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	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
2	Methods to study the effect of solution variables on the conformational dynamics of intrinsically disordered proteins. , 2022, , 551-563.		1
3	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
4	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
5	Intrinsically disordered proteins and proteins with intrinsically disordered regions in neurodegenerative diseases. Biophysical Reviews, 2022, 14, 679-707.	1.5	20
6	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
7	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
8	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
9	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
10	Secondary structure dependence on simulation techniques and force field parameters: from disordered to ordered proteins. Biophysical Reviews, 2021, 13, 1173-1178.	1.5	4
11	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
12	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
13	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
14	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
15	Quantum Chemistry Meets Deep Learning for Complex Carbohydrate and Glycopeptide Species I. Zeitschrift Fur Physikalische Chemie, 2019, 233, 527-550.	1.4	4
16	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
17	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
18	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

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19	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
20	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
21	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
22	Adenosine Triphosphate (ATP) Reduces Amyloid-Î² Protein Misfolding in vitro. Journal of Alzheimer's Disease, 2014, 41, 561-574.	1.2	25
23	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
24	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
25	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
26	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
27	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
28	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
29	Probing and Trapping a Sensitive Conformation: Amyloid-Î² Fibrils, Oligomers, and Dimers. Journal of Alzheimer's Disease, 2012, 32, 197-215.	1.2	23
30	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
31	Amyloid-Î² peptide structure in aqueous solution varies with fragment size. Journal of Chemical Physics, 2011, 135, 205101.	1.2	47
32	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
33	Dynamic and Structural Properties of Aqueous Arsenic Solutions. ChemPhysChem, 2009, 10, 1187-1189.	1.0	7
34	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
35	Coordination Studies of Al-EDTA in Aqueous Solution. Journal of Physical Chemistry A, 2008, 112, 2628-2633.	1.1	29
36	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

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37	Ligand Exchange Reactions in the Formation of Diphosphine-Protected Gold Clusters. Journal of Physical Chemistry C, 2008, 112, 12808-12814.	1.5	34
38	Glycosidic linkage conformation of methyl-Î±-mannopyranoside. Journal of Chemical Physics, 2008, 129, 045102.	1.2	10
39	Preferred conformation of the glycosidic linkage of methyl-Î²-mannose. Journal of Chemical Physics, 2007, 127, 015101.	1.2	23
40	Hydrophobic Interactions of Xenon by Monte Carlo Simulations. Zeitschrift Fur Physikalische Chemie, 2007, 221, 785-799.	1.4	21
41	Water Dissociation in the Presence of Metal Ions. Angewandte Chemie - International Edition, 2007, 46, 7853-7855.	7.2	30
42	Hydrophobic Interactions by Monte Carlo Simulations. Zeitschrift Fur Physikalische Chemie, 2006, 220, 349-369.	1.4	24