limits of protein-ligand binding. *Journal of Chemical Information and Modeling*, **2012**, 52, 2098-106	6.1	31
46	Incorporating dynamics in E. coli dihydrofolate reductase enhances structure-based drug discovery. *Journal of Chemical Information and Modeling*, **2007**, 47, 2358-65	6.1	31
45	Improving protocols for protein mapping through proper comparison to crystallography data. *Journal of Chemical Information and Modeling*, **2013**, 53, 391-402	6.1	29
44	Identifying binding hot spots on protein surfaces by mixed-solvent molecular dynamics: HIV-1 protease as a test case. *Biopolymers*, **2016**, 105, 21-34	2.2	29
43	Parameter choice matters: validating probe parameters for use in mixed-solvent simulations. *Journal of Chemical Information and Modeling*, **2014**, 54, 2190-9	6.1	28
42	Calculation of the pKa values for the ligands and side chains of Escherichia coli D-alanine:D-alanine ligase. *Journal of Medicinal Chemistry*, **1999**, 42, 109-17	8.3	28
41	Chemical probes that selectively recognize the earliest A□ oligomers in complex mixtures. *Journal of the American Chemical Society*, **2010**, 132, 17655-7	16.4	27
40	Refining the multiple protein structure pharmacophore method: consistency across three independent HIV-1 protease models. *Journal of Medicinal Chemistry*, **2006**, 49, 3478-84	8.3	27
39	Conformational Studies of Polyprolines. *Journal of Chemical Theory and Computation*, **2006**, 2, 342-53	6.4	27
38	Inherent versus induced protein flexibility: Comparisons within and between apo and holo structures. *PLoS Computational Biology*, **2019**, 15, e1006705	5	24

37	Updates to Binding MOAD (Mother of All Databases): Polypharmacology Tools and Their Utility in Drug Repurposing. *Journal of Molecular Biology*, **2019**, 431, 2423-2433	6.5	23
36	Differences between high- and low-affinity complexes of enzymes and nonenzymes. *Journal of Medicinal Chemistry*, **2008**, 51, 6432-41	8.3	23
35	How stable is cyclobutyne? The activation energy for the unimolecular rearrangement to butatriene. *Journal of the American Chemical Society*, **1992**, 114, 5344-5348	16.4	21
34	MixMD Probeview: Robust Binding Site Prediction from Cosolvent Simulations. *Journal of Chemical Information and Modeling*, **2018**, 58, 1426-1433	6.1	19
33	The role of tyrosine 71 in modulating the flap conformations of BACE1. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 2247-59	4.2	18
32	Substrate-Competitive Activity-Based Profiling of Ester Prodrug Activating Enzymes. *Molecular Pharmaceutics*, **2015**, 12, 3399-407	5.6	17
31	An allosteric modulator of HIV-1 protease shows equipotent inhibition of wild-type and drug-resistant proteases. *Journal of Medicinal Chemistry*, **2014**, 57, 6468-78	8.3	17
30	Are there physicochemical differences between allosteric and competitive ligands?. *PLoS Computational Biology*, **2017**, 13, e1005813	5	16
29	Free Energies and Entropies of Binding Sites Identified by MixMD Cosolvent Simulations. *Journal of Chemical Information and Modeling*, **2019**, 59, 2035-2045	6.1	14
28	Identification of key hinge residues important for nucleotide-dependent allostery in E. coli Hsp70/DnaK. *PLoS Computational Biology*, **2013**, 9, e1003279	5	13
27	Predicting Displaceable Water Sites Using Mixed-Solvent Molecular Dynamics. *Journal of Chemical Information and Modeling*, **2018**, 58, 305-314	6.1	12
26	Binding to the open conformation of HIV-1 protease. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 2282-90	4.2	12
25	Dynamic behavior of the post-SET loop region of NSD1: Implications for histone binding and drug development. *Protein Science*, **2016**, 25, 1021-9	6.3	12
24	Computational methods for predicting sites of functionally important dynamics. *Journal of Physical Chemistry B*, **2009**, 113, 6613-22	3.4	11
23	ChemTreeMap: an interactive map of biochemical similarity in molecular datasets. *Bioinformatics*, **2016**, 32, 3584-3592	7.2	10
22	Check your confidence: size really does matter. *Journal of Chemical Information and Modeling*, **2013**, 53, 1837-41	6.1	10
21	Automated clustering of probe molecules from solvent mapping of protein surfaces: new algorithms applied to hot-spot mapping and structure-based drug design. *Journal of Computer-Aided Molecular Design*, **2008**, 22, 727-36	4.2	10
20	Multi-targeting Drug Community Challenge. *Cell Chemical Biology*, **2017**, 24, 1434-1435	8.2	9

19	Molecular dynamics of cryptophane and its complexes with tetramethylammonium and neopentane using a continuum solvent model. *Journal of Computational Chemistry*, **1999**, 20, 956-970	3.5	9
18	Clarifying allosteric control of flap conformations in the 1TW7 crystal structure of HIV-1 protease. *Proteins: Structure, Function and Bioinformatics*, **2009**, 74, 872-80	4.2	8
17	Predicting binding sites from unbound versus bound protein structures. *Scientific Reports*, **2020**, 10, 15856	4.9	8
16	Docking studies and ligand recognition in folylpolyglutamate synthetase. *Journal of Medicinal Chemistry*, **2005**, 48, 7764-72	8.3	7
15	Investigations into the stereochemistry of cyclophane-steroid complexes via Monte Carlo simulations. *Tetrahedron*, **1995**, 51, 449-472	2.4	7
14	Identification of Cryptic Binding Sites Using MixMD with Standard and Accelerated Molecular Dynamics. *Journal of Chemical Information and Modeling*, **2021**, 61, 1287-1299	6.1	7
13	Computational methods for identifying a layered allosteric regulatory mechanism for ALS-causing mutations of Cu-Zn superoxide dismutase 1. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 417-27	4.2	6
12	Prevalence of CTX-M extended-spectrum beta-lactamases and sequence type 131 in Korean blood, urine, and rectal Escherichia coli isolates. *Infection, Genetics and Evolution*, **2016**, 41, 292-295	4.5	6
11	Correction to CSAR Benchmark Exercise of 2010: Selection of the Protein□ligand Complexes. *Journal of Chemical Information and Modeling*, **2011**, 51, 2146-2146	6.1	4
10	The role of aspartic acid 143 in E. coli tRNA-guanine transglycosylase: insights from mutagenesis studies and computational modeling. *Biophysical Journal*, **2005**, 89, 1965-77	2.9	4
9	Crowdsourced identification of multi-target kinase inhibitors for RET- and TAU- based disease: The Multi-Targeting Drug DREAM Challenge. *PLoS Computational Biology*, **2021**, 17, e1009302	5	4
8	Overcoming sequence misalignments with weighted structural superposition. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 2523-35	4.2	3
7	Randomized Trial of a Palliative Care Intervention to Improve End-of-Life Care Discussions in Patients With Metastatic Breast Cancer.. *Journal of the National Comprehensive Cancer Network: JNCCN*, **2022**, 20, 136-143	7.3	3
6	Comparing pharmacophore models derived from crystallography and NMR ensembles. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 979-993	4.2	2
5	Mixed-solvent molecular dynamics simulation-based discovery of a putative allosteric site on regulator of G protein signaling 4. *Journal of Computational Chemistry*, **2021**, 42, 2170-2180	3.5	2
4	In silico analysis of SARS-CoV-2 proteins as targets for clinically available drugs.. *Scientific Reports*, **2022**, 12, 5320	4.9	2
3	Computational Identification of Possible Allosteric Sites and Modulators of the SARS-CoV-2 Main Protease.. *Journal of Chemical Information and Modeling*, **2022**, 62, 618-626	6.1	1
2	UPDATING BINDING MOAD □DATA MANAGEMENT AND INFORMATION WORKFLOW. *New Mathematics and Natural Computation*, **2010**, 06, 49-56	0.6	0

1	Chemical validation of a druggable site on Hsp27/HSPB1 using in silico solvent mapping and biophysical methods. *Bioorganic and Medicinal Chemistry*, **2021**, 34, 115990	3.4