Orkide CoÅkuner-Weber

List of Publications by Year
in descending order

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42	914	361045	476904
papers	citations	20 h-index	29 g-index

44	44	44	912
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Structures and Free Energy Landscapes of the A53T Mutant-Type Î±-Synuclein Protein and Impact of A53T Mutation on the Structures of the Wild-Type Î±-Synuclein Protein with Dynamics. ACS Chemical Neuroscience, 2013, 4, 1101-1113.	1.7	66
2	Structures of the E46K Mutant-Type Î±-Synuclein Protein and Impact of E46K Mutation on the Structures of the Wild-Type Î±-Synuclein Protein. ACS Chemical Neuroscience, 2013, 4, 498-508.	1.7	55
3	Insights into the Molecular Mechanisms of Alzheimerâ€™s and Parkinsonâ€™s Diseases with Molecular Simulations: Understanding the Roles of Artificial and Pathological Missense Mutations in Intrinsically Disordered Proteins Related to Pathology. International Journal of Molecular Sciences, 2018, 19, 336.	1.8	51
4	Amyloid-Î² peptide structure in aqueous solution varies with fragment size. Journal of Chemical Physics, 2011, 135, 205101.	1.2	47
5	Transition Metal Ion Interactions with Disordered Amyloid-Î² Peptides in the Pathogenesis of Alzheimerâ€™s Disease: Insights from Computational Chemistry Studies. Journal of Chemical Information and Modeling, 2019, 59, 1782-1805.	2.5	46
6	Structures and free energy landscapes of aqueous zinc(II)-bound amyloid-Î²(1â€“40) and zinc(II)-bound amyloid-Î²(1â€“42) with dynamics. Journal of Biological Inorganic Chemistry, 2012, 17, 927-938.	1.1	40
7	The Structures of the E22Î” Mutant-Type Amyloid-Î² Alloforms and the Impact of E22Î” Mutation on the Structures of the Wild-Type Amyloid-Î² Alloforms. ACS Chemical Neuroscience, 2013, 4, 310-320.	1.7	38
8	How accurate are your simulations? Effects of confined aqueous volume and AMBER FF99SB and CHARMM22/CMAP force field parameters on structural ensembles of intrinsically disordered proteins: Amyloid-Î²₄₂in water. Intrinsically Disordered Proteins, 2017, 5, e1377813.	1.9	37
9	Structures and Free Energy Landscapes of the Wild-Type and A30P Mutant-Type Î±-Synuclein Proteins with Dynamics. ACS Chemical Neuroscience, 2013, 4, 486-497.	1.7	36
10	Ligand Exchange Reactions in the Formation of Diphosphine-Protected Gold Clusters. Journal of Physical Chemistry C, 2008, 112, 12808-12814.	1.5	34
11	Water Dissociation in the Presence of Metal Ions. Angewandte Chemie - International Edition, 2007, 46, 7853-7855.	7.2	30
12	Arginine and Disordered Amyloid-Î² Peptide Structures: Molecular Level Insights into the Toxicity in Alzheimerâ€™s Disease. ACS Chemical Neuroscience, 2013, 4, 1549-1558.	1.7	30
13	Coordination Studies of Al-EDTA in Aqueous Solution. Journal of Physical Chemistry A, 2008, 112, 2628-2633.	1.1	29
14	Tyrosine Regulates Î²-Sheet Structure Formation in Amyloid-Î²₄₂: A New Clustering Algorithm for Disordered Proteins. Journal of Chemical Information and Modeling, 2017, 57, 1342-1358.	2.5	26
15	Adenosine Triphosphate (ATP) Reduces Amyloid-Î² Protein Misfolding in vitro. Journal of Alzheimer's Disease, 2014, 41, 561-574.	1.2	25
16	Hydrophobic Interactions by Monte Carlo Simulations. Zeitschrift Fur Physikalische Chemie, 2006, 220, 349-369.	1.4	24
17	New force field parameters for metalloproteins I: Divalent copper ion centers including three histidine residues and an oxygenâ€ligated amino acid residue. Journal of Computational Chemistry, 2014, 35, 1278-1289.	1.5	24
18	Preferred conformation of the glycosidic linkage of methyl-Î²-mannose. Journal of Chemical Physics, 2007, 127, 015101.	1.2	23

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19	Probing and Trapping a Sensitive Conformation: Amyloid-Î² Fibrils, Oligomers, and Dimers. Journal of Alzheimer's Disease, 2012, 32, 197-215.	1.2	23
20	Intrinsically disordered proteins in various hypotheses on the pathogenesis of Alzheimer's and Parkinson's diseases. Progress in Molecular Biology and Translational Science, 2019, 166, 145-223.	0.9	22
21	Hydrophobic Interactions of Xenon by Monte Carlo Simulations. Zeitschrift Fur Physikalische Chemie, 2007, 221, 785-799.	1.4	21
22	Intrinsically disordered proteins and proteins with intrinsically disordered regions in neurodegenerative diseases. Biophysical Reviews, 2022, 14, 679-707.	1.5	20
23	Divalent copper ion bound amyloid-Î²(40) and amyloid-Î²(42) alloforms are less preferred than divalent zinc ion bound amyloid-Î²(40) and amyloid-Î²(42) alloforms. Journal of Biological Inorganic Chemistry, 2016, 21, 957-973.	1.1	18
24	Current Challenges and Limitations in the Studies of Intrinsically Disordered Proteins in Neurodegenerative Diseases by Computer Simulations. Current Alzheimer Research, 2021, 17, 805-818.	0.7	18
25	Identification of Active Sites of Biomolecules. 1. Methyl-Î±-mannopyranoside and Fe^{III}. Journal of Physical Chemistry A, 2008, 112, 2940-2947.	1.1	16
26	Alanine Scanning Effects on the Biochemical and Biophysical Properties of Intrinsically Disordered Proteins: A Case Study of the Histidine to Alanine Mutations in Amyloid-Î²₄₂. Journal of Chemical Information and Modeling, 2019, 59, 871-884.	2.5	14
27	Single Ion and Dimerization Studies of the Al(III) Ion in Aqueous Solution. Journal of Physical Chemistry A, 2010, 114, 10981-10987.	1.1	13
28	Epitope region identification challenges of intrinsically disordered proteins in neurodegenerative diseases: Secondary structure dependence of Î±â€synuclein on simulation techniques and force field parameters. Chemical Biology and Drug Design, 2020, 96, 659-667.	1.5	13
29	Identification of Active Sites of Biomolecules II: Saccharide and Transition Metal Ion in Aqueous Solution. Journal of Physical Chemistry A, 2009, 113, 2491-2499.	1.1	12
30	Glycosidic linkage conformation of methyl-Î±-mannopyranoside. Journal of Chemical Physics, 2008, 129, 045102.	1.2	10
31	Secondary structure dependence of amyloidâ€Î²(1â€“40) on simulation techniques and force field parameters. Chemical Biology and Drug Design, 2021, 97, 1100-1108.	1.5	10
32	Molecular simulations of IDPs: From ensemble generation to IDP interactions leading to disorder-to-order transitions. Progress in Molecular Biology and Translational Science, 2021, 183, 135-185.	0.9	9
33	Dynamic and Structural Properties of Aqueous Arsenic Solutions. ChemPhysChem, 2009, 10, 1187-1189.	1.0	7
34	Revisiting Cu(II) Bound Amyloid-Î²40 and Amyloid-Î²42 Peptides: Varying Coordination Chemistries. Journal of the Turkish Chemical Society, Section A: Chemistry, 2018, 5, 981-1008.	0.4	6
35	Structures of the Wild-Type and S59L Mutant CHCHD10 Proteins Important in Amyotrophic Lateral Sclerosisâ€“Frontotemporal Dementia. ACS Chemical Neuroscience, 2022, 13, 1273-1280.	1.7	6
36	Quantum Chemistry Meets Deep Learning for Complex Carbohydrate and Glycopeptide Species I. Zeitschrift Fur Physikalische Chemie, 2019, 233, 527-550.	1.4	4

#	Article	IF	Citations
37	Secondary structure dependence on simulation techniques and force field parameters: from disordered to ordered proteins. Biophysical Reviews, 2021, 13, 1173-1178.	1.5	4
38	BMP-2 and BMP-9 binding specificities with ALK-3 in aqueous solution with dynamics. Journal of Molecular Graphics and Modelling, 2017, 77, 181-188.	1.3	3
39	Structures of <scp>MERSâ€CoV</scp> macro domain in aqueous solution with dynamics: Impacts of parallel tempering simulation techniques and <scp>CHARMM36m</scp> and <scp>AMBER99SB</scp> force field parameters. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1289-1299.	1.5	2
40	Methods to study the effect of solution variables on the conformational dynamics of intrinsically disordered proteins. , 2022, , 551-563.		1
41	From Quantum Mechanics, Classical Mechanics, and Bioinformatics to Artificial Intelligence Studies in Neurodegenerative Diseases. Methods in Molecular Biology, 2022, 2340, 139-173.	0.4	1
42	Challenges and limitations in the studies of glycoproteins: A computational chemist's perspective. Proteins: Structure, Function and Bioinformatics, 2022, 90, 322-339.	1.5	0