Olgun Guvench

List of Publications by Year
in descending order

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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	Pyranose Ring Puckering Thermodynamics for Glycan Monosaccharides Associated with Vertebrate Proteins. International Journal of Molecular Sciences, 2022, 23, 473.	1.8	11
2	Sulfation and Calcium Favor Compact Conformations of Chondroitin in Aqueous Solutions. ACS Omega, 2021, 6, 13204-13217.	1.6	13
3	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
4	Efficient Construction of Atomic-Resolution Models of Non-Sulfated Chondroitin Glycosaminoglycan Using Molecular Dynamics Data. Biomolecules, 2020, 10, 537.	1.8	16
5	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
6	Computational functional group mapping for drug discovery. Drug Discovery Today, 2016, 21, 1928-1931.	3.2	19
7	Folding of Fibroblast Growth Factor 1 Is Critical for Its Nonclassical Release. Biochemistry, 2016, 55, 1159-1167.	1.2	8
8	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
9	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
10	Site Identification by Ligand Competitive Saturation (SILCS) Simulations for Fragment-Based Drug Design. Methods in Molecular Biology, 2015, 1289, 75-87.	0.4	37
11	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
12	CD44 Receptor Unfolding Enhances Binding by Freeing Basic Amino Acids to Contact Carbohydrate Ligand. Biophysical Journal, 2013, 105, 1217-1226.	0.2	21
13	Peptide Backbone Sampling Convergence with the Adaptive Biasing Force Algorithm. Journal of Physical Chemistry B, 2013, 117, 518-526.	1.2	20
14	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
15	Balancing target flexibility and target denaturation in computational fragmentâ€based inhibitor discovery. Journal of Computational Chemistry, 2012, 33, 1880-1891.	1.5	36
16	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
17	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
18	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

#	Article	IF	Citations
19	Computational Fragment-Based Binding Site Identification by Ligand Competitive Saturation. PLoS Computational Biology, 2009, 5, e1000435.	1.5	208
20	Computational evaluation of proteinâ€“small molecule binding. Current Opinion in Structural Biology, 2009, 19, 56-61.	2.6	73
21	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
22	CHARMM Additive All-Atom Force Field for Glycosidic Linkages between Hexopyranoses. Journal of Chemical Theory and Computation, 2009, 5, 2353-2370.	2.3	578
23	Automated conformational energy fitting for force-field development. Journal of Molecular Modeling, 2008, 14, 667-679.	0.8	104
24	Additive empirical force field for hexopyranose monosaccharides. Journal of Computational Chemistry, 2008, 29, 2543-2564.	1.5	483
25	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
26	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
27	Quantum Mechanical Analysis of 1,2-Ethanediol Conformational Energetics and Hydrogen Bonding. Journal of Physical Chemistry A, 2006, 110, 9934-9939.	1.1	30