Bogdan Lesyng

List of Publications by Year
in descending order

22	463	759233 12	794594 19
papers	citations	h-index	g-index

22	22	22	694
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Structural characterisation of inhibitory and non-inhibitory MMP-9â€“TIMP-1 complexes and implications for regulatory mechanisms of MMP-9. Scientific Reports, 2021, 11, 13376.	3.3	18
2	Exploring Covalent Docking Mechanisms of Boron-Based Inhibitors to Class A, C and D Î²-Lactamases Using Time-dependent Hybrid QM/MM Simulations. Frontiers in Molecular Biosciences, 2021, 8, 633181.	3.5	4
3	DAMA: a method for computing multiple alignments of protein structures using local structure descriptors. Bioinformatics, 2021, , .	4.1	2
4	A novel formulation of an approximate valence bond model (AVB2) and its application to the tautomeric forms of porphyrin and porphycene. Journal of Molecular Modeling, 2019, 25, 155.	1.8	0
5	Synthesis, structural and antimicrobial studies of type II topoisomerase-targeted copper(II) complexes of 1,3-disubstituted thiourea ligands. Journal of Inorganic Biochemistry, 2018, 182, 61-70.	3.5	25
6	Surface markers of cancer stem-like cells of ovarian cancer and their clinical relevance. Wspolczesna Onkologia, 2018, 2018, 48-55.	1.4	30
7	ResiCon: a method for the identification of dynamic domains, hinges and interfacial regions in proteins. Bioinformatics, 2016, 32, 25-34.	4.1	10
8	Toward the identification of molecular cogs. Journal of Computational Chemistry, 2016, 37, 848-860.	3.3	0
9	A novel method to compare protein structures using local descriptors. BMC Bioinformatics, 2011, 12, 344.	2.6	25
10	Parallelization of the quantum dynamics code for cluster architecture and its applications to the Gross-Pitaevskii equation. International Journal of Quantum Chemistry, 2006, 106, 664-669.	2.0	0
11	Generalized Born Model:Â Analysis, Refinement, and Applications to Proteins. Journal of Physical Chemistry B, 2004, 108, 18368-18376.	2.6	115
12	Class IV Charge Model for the Self-Consistent Charge Density-Functional Tight-Binding Method. Journal of Physical Chemistry A, 2004, 108, 2545-2549.	2.5	51
13	DFT calculations and parameterization of the approximate valence bond method to describe the phosphoryl transfer reaction in a model system. International Journal of Quantum Chemistry, 2002, 90, 1129-1139.	2.0	3
14	Structural basis of oncogenic activation caused by point mutations in the kinase domain of the MET proto-oncogene: Modeling studies. Proteins: Structure, Function and Bioinformatics, 2001, 44, 32-43.	2.6	60
15	Structure-based sequence alignment for the Î²-trefoil subdomain of the clostridial neurotoxin family provides residue level information about the putative ganglioside binding site. FEBS Letters, 2000, 482, 119-124.	2.8	39
16	A Mezoscopic Model of Nucleic Acids. Part 1. Lagrangian and Quaternion Molecular Dynamics. Journal of Biomolecular Structure and Dynamics, 2000, 17, 1097-1108.	3.5	15
17	A Mezoscopic Model of Nucleic Acids. Part 2. An Effective Potential Energy Function for DNA. Journal of Biomolecular Structure and Dynamics, 2000, 17, 1109-1115.	3.5	11
18	Conformational Correlations in DNA. Molecular Dynamics Studies. Molecular Simulation, 1997, 19, 247-266.	2.0	3

#	Article	IF	Citations
19	Lagrangian molecular dynamics using selected conformational degrees of freedom, with application to the pseudorotation dynamics of furanose rings. Biopolymers, 1994, 34, 383-392.	2.4	16
20	Why isoguanine and isocytosine are not the components of the genetic code. International Journal of Quantum Chemistry, 1985, 28, 209-216.	2.0	6
21	The Tautomerism of Cytosine and Hydroxycytosine. A Quantum-Mechanical Study. Zeitschrift Fur Naturforschung - Section C Journal of Biosciences, 1982, 37, 937-941.	1.4	15
22	Effect of water on the tautomeric equilibrium of 2-oxopyridine. A Monte Carlo simulation study. International Journal of Quantum Chemistry, 1981, 20, 359-364.	2.0	15