Woody Sherman

List of Publications by Year
in descending order

94 papers	17,633 citations	38742 50 h-index	45317 90 g-index
103 all docs	103 docs citations	103 times ranked	19688 citing authors

#	Article	IF	Citations
1	Precise Binding Free Energy Calculations for Multiple Molecules Using an Optimal Measurement Network of Pairwise Differences. Journal of Chemical Theory and Computation, 2022, 18, 650-663.	5.3	7
2	Upgrade of FPGA Range-Limited Molecular Dynamics to Handle Hundreds of Processors. , 2021, , .		6
3	Physics-based modeling provides predictive understanding of selectively promiscuous substrate binding by Hsp70 chaperones. PLoS Computational Biology, 2021, 17, e1009567.	3.2	9
4	System-Level Modeling of GPU/FPGA Clusters for Molecular Dynamics Simulations. , 2021, , .		6
5	Fast Equilibration of Water between Buried Sites and the Bulk by Molecular Dynamics with Parallel Monte Carlo Water Moves on Graphical Processing Units. Journal of Chemical Theory and Computation, 2021, 17, 7366-7372.	5.3	16
6	Improved Alchemical Free Energy Calculations with Optimized Smoothstep Softcore Potentials. Journal of Chemical Theory and Computation, 2020, 16, 5512-5525.	5.3	35
7	Accounting for the Central Role of Interfacial Water in Proteinâ€“Ligand Binding Free Energy Calculations. Journal of Chemical Theory and Computation, 2020, 16, 7883-7894.	5.3	24
8	Alchemical Binding Free Energy Calculations in AMBER20: Advances and Best Practices for Drug Discovery. Journal of Chemical Information and Modeling, 2020, 60, 5595-5623.	5.4	177
9	Rigorous Free Energy Simulations in Virtual Screening. Journal of Chemical Information and Modeling, 2020, 60, 4153-4169.	5.4	114
10	Mechanism of biomolecular recognition of trimethyllysine by the fluorinated aromatic cage of KDM5A PHD3 finger. Communications Chemistry, 2020, 3, .	4.5	13
11	A Communication-Efficient Multi-Chip Design for Range-Limited Molecular Dynamics. , 2020, , .		3
12	Molecular Dynamics Range-Limited Force Evaluation Optimized for FPGAs. , 2019, , .		13
13	Fully integrated FPGA molecular dynamics simulations. , 2019, , .		32
14	Large-Scale Validation of Mixed-Solvent Simulations to Assess Hotspots at Proteinâ€“Protein Interaction Interfaces. Journal of Chemical Information and Modeling, 2018, 58, 784-793.	5.4	29
15	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.	3.1	8
16	Waterâ€Restructuring Mutations Can Reverse the Thermodynamic Signature of Ligand Binding to Human Carbonic Anhydrase. Angewandte Chemie - International Edition, 2017, 56, 3833-3837.	13.8	28
17	Waterâ€Restructuring Mutations Can Reverse the Thermodynamic Signature of Ligand Binding to Human Carbonic Anhydrase. Angewandte Chemie, 2017, 129, 3891-3895.	2.0	6
18	Deciphering Cryptic Binding Sites on Proteins by Mixed-Solvent Molecular Dynamics. Journal of Chemical Information and Modeling, 2017, 57, 1388-1401.	5.4	60

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19	Predicting the Effect of Amino Acid Single-Point Mutations on Protein Stabilityâ€"Large-Scale Validation of MD-Based Relative Free Energy Calculations. Journal of Molecular Biology, 2017, 429, 948-963.	4.2	89
20	A Water-Bridged Cysteine-Cysteine Redox Regulation Mechanism in Bacterial Protein Tyrosine Phosphatases. CheM, 2017, 3, 665-677.	11.7	18
21	The Hsp70 interdomain linker is a dynamic switch that enables allosteric communication between two structured domains. Journal of Biological Chemistry, 2017, 292, 14765-14774.	3.4	53
22	Relative Binding Free Energy Calculations in Drug Discovery: Recent Advances and Practical Considerations. Journal of Chemical Information and Modeling, 2017, 57, 2911-2937.	5.4	458
23	Calculating Water Thermodynamics in the Binding Site of Proteins â€" Applications of WaterMap to Drug Discovery. Current Topics in Medicinal Chemistry, 2017, 17, 2586-2598.	2.1	58
24	Differential Water Thermodynamics Determine PI3K-Beta/Delta Selectivity for Solvent-Exposed Ligand Modifications. Journal of Chemical Information and Modeling, 2016, 56, 886-894.	5.4	31
25	Molecular dynamics techniques for modeling G protein-coupled receptors. Current Opinion in Pharmacology, 2016, 30, 69-75.	3.5	26
26	Predicting Binding Affinities for GPCR Ligands Using Free-Energy Perturbation. ACS Omega, 2016, 1, 293-304.	3.5	108
27	In search of novel ligands using a structure-based approach: a case study on the adenosine A2A receptor. Journal of Computer-Aided Molecular Design, 2016, 30, 863-874.	2.9	20
28	AutoQSAR: an automated machine learning tool for best-practice quantitative structureâ€"activity relationship modeling. Future Medicinal Chemistry, 2016, 8, 1825-1839.	2.3	102
29	Relative Binding Free Energy Calculations Applied to Protein Homology Models. Journal of Chemical Information and Modeling, 2016, 56, 2388-2400.	5.4	60
30	Automated Protocol for Large-Scale Modeling of Gene Expression Data. Journal of Chemical Information and Modeling, 2016, 56, 2216-2224.	5.4	5
31	Highly efficient implementation of pseudospectral timeâ€dependent densityâ€functional theory for the calculation of excitation energies of large molecules. Journal of Computational Chemistry, 2016, 37, 1425-1441.	3.3	29
32	11th German Conference on Chemoinformatics (GCC 2015). Journal of Cheminformatics, 2016, 8, 18.	6.1	1
33	On the Rational Design of Zeolite Clusters. ACS Catalysis, 2015, 5, 2859-2865.	11.2	25
34	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, 2695-2703.	13.7	931
35	Interactions between Hofmeister Anions and the Binding Pocket of a Protein. Journal of the American Chemical Society, 2015, 137, 3859-3866.	13.7	89
36	Accurate Binding Free Energy Predictions in Fragment Optimization. Journal of Chemical Information and Modeling, 2015, 55, 2411-2420.	5.4	119

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37	Docking and Virtual Screening Strategies for GPCR Drug Discovery. Methods in Molecular Biology, 2015, 1335, 251-276.	0.9	17
38	Chemical basis for the recognition of trimethyllysine by epigenetic reader proteins. Nature Communications, 2015, 6, 8911.	12.8	72
39	Exploring conformational search protocols for ligand-based virtual screening and 3-D QSAR modeling. Journal of Computer-Aided Molecular Design, 2015, 29, 165-182.	2.9	31
40	Physicsâ€based enzyme design: Predicting binding affinity and catalytic activity. Proteins: Structure, Function and Bioinformatics, 2014, 82, 3397-3409.	2.6	39
41	Structure-based approach to the prediction of disulfide bonds in proteins. Protein Engineering, Design and Selection, 2014, 27, 365-374.	2.1	73
42	Mechanistic and Computational Studies of the Reductive Half-Reaction of Tyrosine to Phenylalanine Active Site Variants of <scp>d</scp>-Arginine Dehydrogenase. Biochemistry, 2014, 53, 6574-6583.	2.5	13
43	Selecting an Optimal Number of Binding Site Waters To Improve Virtual Screening Enrichments Against the Adenosine A_{2A} Receptor. Journal of Chemical Information and Modeling, 2014, 54, 1737-1746.	5.4	49
44	A Computational Approach to Enzyme Design: Predicting Ï‰-Aminotransferase Catalytic Activity Using Docking and MM-GBSA Scoring. Journal of Chemical Information and Modeling, 2014, 54, 2334-2346.	5.4	78
45	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, 2697-2717.	5.4	72
46	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, .	6.1	0
47	Predicting GPCR Promiscuity Using Binding Site Features. Journal of Chemical Information and Modeling, 2014, 54, 184-194.	5.4	19
48	Synthesis, biological evaluation, hydration site thermodynamics, and chemical reactivity analysis of Î±-keto substituted peptidomimetics for the inhibition of Plasmodium falciparum. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 1274-1279.	2.2	16
49	The Binding of Benzoarylsulfonamide Ligands to Human Carbonic Anhydrase is Insensitive to Formal Fluorination of the Ligand. Angewandte Chemie - International Edition, 2013, 52, 7714-7717.	13.8	47
50	Improved Docking of Polypeptides with Glide. Journal of Chemical Information and Modeling, 2013, 53, 1689-1699.	5.4	1,407
51	Kernel-Based Partial Least Squares: Application to Fingerprint-Based QSAR with Model Visualization. Journal of Chemical Information and Modeling, 2013, 53, 2312-2321.	5.4	53
52	Structure-Based Virtual Screening of MT₂ Melatonin Receptor: Influence of Template Choice and Structural Refinement. Journal of Chemical Information and Modeling, 2013, 53, 821-835.	5.4	32
53	Contributions of water transfer energy to proteinâ€ligand association and dissociation barriers: Watermap analysis of a series of p38Î± MAP kinase inhibitors. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1509-1526.	2.6	55
54	Allosteric Inhibition of the NS2B-NS3 Protease from Dengue Virus. ACS Chemical Biology, 2013, 8, 2744-2752.	3.4	101

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55	Water Networks Contribute to Enthalpy/Entropy Compensation in Proteinâ€“Ligand Binding. Journal of the American Chemical Society, 2013, 135, 15579-15584.	13.7	288
56	Modeling Local Structural Rearrangements Using FEP/REST: Application to Relative Binding Affinity Predictions of CDK2 Inhibitors. Journal of Chemical Theory and Computation, 2013, 9, 1282-1293.	5.3	179
57	Protein and ligand preparation: parameters, protocols, and influence on virtual screening enrichments. Journal of Computer-Aided Molecular Design, 2013, 27, 221-234.	2.9	3,989
58	Type II Kinase Inhibitors Show an Unexpected Inhibition Mode against Parkinsonâ€™s Disease-Linked LRRK2 Mutant G2019S. Biochemistry, 2013, 52, 1725-1736.	2.5	54
59	Boosting Virtual Screening Enrichments with Data Fusion: Coalescing Hits from Two-Dimensional Fingerprints, Shape, and Docking. Journal of Chemical Information and Modeling, 2013, 53, 1531-1542.	5.4	67
60	Novel Inverse Binding Mode of Indirubin Derivatives Yields Improved Selectivity for DYRK Kinases. ACS Medicinal Chemistry Letters, 2013, 4, 22-26.	2.8	65
61	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.	5.3	34
62	Applying Physics-Based Scoring to Calculate Free Energies of Binding for Single Amino Acid Mutations in Protein-Protein Complexes. PLoS ONE, 2013, 8, e82849.	2.5	193
63	Close intramolecular sulfurâ€“oxygen contacts: modified force field parameters for improved conformation generation. Journal of Computer-Aided Molecular Design, 2012, 26, 1195-1205.	2.9	21
64	Hole filling and library optimization: Application to commercially available fragment libraries. Bioorganic and Medicinal Chemistry, 2012, 20, 5379-5387.	3.0	16
65	Current Assessment of Docking into GPCR Crystal Structures and Homology Models: Successes, Challenges, and Guidelines. Journal of Chemical Information and Modeling, 2012, 52, 3263-3277.	5.4	86
66	Consensus Induced Fit Docking (cIFD): methodology, validation, and application to the discovery of novel Crm1 inhibitors. Journal of Computer-Aided Molecular Design, 2012, 26, 1217-1228.	2.9	62
67	Exploring Protein Flexibility: Incorporating Structural Ensembles From Crystal Structures and Simulation into Virtual Screening Protocols. Journal of Physical Chemistry B, 2012, 116, 6952-6959.	2.6	77
68	Improving the Prediction of Absolute Solvation Free Energies Using the Next Generation OPLS Force Field. Journal of Chemical Theory and Computation, 2012, 8, 2553-2558.	5.3	239
69	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, 871-883.	2.6	118
70	Rational Approaches to Improving Selectivity in Drug Design. Journal of Medicinal Chemistry, 2012, 55, 1424-1444.	6.4	248
71	Computer-Aided Drug Design of Falcipain Inhibitors: Virtual Screening, Structureâ€“Activity Relationships, Hydration Site Thermodynamics, and Reactivity Analysis. Journal of Chemical Information and Modeling, 2012, 52, 696-710.	5.4	39
72	Generation of Receptor Structural Ensembles for Virtual Screening Using Binding Site Shape Analysis and Clustering. Chemical Biology and Drug Design, 2012, 80, 182-193.	3.2	71

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73	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, 2455-2466.	5.4	190
74	Generation of structure-based pharmacophores using energetic analysis â€“ application on fragment docking. Journal of Cheminformatics, 2011, 3, .	6.1	1
75	Contribution of Explicit Solvent Effects to the Binding Affinity of Smallâ€Molecule Inhibitors in Blood Coagulation Factor Serine Proteases. ChemMedChem, 2011, 6, 1049-1066.	3.2	116
76	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, 17889-17894.	7.1	304
77	Large-Scale Systematic Analysis of 2D Fingerprint Methods and Parameters to Improve Virtual Screening Enrichments. Journal of Chemical Information and Modeling, 2010, 50, 771-784.	5.4	301
78	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, 1509-1519.	5.3	1,360
79	Understanding Kinase Selectivity Through Energetic Analysis of Binding Site Waters. ChemMedChem, 2010, 5, 618-627.	3.2	112
80	Analysis and comparison of 2D fingerprints: Insights into database screening performance using eight fingerprint methods. Journal of Molecular Graphics and Modelling, 2010, 29, 157-170.	2.4	390
81	New hypotheses about the structureâ€“function of proprotein convertase subtilisin/kexin type 9: Analysis of the epidermal growth factorâ€like repeat A docking site using WaterMap. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2571-2586.	2.6	65
82	Probing the Î±â€Helical Structural Stability of Stapled p53 Peptides: Molecular Dynamics Simulations and Analysis. Chemical Biology and Drug Design, 2010, 75, 348-359.	3.2	351
83	Computational Approaches for Fragment-Based and De Novo Design. Current Topics in Medicinal Chemistry, 2010, 10, 14-32.	2.1	100
84	Hydration Site Thermodynamics Explain SARs for Triazolylpurines Analogues Binding to the A2A Receptor. ACS Medicinal Chemistry Letters, 2010, 1, 160-164.	2.8	95
85	ConfGen: A Conformational Search Method for Efficient Generation of Bioactive Conformers. Journal of Chemical Information and Modeling, 2010, 50, 534-546.	5.4	369
86	Energetic analysis of fragment docking and application to structure-based pharmacophore hypothesis generation. Journal of Computer-Aided Molecular Design, 2009, 23, 541-554.	2.9	147
87	Highâ€energy water sites determine peptide binding affinity and specificity of PDZ domains. Protein Science, 2009, 18, 1609-1619.	7.6	100
88	Novel Method for Generating Structure-Based Pharmacophores Using Energetic Analysis. Journal of Chemical Information and Modeling, 2009, 49, 2356-2368.	5.4	279
89	Improving database enrichment through ensemble docking. Journal of Computer-Aided Molecular Design, 2008, 22, 621-627.	2.9	63
90	Novel Method for Probing the Specificity Binding Profile of Ligands: Applications to HIV Protease. Chemical Biology and Drug Design, 2008, 71, 387-407.	3.2	26

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91	Novel Procedure for Modeling Ligand/Receptor Induced Fit Effects. Journal of Medicinal Chemistry, 2006, 49, 534-553.	6.4	1,671
92	Use of an Induced Fit Receptor Structure in Virtual Screening. Chemical Biology and Drug Design, 2006, 67, 83-84.	3.2	550
93	Affinity enhancement of an in vivo matured therapeutic antibody using structure-based computational design. Protein Science, 2006, 15, 949-960.	7.6	160
94	Free Energy Methods in Drug Discoveryâ€"Introduction. ACS Symposium Series, 0, , 1-38.	0.5	24