Franci Merzel

List of Publications by Year
in descending order

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41 papers	1,316 citations	430442 18 h-index	344852 36 g-index
41 all docs	41 docs citations	41 times ranked	1790 citing authors

#	Article	IF	Citations
1	Is the first hydration shell of lysozyme of higher density than bulk water?. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 5378-5383.	3.3	355
2	Origin of hydrophobicity and enhanced water hydrogen bond strength near purely hydrophobic solutes. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 322-327.	3.3	169
3	Structural basis for the multitasking nature of the potato virus Y coat protein. Science Advances, 2019, 5, eaaw3808.	4.7	61
4	Structure, dynamics and reactions of protein hydration water. Philosophical Transactions of the Royal Society B: Biological Sciences, 2004, 359, 1181-1190.	1.8	57
5	SASSIM: a method for calculating small-angle X-ray and neutron scattering and the associated molecular envelope from explicit-atom models of solvated proteins. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 242-249.	2.5	54
6	Molecular dynamics integration and molecular vibrational theory. I. New symplectic integrators. Journal of Chemical Physics, 2005, 122, 174101.	1.2	54
7	Liquid-Ordered Phase Formation in Cholesterol/Sphingomyelin Bilayers: All-Atom Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 15795-15802.	1.2	46
8	Lattice Dynamics of a Protein Crystal. Physical Review Letters, 2007, 99, 138101.	2.9	45
9	Vibrational Softening of a Protein on Ligand Binding. Journal of Physical Chemistry B, 2011, 115, 6811-6817.	1.2	39
10	Increase of both Order and Disorder in the First Hydration Shell with Increasing Solute Polarity. Physical Review Letters, 2011, 107, 267801.	2.9	36
11	An Efficient Symplectic Integration Algorithm for Molecular Dynamics Simulations. Journal of Chemical Information and Computer Sciences, 1995, 35, 321-326.	2.8	35
12	Protein hydration water: Structure and thermodynamics. Journal of Molecular Liquids, 2002, 101, 27-33.	2.3	35
13	Physical Origin Underlying the Entropy Loss upon Hydrophobic Hydration. Journal of the American Chemical Society, 2012, 134, 17574-17581.	6.6	33
14	High-solar-absorptance CSP coating characterization and reliability testing with isothermal and cyclic loads for service-life prediction. Energy and Environmental Science, 2019, 12, 1679-1694.	15.6	33
15	Modus operandi of controlled release from mesoporous matrices: a theoretical perspective. Physical Chemistry Chemical Physics, 2011, 13, 15311.	1.3	24
16	Polymorphisms of CYP51A1 from Cholesterol Synthesis: Associations with Birth Weight and Maternal Lipid Levels and Impact on CYP51 Protein Structure. PLoS ONE, 2013, 8, e82554.	1.1	24
17	High-Density Hydration Layer of Lysozymes:Â Molecular Dynamics Decomposition of Solution Scattering Data. Journal of Chemical Information and Modeling, 2005, 45, 1593-1599.	2.5	23
18	Probing Amyloid-Beta Fibril Stability by Increasing Ionic Strengths. Journal of Physical Chemistry B, 2011, 115, 2075-2081.	1.2	20

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19	Split Integration Symplectic Method for Molecular Dynamics Integration. Journal of Chemical Information and Computer Sciences, 1997, 37, 1048-1054.	2.8	17
20	Quantitative structure-activation barrier relationship modeling for Diels-Alder ligations utilizing quantum chemical structural descriptors. Chemistry Central Journal, 2013, 7, 171.	2.6	16
21	Decoupling between the translation and rotation of water in the proximity of a protein molecule. Physical Chemistry Chemical Physics, 2020, 22, 18132-18140.	1.3	16
22	Allostery and Conformational Dynamics in cAMP-binding Acyltransferases. Journal of Biological Chemistry, 2014, 289, 16588-16600.	1.6	15
23	Why do water molecules around small hydrophobic solutes form stronger hydrogen bonds than in the bulk?. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129537.	1.1	13
24	Nucleotide-Specific Autoinhibition of Full-Length K-Ras4B Identified by Extensive Conformational Sampling. Frontiers in Molecular Biosciences, 2020, 7, 145.	1.6	11
25	NMscatt: a program for calculating inelastic scattering from large biomolecular systems using classical force-field simulations. Computer Physics Communications, 2007, 177, 530-538.	3.0	10
26	New force field for calcium binding sites in annexinâ€“membrane complexes. Journal of Computational Chemistry, 2006, 27, 446-452.	1.5	9
27	The Complexity of Parallel Symplectic Molecular Dynamics Algorithms. Journal of Chemical Information and Computer Sciences, 1997, 37, 1055-1062.	2.8	8
28	Soft Collective Fluctuations Governing Hydrophobic Association. Physical Review Letters, 2013, 111, 127801.	2.9	8
29	The amide III vibrational circular dichroism band as a probe to detect conformational preferences of alanine dipeptide in water. Biopolymers, 2014, 101, 814-818.	1.2	8
30	A novel synthetic luteinizing hormone-releasing hormone (LHRH) analogue coupled with modified Î²-cyclodextrin: Insight into its intramolecular interactions. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 159-168.	1.1	8
31	Evaluation of Selected CYP51A1 Polymorphisms in View of Interactions with Substrate and Redox Partner. Frontiers in Pharmacology, 2017, 8, 417.	1.6	7
32	Spectroscopic Characterization of Omeprazole and Its Salts. Journal of Spectroscopy, 2017, 2017, 1-11.	0.6	5
33	High-temperature â€œion baseballâ€•for enhancing concentrated solar power efficiency. Solar Energy Materials and Solar Cells, 2019, 200, 109974.	3.0	5
34	Endogenous modulators of neurotrophin signaling: Landscape of the transient ATP-NGF interactions. Computational and Structural Biotechnology Journal, 2021, 19, 2938-2949.	1.9	5
35	Ion-size effect within the aqueous solution interface at the Pt(111) surface: molecular dynamics studies. Physical Chemistry Chemical Physics, 2010, 12, 13566.	1.3	4
36	Molecular Dynamics-Derived Pharmacophore Model Explaining the Nonselective Aspect of KV10.1 Pore Blockers. International Journal of Molecular Sciences, 2021, 22, 8999.	1.8	3

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37	Computational Complexity of Split Symplectic MD Integration Method. Advances in Parallel Computing, 1998, 12, 541-548.	0.3	2
38	Long Time Step MD Simulations Using Split Integration Symplectic Method. Lecture Notes in Computational Science and Engineering, 1999, , 332-348.	0.1	2
39	Direct orbital-free calculations using DFT and one-electron Green's functions: applications to atoms. Chemical Physics Letters, 1996, 263, 507-512.	1.2	1
40	Molecular electronic structure problem solved by numerical one-electron Green's functions. International Journal of Quantum Chemistry, 2004, 96, 554-561.	1.0	0
41	Normal modes and neutrons: defining collective, functional biomolecular motions. Neutron News, 2012, 23, 26-30.	0.1	0