Woody Sherman

List of Publications by Year in Descending Order

91 papers	12,456 citations	47 h-index	103 g-index
103 ext. papers	15,041 ext. citations	5.9 avg, IF	6.53 L-index

#	Paper	IF	Citations
91	Physics-based modeling provides predictive understanding of selectively promiscuous substrate binding by Hsp70 chaperones. *PLoS Computational Biology*, **2021**, 17, e1009567	5	1
90	Rigorous Free Energy Simulations in Virtual Screening. *Journal of Chemical Information and Modeling*, **2020**, 60, 4153-4169	6.1	54
89	Mechanism of biomolecular recognition of trimethyllysine by the fluorinated aromatic cage of KDM5A PHD3 finger. *Communications Chemistry*, **2020**, 3,	6.3	4
88	Improved Alchemical Free Energy Calculations with Optimized Smoothstep Softcore Potentials. *Journal of Chemical Theory and Computation*, **2020**, 16, 5512-5525	6.4	17
87	Accounting for the Central Role of Interfacial Water in Protein-Ligand Binding Free Energy Calculations. *Journal of Chemical Theory and Computation*, **2020**, 16, 7883-7894	6.4	6
86	Alchemical Binding Free Energy Calculations in AMBER20: Advances and Best Practices for Drug Discovery. *Journal of Chemical Information and Modeling*, **2020**, 60, 5595-5623	6.1	56
85	Fully integrated FPGA molecular dynamics simulations **2019**,		11
84	**2019**,		5
83	Large-Scale Validation of Mixed-Solvent Simulations to Assess Hotspots at Protein-Protein Interaction Interfaces. *Journal of Chemical Information and Modeling*, **2018**, 58, 784-793	6.1	16
82	On the Rational Design of Zeolite Clusters for Converging Reaction Barriers: Quantum Study of Aldol Kinetics Confined in HZSM-5. *Journal of Physical Chemistry C*, **2018**, 122, 23230-23241	3.8	3
81	Water-Restructuring Mutations Can Reverse the Thermodynamic Signature of Ligand Binding to Human Carbonic Anhydrase. *Angewandte Chemie - International Edition*, **2017**, 56, 3833-3837	16.4	24
80	Water-Restructuring Mutations Can Reverse the Thermodynamic Signature of Ligand Binding to Human Carbonic Anhydrase. *Angewandte Chemie*, **2017**, 129, 3891-3895	3.6	2
79	Deciphering Cryptic Binding Sites on Proteins by Mixed-Solvent Molecular Dynamics. *Journal of Chemical Information and Modeling*, **2017**, 57, 1388-1401	6.1	41
78	Predicting the Effect of Amino Acid Single-Point Mutations on Protein Stability-Large-Scale Validation of MD-Based Relative Free Energy Calculations. *Journal of Molecular Biology*, **2017**, 429, 948-963	6.5	54
77	A Water-Bridged Cysteine-Cysteine Redox Regulation Mechanism in Bacterial Protein Tyrosine Phosphatases. *CheM*, **2017**, 3, 665-677	16.2	13
76	The Hsp70 interdomain linker is a dynamic switch that enables allosteric communication between two structured domains. *Journal of Biological Chemistry*, **2017**, 292, 14765-14774	5.4	37
75	Relative Binding Free Energy Calculations in Drug Discovery: Recent Advances and Practical Considerations. *Journal of Chemical Information and Modeling*, **2017**, 57, 2911-2937	6.1	254

74	Calculating Water Thermodynamics in the Binding Site of Proteins - Applications of WaterMap to Drug Discovery. *Current Topics in Medicinal Chemistry*, **2017**, 17, 2586-2598	3	41
73	Predicting Binding Affinities for GPCR Ligands Using Free-Energy Perturbation. *ACS Omega*, **2016**, 1, 293-304	3.9	81
72	In search of novel ligands using a structure-based approach: a case study on the adenosine A receptor. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 863-874	4.2	13
71	AutoQSAR: an automated machine learning tool for best-practice quantitative structure-activity relationship modeling. *Future Medicinal Chemistry*, **2016**, 8, 1825-1839	4.1	50
70	Improving Force Field Parameters for Small-Molecule Conformation Generation **2016**, 57-85		
69	Relative Binding Free Energy Calculations Applied to Protein Homology Models. *Journal of Chemical Information and Modeling*, **2016**, 56, 2388-2400	6.1	40
68	Automated Protocol for Large-Scale Modeling of Gene Expression Data. *Journal of Chemical Information and Modeling*, **2016**, 56, 2216-2224	6.1	3
67	Highly efficient implementation of pseudospectral time-dependent density-functional theory for the calculation of excitation energies of large molecules. *Journal of Computational Chemistry*, **2016**, 37, 1425-41	3.5	17
66	11th German Conference on Chemoinformatics (GCC 2015) : Fulda, Germany. 8-10 November 2015. *Journal of Cheminformatics*, **2016**, 8, 18	8.6	
65	Differential Water Thermodynamics Determine PI3K-Beta/Delta Selectivity for Solvent-Exposed Ligand Modifications. *Journal of Chemical Information and Modeling*, **2016**, 56, 886-94	6.1	26
64	Molecular dynamics techniques for modeling G protein-coupled receptors. *Current Opinion in Pharmacology*, **2016**, 30, 69-75	5.1	24
63	Interactions between Hofmeister anions and the binding pocket of a protein. *Journal of the American Chemical Society*, **2015**, 137, 3859-66	16.4	76
62	Accurate Binding Free Energy Predictions in Fragment Optimization. *Journal of Chemical Information and Modeling*, **2015**, 55, 2411-20	6.1	83
61	Docking and Virtual Screening Strategies for GPCR Drug Discovery. *Methods in Molecular Biology*, **2015**, 1335, 251-76	1.4	14
60	Chemical basis for the recognition of trimethyllysine by epigenetic reader proteins. *Nature Communications*, **2015**, 6, 8911	17.4	57
59	Exploring conformational search protocols for ligand-based virtual screening and 3-D QSAR modeling. *Journal of Computer-Aided Molecular Design*, **2015**, 29, 165-82	4.2	25
58	On the Rational Design of Zeolite Clusters. *ACS Catalysis*, **2015**, 5, 2859-2865	13.1	21
57	Accurate and reliable prediction of relative ligand binding potency in prospective drug discovery by way of a modern free-energy calculation protocol and force field. *Journal of the American Chemical Society*, **2015**, 137, 2695-703	16.4	633

56	Selecting an optimal number of binding site waters to improve virtual screening enrichments against the adenosine A2A receptor. *Journal of Chemical Information and Modeling*, **2014**, 54, 1737-46	6.1	43
55	A computational approach to enzyme design: predicting Ɛ-aminotransferase catalytic activity using docking and MM-GBSA scoring. *Journal of Chemical Information and Modeling*, **2014**, 54, 2334-46	6.1	62
54	Improving docking results via reranking of ensembles of ligand poses in multiple X-ray protein conformations with MM-GBSA. *Journal of Chemical Information and Modeling*, **2014**, 54, 2697-717	6.1	60
53	Impact of binding site waters on inhibitor design: contemplating a novel inverse binding mode of indirubin derivatives in DYRK kinases. *Journal of Cheminformatics*, **2014**, 6,	8.6	78
52	Predicting GPCR promiscuity using binding site features. *Journal of Chemical Information and Modeling*, **2014**, 54, 184-94	6.1	17
51	Synthesis, biological evaluation, hydration site thermodynamics, and chemical reactivity analysis of β-keto substituted peptidomimetics for the inhibition of Plasmodium falciparum. *Bioorganic and Medicinal Chemistry Letters*, **2014**, 24, 1274-9	2.9	13
50	Physics-based enzyme design: predicting binding affinity and catalytic activity. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 3397-409	4.2	29
49	Structure-based approach to the prediction of disulfide bonds in proteins. *Protein Engineering, Design and Selection*, **2014**, 27, 365-74	1.9	39
48	Mechanistic and computational studies of the reductive half-reaction of tyrosine to phenylalanine active site variants of D-arginine dehydrogenase. *Biochemistry*, **2014**, 53, 6574-83	3.2	10
47	The binding of benzoarylsulfonamide ligands to human carbonic anhydrase is insensitive to formal fluorination of the ligand. *Angewandte Chemie - International Edition*, **2013**, 52, 7714-7	16.4	43
46	Improved docking of polypeptides with Glide. *Journal of Chemical Information and Modeling*, **2013**, 53, 1689-99	6.1	815
45	Kernel-based partial least squares: application to fingerprint-based QSAR with model visualization. *Journal of Chemical Information and Modeling*, **2013**, 53, 2312-21	6.1	46
44	The Binding of Benzoarylsulfonamide Ligands to Human Carbonic Anhydrase is Insensitive to Formal Fluorination of the Ligand. *Angewandte Chemie*, **2013**, 125, 7868-7871	3.6	11
43	Structure-based virtual screening of MT2 melatonin receptor: influence of template choice and structural refinement. *Journal of Chemical Information and Modeling*, **2013**, 53, 821-35	6.1	28
42	Contributions of water transfer energy to protein-ligand association and dissociation barriers: Watermap analysis of a series of p38 MAP kinase inhibitors. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 1509-26	4.2	46
41	Allosteric inhibition of the NS2B-NS3 protease from dengue virus. *ACS Chemical Biology*, **2013**, 8, 2744-52	4.9	66
40	Water networks contribute to enthalpy/entropy compensation in protein-ligand binding. *Journal of the American Chemical Society*, **2013**, 135, 15579-84	16.4	230
39	Modeling Local Structural Rearrangements Using FEP/REST: Application to Relative Binding Affinity Predictions of CDK2 Inhibitors. *Journal of Chemical Theory and Computation*, **2013**, 9, 1282-93	6.4	128

38	Protein and ligand preparation: parameters, protocols, and influence on virtual screening enrichments. *Journal of Computer-Aided Molecular Design*, **2013**, 27, 221-34	4.2	2521
37	Type II kinase inhibitors show an unexpected inhibition mode against Parkinson's disease-linked LRRK2 mutant G2019S. *Biochemistry*, **2013**, 52, 1725-36	3.2	44
36	Boosting virtual screening enrichments with data fusion: coalescing hits from two-dimensional fingerprints, shape, and docking. *Journal of Chemical Information and Modeling*, **2013**, 53, 1531-42	6.1	54
35	Novel Inverse Binding Mode of Indirubin Derivatives Yields Improved Selectivity for DYRK Kinases. *ACS Medicinal Chemistry Letters*, **2013**, 4, 22-26	4.3	57
34	Improving the Resistance Profile of Hepatitis C NS3/4A Inhibitors: Dynamic Substrate Envelope Guided Design. *Journal of Chemical Theory and Computation*, **2013**, 9, 5693-5705	6.4	30
33	Applying physics-based scoring to calculate free energies of binding for single amino acid mutations in protein-protein complexes. *PLoS ONE*, **2013**, 8, e82849	3.7	116
32	Generation of receptor structural ensembles for virtual screening using binding site shape analysis and clustering. *Chemical Biology and Drug Design*, **2012**, 80, 182-93	2.9	62
31	Close intramolecular sulfur-oxygen contacts: modified force field parameters for improved conformation generation. *Journal of Computer-Aided Molecular Design*, **2012**, 26, 1195-205	4.2	18
30	Hole filling and library optimization: application to commercially available fragment libraries. *Bioorganic and Medicinal Chemistry*, **2012**, 20, 5379-87	3.4	12
29	Current assessment of docking into GPCR crystal structures and homology models: successes, challenges, and guidelines. *Journal of Chemical Information and Modeling*, **2012**, 52, 3263-77	6.1	74
28	Consensus Induced Fit Docking (cIFD): methodology, validation, and application to the discovery of novel Crm1 inhibitors. *Journal of Computer-Aided Molecular Design*, **2012**, 26, 1217-28	4.2	54
27	Exploring protein flexibility: incorporating structural ensembles from crystal structures and simulation into virtual screening protocols. *Journal of Physical Chemistry B*, **2012**, 116, 6952-9	3.4	71
26	Improving the Prediction of Absolute Solvation Free Energies Using the Next Generation OPLS Force Field. *Journal of Chemical Theory and Computation*, **2012**, 8, 2553-8	6.4	159
25	Thermodynamic analysis of water molecules at the surface of proteins and applications to binding site prediction and characterization. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 871-83	4.2	105
24	Rational approaches to improving selectivity in drug design. *Journal of Medicinal Chemistry*, **2012**, 55, 1424-44	8.3	189
23	Computer-aided drug design of falcipain inhibitors: virtual screening, structure-activity relationships, hydration site thermodynamics, and reactivity analysis. *Journal of Chemical Information and Modeling*, **2012**, 52, 696-710	6.1	37
22	Rapid shape-based ligand alignment and virtual screening method based on atom/feature-pair similarities and volume overlap scoring. *Journal of Chemical Information and Modeling*, **2011**, 51, 2455-66	6.1	147
21	Contribution of explicit solvent effects to the binding affinity of small-molecule inhibitors in blood coagulation factor serine proteases. *ChemMedChem*, **2011**, 6, 1049-66	3.7	103

20	Mechanism of the hydrophobic effect in the biomolecular recognition of arylsulfonamides by carbonic anhydrase. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 17889-94	11.5	268
19	Probing the alpha-helical structural stability of stapled p53 peptides: molecular dynamics simulations and analysis. *Chemical Biology and Drug Design*, **2010**, 75, 348-59	2.9	309
18	Computational approaches for fragment-based and de novo design. *Current Topics in Medicinal Chemistry*, **2010**, 10, 14-32	3	87
17	Hydration Site Thermodynamics Explain SARs for Triazolylpurines Analogues Binding to the A2A Receptor. *ACS Medicinal Chemistry Letters*, **2010**, 1, 160-4	4.3	91
16	ConfGen: a conformational search method for efficient generation of bioactive conformers. *Journal of Chemical Information and Modeling*, **2010**, 50, 534-46	6.1	303
15	Large-scale systematic analysis of 2D fingerprint methods and parameters to improve virtual screening enrichments. *Journal of Chemical Information and Modeling*, **2010**, 50, 771-84	6.1	227
14	Prediction of Absolute Solvation Free Energies using Molecular Dynamics Free Energy Perturbation and the OPLS Force Field. *Journal of Chemical Theory and Computation*, **2010**, 6, 1509-19	6.4	959
13	Understanding kinase selectivity through energetic analysis of binding site waters. *ChemMedChem*, **2010**, 5, 618-27	3.7	99
12	Analysis and comparison of 2D fingerprints: insights into database screening performance using eight fingerprint methods. *Journal of Molecular Graphics and Modelling*, **2010**, 29, 157-70	2.8	275
11	New hypotheses about the structure-function of proprotein convertase subtilisin/kexin type 9: analysis of the epidermal growth factor-like repeat A docking site using WaterMap. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 2571-86	4.2	53
10	Energetic analysis of fragment docking and application to structure-based pharmacophore hypothesis generation. *Journal of Computer-Aided Molecular Design*, **2009**, 23, 541-54	4.2	125
9	High-energy water sites determine peptide binding affinity and specificity of PDZ domains. *Protein Science*, **2009**, 18, 1609-19	6.3	94
8	Novel method for generating structure-based pharmacophores using energetic analysis. *Journal of Chemical Information and Modeling*, **2009**, 49, 2356-68	6.1	224
7	Improving database enrichment through ensemble docking. *Journal of Computer-Aided Molecular Design*, **2008**, 22, 621-7	4.2	56
6	Novel method for probing the specificity binding profile of ligands: applications to HIV protease. *Chemical Biology and Drug Design*, **2008**, 71, 387-407	2.9	22
5	Novel procedure for modeling ligand/receptor induced fit effects. *Journal of Medicinal Chemistry*, **2006**, 49, 534-53	8.3	1320
4	Use of an induced fit receptor structure in virtual screening. *Chemical Biology and Drug Design*, **2006** , 67, 83-4	2.9	376
3	Affinity enhancement of an in vivo matured therapeutic antibody using structure-based computational design. *Protein Science*, **2006**, 15, 949-60	6.3	137

2	Accounting for the Central Role of Interfacial Water in Protein-Ligand Binding Free Energy Calculations		2
1	Free Energy Methods in Drug Discovery: Introduction. *ACS Symposium Series*, 1-38	0.4	3