Ebru Demet Akten

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	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
2	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
3	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
4	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
5	How an Inhibitor Bound to Subunit Interface Alters Triosephosphate Isomerase Dynamics. Biophysical Journal, 2015, 109, 1169-1178.	0.5	28
6	Effect of intracellular loop 3 on intrinsic dynamics of human Î²2-adrenergic receptor. BMC Structural Biology, 2013, 13, 29.	2.3	25
7	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
8	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
9	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
10	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
11	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
12	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
13	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
14	Molecular Docking Study Based on Pharmacophore Modeling for Novel PhosphodiesteraseIV Inhibitors. Molecular Informatics, 2012, 31, 459-471.	2.5	5
15	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
16	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
17	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
18	Editorial: Understanding Protein Dynamics, Binding and Allostery for Drug Design. Frontiers in Molecular Biosciences, 2021, 8, 681364.	3.5	2

#	Article	IF	Citations
19	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
20	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
21	Effect of Intracellular Loop 3 on Intrinsic Dynamics of Human Î²2-Adrenergic Receptor. Biophysical Journal, 2014, 106, 53a.	0.5	1
22	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