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	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
2	Endogenous modulators of neurotrophin signaling: Landscape of the transient ATP-NGF interactions. Computational and Structural Biotechnology Journal, 2021, 19, 2938-2949.	1.9	5
3	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
4	Nucleotide-Specific Autoinhibition of Full-Length K-Ras4B Identified by Extensive Conformational Sampling. Frontiers in Molecular Biosciences, 2020, 7, 145.	1.6	11
5	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
6	Structural basis for the multitasking nature of the potato virus Y coat protein. Science Advances, 2019, 5, eaaw3808.	4.7	61
7	High-temperature â€œion baseballâ€•for enhancing concentrated solar power efficiency. Solar Energy Materials and Solar Cells, 2019, 200, 109974.	3.0	5
8	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
9	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
10	Evaluation of Selected CYP51A1 Polymorphisms in View of Interactions with Substrate and Redox Partner. Frontiers in Pharmacology, 2017, 8, 417.	1.6	7
11	Spectroscopic Characterization of Omeprazole and Its Salts. Journal of Spectroscopy, 2017, 2017, 1-11.	0.6	5
12	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
13	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
14	Allostery and Conformational Dynamics in cAMP-binding Acyltransferases. Journal of Biological Chemistry, 2014, 289, 16588-16600.	1.6	15
15	Soft Collective Fluctuations Governing Hydrophobic Association. Physical Review Letters, 2013, 111, 127801.	2.9	8
16	Quantitative structure-activation barrier relationship modeling for Diels-Alder ligations utilizing quantum chemical structural descriptors. Chemistry Central Journal, 2013, 7, 171.	2.6	16
17	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
18	Normal modes and neutrons: defining collective, functional biomolecular motions. Neutron News, 2012, 23, 26-30.	0.1	0

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19	Physical Origin Underlying the Entropy Loss upon Hydrophobic Hydration. Journal of the American Chemical Society, 2012, 134, 17574-17581.	6.6	33
20	Modus operandi of controlled release from mesoporous matrices: a theoretical perspective. Physical Chemistry Chemical Physics, 2011, 13, 15311.	1.3	24
21	Vibrational Softening of a Protein on Ligand Binding. Journal of Physical Chemistry B, 2011, 115, 6811-6817.	1.2	39
22	Increase of both Order and Disorder in the First Hydration Shell with Increasing Solute Polarity. Physical Review Letters, 2011, 107, 267801.	2.9	36
23	Probing Amyloid-Beta Fibril Stability by Increasing Ionic Strengths. Journal of Physical Chemistry B, 2011, 115, 2075-2081.	1.2	20
24	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
25	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
26	Lattice Dynamics of a Protein Crystal. Physical Review Letters, 2007, 99, 138101.	2.9	45
27	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
28	New force field for calcium binding sites in annexinâ€“membrane complexes. Journal of Computational Chemistry, 2006, 27, 446-452.	1.5	9
29	Molecular dynamics integration and molecular vibrational theory. I. New symplectic integrators. Journal of Chemical Physics, 2005, 122, 174101.	1.2	54
30	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
31	Structure, dynamics and reactions of protein hydration water. Philosophical Transactions of the Royal Society B: Biological Sciences, 2004, 359, 1181-1190.	1.8	57
32	Molecular electronic structure problem solved by numerical one-electron Green's functions. International Journal of Quantum Chemistry, 2004, 96, 554-561.	1.0	0
33	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
34	Protein hydration water: Structure and thermodynamics. Journal of Molecular Liquids, 2002, 101, 27-33.	2.3	35
35	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
36	Long Time Step MD Simulations Using Split Integration Symplectic Method. Lecture Notes in Computational Science and Engineering, 1999, , 332-348.	0.1	2

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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	Split Integration Symplectic Method for Molecular Dynamics Integration. Journal of Chemical Information and Computer Sciences, 1997, 37, 1048-1054.	2.8	17
39	The Complexity of Parallel Symplectic Molecular Dynamics Algorithms. Journal of Chemical Information and Computer Sciences, 1997, 37, 1055-1062.	2.8	8
40	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
41	An Efficient Symplectic Integration Algorithm for Molecular Dynamics Simulations. Journal of Chemical Information and Computer Sciences, 1995, 35, 321-326.	2.8	35