Andreas Vitalis

List of Publications by Year
in descending order

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36 papers	2,593 citations	304743 22 h-index	345221 36 g-index
36 all docs	36 docs citations	36 times ranked	2745 citing authors

#	Article	IF	Citations
1	Antibody binding modulates the dynamics ofÂtheÂmembrane-bound prion protein. Biophysical Journal, 2022, 121, 2813-2825.	0.5	3
2	Unsupervised Methods for Detection of Neural States: Case Study of Hippocampal-Amygdala Interactions. ENeuro, 2021, 8, ENEURO.0484-20.2021.	1.9	2
3	An ABSINTH-Based Protocol for Predicting Binding Affinities between Proteins and Small Molecules. Journal of Chemical Information and Modeling, 2020, 60, 5188-5202.	5.4	5
4	<scp>Sapphire</scp>-Based Clustering. Journal of Chemical Theory and Computation, 2020, 16, 6383-6396.	5.3	13
5	On the removal of initial state bias from simulation data. Journal of Chemical Physics, 2019, 150, 104105.	3.0	12
6	Unsupervised identification of states from voltage recordings of neural networks. Journal of Neuroscience Methods, 2019, 318, 104-117.	2.5	3
7	Precise estimation of transfer free energies for ionic species between similar media. Physical Chemistry Chemical Physics, 2018, 20, 27003-27010.	2.8	1
8	Amyloid Î² Fibril Elongation by Monomers Involves Disorder at the Tip. Journal of Chemical Theory and Computation, 2017, 13, 5117-5130.	5.3	34
9	The ATAD2 bromodomain binds different acetylation marks on the histone H4 in similar fuzzy complexes. Journal of Biological Chemistry, 2017, 292, 16734-16745.	3.4	26
10	Focused conformational sampling in proteins. Journal of Chemical Physics, 2017, 147, 195102.	3.0	8
11	Dynamic microfluidic control of supramolecular peptide self-assembly. Nature Communications, 2016, 7, 13190.	12.8	89
12	Quantitative Assessments of the Distinct Contributions of Polypeptide Backbone Amides versus Side Chain Groups to Chain Expansion via Chemical Denaturation. Journal of the American Chemical Society, 2015, 137, 2984-2995.	13.7	104
13	Weighted Distance Functions Improve Analysis of High-Dimensional Data: Application to Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2015, 11, 5481-5492.	5.3	11
14	A molecular simulation protocol to avoid sampling redundancy and discover new states. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 889-902.	2.4	25
15	A simple molecular mechanics integrator in mixed rigid body and dihedral angle space. Journal of Chemical Physics, 2014, 141, 034105.	3.0	17
16	Equilibrium Sampling Approach to the Interpretation of Electron Density Maps. Structure, 2014, 22, 156-167.	3.3	9
17	High-Resolution Visualisation of the States and Pathways Sampled in Molecular Dynamics Simulations. Scientific Reports, 2014, 4, 6264.	3.3	17
18	A scalable algorithm to order and annotate continuous observations reveals the metastable states visited by dynamical systems. Computer Physics Communications, 2013, 184, 2446-2453.	7.5	24

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19	Improved Atomistic Monte Carlo Simulations Demonstrate That Poly-<scp>l</scp>-Proline Adopts Heterogeneous Ensembles of Conformations of Semi-Rigid Segments Interrupted by Kinks. Journal of Physical Chemistry B, 2012, 116, 6862-6871.	2.6	39
20	Efficient Construction of Mesostate Networks from Molecular Dynamics Trajectories. Journal of Chemical Theory and Computation, 2012, 8, 1108-1120.	5.3	42
21	50 Years of Lifsonâ€“Roig Models: Application to Molecular Simulation Data. Journal of Chemical Theory and Computation, 2012, 8, 363-373.	5.3	21
22	Assessing the contribution of heterogeneous distributions of oligomers to aggregation mechanisms of polyglutamine peptides. Biophysical Chemistry, 2011, 159, 14-23.	2.8	103
23	Disordered Binding of Small Molecules to AÎ²(12â€“28). Journal of Biological Chemistry, 2011, 286, 41578-41588.	3.4	46
24	Net charge per residue modulates conformational ensembles of intrinsically disordered proteins. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 8183-8188.	7.1	484
25	Modulation of Polyglutamine Conformations and Dimer Formation by the N-Terminus of Huntingtin. Journal of Molecular Biology, 2010, 396, 1295-1309.	4.2	122
26	Micelle-Like Architecture of the Monomer Ensemble of Alzheimerâ€™s Amyloid-Î² Peptide in Aqueous Solution and Its Implications for AÎ² Aggregation. Journal of Molecular Biology, 2010, 403, 148-165.	4.2	71
27	New Estimators for Calculating Solvation Entropy and Enthalpy and Comparative Assessments of Their Accuracy and Precision. Journal of Physical Chemistry B, 2010, 114, 8166-8180.	2.6	23
28	ABSINTH: A new continuum solvation model for simulations of polypeptides in aqueous solutions. Journal of Computational Chemistry, 2009, 30, 673-699.	3.3	307
29	Thermodynamics of Î²-Sheet Formation in Polyglutamine. Biophysical Journal, 2009, 97, 303-311.	0.5	83
30	Chapter 3 Methods for Monte Carlo Simulations of Biomacromolecules. Annual Reports in Computational Chemistry, 2009, 5, 49-76.	1.7	110
31	Atomistic Simulations of the Effects of Polyglutamine Chain Length and Solvent Quality on Conformational Equilibria and Spontaneous Homodimerization. Journal of Molecular Biology, 2008, 384, 279-297.	4.2	113
32	A polymer physics perspective on driving forces and mechanisms for protein aggregation. Archives of Biochemistry and Biophysics, 2008, 469, 132-141.	3.0	151
33	Quantitative Characterization of Intrinsic Disorder in Polyglutamine: Insights from Analysis Based on Polymer Theories. Biophysical Journal, 2007, 93, 1923-1937.	0.5	140
34	Characterizing the conformational ensemble of monomeric polyglutamine. Proteins: Structure, Function and Bioinformatics, 2005, 63, 297-311.	2.6	124
35	PELE:Â Protein Energy Landscape Exploration. A Novel Monte Carlo Based Technique. Journal of Chemical Theory and Computation, 2005, 1, 1304-1311.	5.3	190
36	ISIM: A Program for Grand Canonical Monte Carlo Simulations of the Ionic Environment of Biomolecules. Molecular Simulation, 2004, 30, 45-61.	2.0	21