Vania Calandrini

List of Publications by Year
in descending order

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29	499	567281 15	677142 22
papers	citations	h-index	g-index

30	30	30	701
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Relaxation dynamics of lysozyme in solution under pressure: Combining molecular dynamics simulations and quasielastic neutron scattering. Chemical Physics, 2008, 345, 289-297.	1.9	47
2	Fractional protein dynamics seen by nuclear magnetic resonance spectroscopy: Relating molecular dynamics simulation and experiment. Journal of Chemical Physics, 2010, 133, 145101.	3.0	42
3	nMoldyn - Interfacing spectroscopic experiments, molecular dynamics simulations and models for time correlation functions. Â‰cole ThÃ©matique De La SociÃ©tÃ© FranÃ§aise De La Neutronique, 2011, 12, 201-232.	0.2	38
4	Conformational transition of DNA bound to Hfq probed by infrared spectroscopy. Physical Chemistry Chemical Physics, 2011, 13, 1222-1229.	2.8	34
5	Diffusive dynamics of water in tert-butyl alcohol/water mixtures. Journal of Chemical Physics, 2004, 120, 4759-4767.	3.0	32
6	Platination of the copper transporter ATP7A involved in anticancer drug resistance. Dalton Transactions, 2014, 43, 12085.	3.3	29
7	Rotational and translational dynamics of lysozyme in waterâ€“glycerol solution. Colloids and Surfaces B: Biointerfaces, 2001, 21, 311-316.	5.0	26
8	Estimating the influence of finite instrumental resolution on elastic neutron scattering intensities from proteins. Journal of Chemical Physics, 2007, 126, 125107.	3.0	21
9	Influence of pressure on the slow and fast fractional relaxation dynamics in lysozyme: A simulation study. Journal of Chemical Physics, 2008, 128, 065102.	3.0	21
10	Computational metallomics of the anticancer drug cisplatin. Journal of Inorganic Biochemistry, 2015, 153, 231-238.	3.5	20
11	Open Boundary Simulations of Proteins and Their Hydration Shells by Hamiltonian Adaptive Resolution Scheme. Journal of Chemical Theory and Computation, 2017, 13, 5647-5657.	5.3	20
12	Role of hydrophobic interactions on the stabilisation of native state of globular proteins. Chemical Physics Letters, 2000, 324, 344-348.	2.6	18
13	Molecular Dynamics Simulations of the [2Feâ€“2S] Cluster-Binding Domain of NEET Proteins Reveal Key Molecular Determinants That Induce Their Cluster Transfer/Release. Journal of Physical Chemistry B, 2017, 121, 10648-10656.	2.6	18
14	Protein dynamics from a NMR perspective: Networks of coupled rotators and fractional Brownian dynamics. Journal of Chemical Physics, 2008, 128, 145102.	3.0	16
15	Open-Boundary Molecular Mechanics/Coarse-Grained Framework for Simulations of Low-Resolution G-Protein-Coupled Receptorâ€“Ligand Complexes. Journal of Chemical Theory and Computation, 2019, 15, 2101-2109.	5.3	16
16	Adaptation of Extremophilic Proteins with Temperature and Pressure: Evidence from Initiation Factor 6. Journal of Physical Chemistry B, 2015, 119, 7860-7873.	2.6	15
17	Conformational changes of proteins in aqueous solution induced by temperature in the pre-melting region. Physical Chemistry Chemical Physics, 2001, 3, 3811-3813.	2.8	14
18	Structural Biology of Cisplatin Complexes with Cellular Targets: The Adduct with Human Copper Chaperone Atox1 in Aqueous Solution. Chemistry - A European Journal, 2014, 20, 11719-11725.	3.3	14

#	Article	IF	Citations
19	Effect of Trehalose on Alkaline Transition of Cytochrome-c. Journal of Physical Chemistry B, 2000, 104, 6889-6893.	2.6	13
20	From NMR Relaxation to Fractional Brownian Dynamics in Proteins: Results from a Virtual Experiment. Journal of Physical Chemistry B, 2011, 115, 12370-12379.	2.6	13
21	Effect of 1-alkanols on the native conformation of Lysozyme. Physical Chemistry Chemical Physics, 2000, 2, 4143-4146.	2.8	6
22	Subdiffusive-Brownian crossover in membrane proteins: a Generalized Langevin Equation-based approach. Biophysical Journal, 2021, 120, 4722-4737.	0.5	6
23	Pressure effect on water dynamics in tert-butyl alcohol/water solutions. Journal of Physics Condensed Matter, 2006, 18, S2363-S2371.	1.8	4
24	Structural predictions of neurobiologically relevant G-protein coupled receptors and intrinsically disordered proteins. Archives of Biochemistry and Biophysics, 2015, 582, 91-100.	3.0	4
25	Water dynamics in dilute aqueous solutions of small apolar solutes by quasi-elastic neutron scattering. Applied Physics A: Materials Science and Processing, 2002, 74, s1339-s1341.	2.3	3
26	Role of effective atomic masses in memory function-based models for liquids: A simulation study of liquid water. Journal of Chemical Physics, 2006, 125, 236102.	3.0	3
27	Hydrodynamics of immiscible binary fluids with viscosity contrast: a multiparticle collision dynamics approach. Soft Matter, 2021, 17, 7978-7990.	2.7	3
28	Scaling laws and memory effects in the dynamics of liquids and proteins. Physics of Particles and Nuclei Letters, 2008, 5, 189-195.	0.4	2
29	Rigid Molecule Approximation in Memory Function-based Models for Molecular Liquids: Application to Liquid Water. Zeitschrift Fur Physikalische Chemie, 2009, 223, 957-978.	2.8	1