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List of Publications by Year
in descending order

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Version: 2024-02-01

27 papers	2,770 citations	393982 19 h-index	525886 27 g-index
28 all docs	28 docs citations	28 times ranked	3017 citing authors

#	Article	IF	Citations
1	CHARMM Additive All-Atom Force Field for Glycosidic Linkages between Hexopyranoses. Journal of Chemical Theory and Computation, 2009, 5, 2353-2370.	2.3	578
2	CHARMM Additive All-Atom Force Field for Carbohydrate Derivatives and Its Utility in Polysaccharide and Carbohydrateâ€“Protein Modeling. Journal of Chemical Theory and Computation, 2011, 7, 3162-3180.	2.3	559
3	Additive empirical force field for hexopyranose monosaccharides. Journal of Computational Chemistry, 2008, 29, 2543-2564.	1.5	483
4	Computational Fragment-Based Binding Site Identification by Ligand Competitive Saturation. PLoS Computational Biology, 2009, 5, e1000435.	1.5	208
5	CHARMM Additive All-Atom Force Field for Acyclic Polyalcohols, Acyclic Carbohydrates, and Inositol. Journal of Chemical Theory and Computation, 2009, 5, 1315-1327.	2.3	150
6	Reproducing Crystal Binding Modes of Ligand Functional Groups Using Site-Identification by Ligand Competitive Saturation (SILCS) Simulations. Journal of Chemical Information and Modeling, 2011, 51, 877-896.	2.5	105
7	Automated conformational energy fitting for force-field development. Journal of Molecular Modeling, 2008, 14, 667-679.	0.8	104
8	CHARMM Additive All-Atom Force Field for Phosphate and Sulfate Linked to Carbohydrates. Journal of Chemical Theory and Computation, 2012, 8, 759-776.	2.3	100
9	Computational evaluation of proteinâ€“small molecule binding. Current Opinion in Structural Biology, 2009, 19, 56-61.	2.6	73
10	Identification of Small Molecular Weight Inhibitors of Src Homology 2 Domain-Containing Tyrosine Phosphatase 2 (SHP-2) via in Silico Database Screening Combined with Experimental Assay. Journal of Medicinal Chemistry, 2008, 51, 7396-7404.	2.9	39
11	Site Identification by Ligand Competitive Saturation (SILCS) Simulations for Fragment-Based Drug Design. Methods in Molecular Biology, 2015, 1289, 75-87.	0.4	37
12	Balancing target flexibility and target denaturation in computational fragmentâ€based inhibitor discovery. Journal of Computational Chemistry, 2012, 33, 1880-1891.	1.5	36
13	Terminal sialic acids on CD44 N-glycans can block hyaluronan binding by forming competing intramolecular contacts with arginine sidechains. Proteins: Structure, Function and Bioinformatics, 2014, 82, 3079-3089.	1.5	34
14	Quantum Mechanical Analysis of 1,2-Ethanediol Conformational Energetics and Hydrogen Bonding. Journal of Physical Chemistry A, 2006, 110, 9934-9939.	1.1	30
15	Mechanism of Binding Site Conformational Switching in the CD44â€“Hyaluronan Proteinâ€“Carbohydrate Binding Interaction. Journal of Molecular Biology, 2011, 406, 631-647.	2.0	28
16	Revealing the Mechanisms of Protein Disorder and N-Glycosylation in CD44-Hyaluronan Binding Using Molecular Simulation. Frontiers in Immunology, 2015, 6, 305.	2.2	28
17	Sulfation and Cation Effects on the Conformational Properties of the Glycan Backbone of Chondroitin Sulfate Disaccharides. Journal of Physical Chemistry B, 2015, 119, 6063-6073.	1.2	28
18	CD44 Receptor Unfolding Enhances Binding by Freeing Basic Amino Acids to Contact Carbohydrate Ligand. Biophysical Journal, 2013, 105, 1217-1226.	0.2	21

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19	Peptide Backbone Sampling Convergence with the Adaptive Biasing Force Algorithm. Journal of Physical Chemistry B, 2013, 117, 518-526.	1.2	20
20	Computational functional group mapping for drug discovery. Drug Discovery Today, 2016, 21, 1928-1931.	3.2	19
21	Efficient Construction of Atomic-Resolution Models of Non-Sulfated Chondroitin Glycosaminoglycan Using Molecular Dynamics Data. Biomolecules, 2020, 10, 537.	1.8	16
22	Tyr66 acts as a conformational switch in the closed-to-open transition of the SHP-2 N-SH2-domain phosphotyrosine-peptide binding cleft. BMC Structural Biology, 2007, 7, 14.	2.3	13
23	Constructing 3-Dimensional Atomic-Resolution Models of Nonsulfated Glycosaminoglycans with Arbitrary Lengths Using Conformations from Molecular Dynamics. International Journal of Molecular Sciences, 2020, 21, 7699.	1.8	13
24	Sulfation and Calcium Favor Compact Conformations of Chondroitin in Aqueous Solutions. ACS Omega, 2021, 6, 13204-13217.	1.6	13
25	Rigidity and flexibility in the tetrasaccharide linker of proteoglycans from atomicâ€resolution molecular simulation. Journal of Computational Chemistry, 2017, 38, 1438-1446.	1.5	12
26	Pyranose Ring Puckering Thermodynamics for Glycan Monosaccharides Associated with Vertebrate Proteins. International Journal of Molecular Sciences, 2022, 23, 473.	1.8	11
27	Folding of Fibroblast Growth Factor 1 Is Critical for Its Nonclassical Release. Biochemistry, 2016, 55, 1159-1167.	1.2	8