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List of Publications by Year
in descending order

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22 papers	607 citations	1040056 9 h-index	713466 21 g-index
22 all docs	22 docs citations	22 times ranked	780 citing authors

#	Article	IF	Citations
1	Drug repositioning to propose alternative modulators for glucocorticoid receptor through structure-based virtual screening. Journal of Biomolecular Structure and Dynamics, 2022, 40, 11418-11433.	3.5	2
2	Potential allosteric sites captured in glycolytic enzymes via residue-based network models: Phosphofructokinase, glyceraldehyde-3-phosphate dehydrogenase and pyruvate kinase. Biophysical Chemistry, 2022, 280, 106701.	2.8	5
3	Altered Dynamics of S. aureus Phosphofructokinase via Bond Restraints at Two Distinct Allosteric Binding Sites. Journal of Molecular Biology, 2022, 434, 167646.	4.2	2
4	Editorial: Understanding Protein Dynamics, Binding and Allostery for Drug Design. Frontiers in Molecular Biosciences, 2021, 8, 681364.	3.5	2
5	Distinctive communication networks in inactive states of Î²₂â€adrenergic receptor: Mutual information and entropy transfer analysis. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1458-1471.	2.6	6
6	Identification of Alternative Allosteric Sites in Glycolytic Enzymes for Potential Use as Species-Specific Drug Targets. Frontiers in Molecular Biosciences, 2020, 7, 88.	3.5	17
7	Intrinsic Dynamics and Causality in Correlated Motions Unraveled in Two Distinct Inactive States of Human Î²₂-Adrenergic Receptor. Journal of Physical Chemistry B, 2019, 123, 3630-3642.	2.6	3
8	Ligandâ€binding affinity of alternative conformers of human Î² 2 â€adrenergic receptor in the presence of intracellular loop 3 (ICL 3) and their potential use in virtual screening studies. Chemical Biology and Drug Design, 2019, 93, 883-899.	3.2	9
9	Assessing proteinâ€“ligand binding modes with computational tools: the case of PDE4B. Journal of Computer-Aided Molecular Design, 2017, 31, 563-575.	2.9	1
10	Investigation of allosteric coupling in human Î²2-adrenergic receptor in the presence of intracellular loop 3. BMC Structural Biology, 2016, 16, 9.	2.3	18
11	Structural analysis of peptide fragments following the hydrolysis of bovine serum albumin by trypsin and chymotrypsin. Journal of Biomolecular Structure and Dynamics, 2016, 34, 1092-1100.	3.5	6
12	How an Inhibitor Bound to Subunit Interface Alters Triosephosphate Isomerase Dynamics. Biophysical Journal, 2015, 109, 1169-1178.	0.5	28
13	Transmembrane helix 6 observed at the interface of Î²2AR homodimers in blind docking studies. Journal of Biomolecular Structure and Dynamics, 2015, 33, 1503-1515.	3.5	3
14	Discovery of high affinity ligands for Î² 2 -adrenergic receptor through pharmacophore-based high-throughput virtual screening and docking. Journal of Molecular Graphics and Modelling, 2014, 53, 148-160.	2.4	6
15	Effect of Intracellular Loop 3 on Intrinsic Dynamics of Human Î²2-Adrenergic Receptor. Biophysical Journal, 2014, 106, 53a.	0.5	1
16	Effect of intracellular loop 3 on intrinsic dynamics of human Î²2-adrenergic receptor. BMC Structural Biology, 2013, 13, 29.	2.3	25
17	Molecular Docking Study Based on Pharmacophore Modeling for Novel PhosphodiesteraseIV Inhibitors. Molecular Informatics, 2012, 31, 459-471.	2.5	5
18	Blind Dockings of Benzothiazoles to Multiple Receptor Conformations of Triosephosphate Isomerase from Trypanosoma cruzi and Human. Molecular Informatics, 2011, 30, 986-995.	2.5	12

#	Article	IF	Citations
19	A Docking Study Using Atomistic Conformers Generated via Elastic Network Model for Cyclosporin A/Cyclophilin A Complex. Journal of Biomolecular Structure and Dynamics, 2009, 27, 13-25.	3.5	42
20	Monte Carlo Simulation of Single- and Binary-Component Adsorption of CO2, N2, and H2in Zeolite Na-4A. Energy & Fuels, 2003, 17, 977-983.	5.1	165
21	Atomistic Simulations of CO2and N2Adsorption in Silica Zeolites:Â The Impact of Pore Size and Shapeâ€. Journal of Physical Chemistry B, 2002, 106, 8367-8375.	2.6	205
22	Monte Carlo Simulation of Head-to-Head, Tail-to-Tail Polypropylene and Its Mixing with Polyethylene in the Melt. Macromolecules, 2001, 34, 3389-3395.	4.8	44