

Artur Geldon

List of Publications by Year in descending order

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53
papers

861
citations

471371

17
h-index

580701

25
g-index

53
all docs

53
docs citations

53
times ranked

1097
citing authors

#	ARTICLE	IF	CITATIONS
1	Prediction of protein assemblies, the next frontier: The <sc>CASP14â€œCAPRI</sc> experiment. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1800-1823.	1.5	73
2	Structural insights into the activation mechanisms of human HtrA serine proteases. Archives of Biochemistry and Biophysics, 2017, 621, 6-23.	1.4	53
3	Performance of protein-structure predictions with the physics-based UNRES force field in CASP11. Bioinformatics, 2016, 32, 3270-3278.	1.8	44
4	Analysis of interactions responsible for vasopressin binding to human neurohypophyseal hormone receptorsâ€œ” molecular dynamics study of the activated receptorâ€œ” vasopressinâ€œ”G± systems. Journal of Peptide Science, 2006, 12, 180-189.	0.8	33
5	Temperature-induced changes of HtrA2(Omi) protease activity and structure. Cell Stress and Chaperones, 2013, 18, 35-51.	1.2	33
6	Preliminary studies on trigonelline as potential anti-Alzheimer disease agent: Determination by hydrophilic interaction liquid chromatography and modeling of interactions with beta-amyloid. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2014, 968, 101-104.	1.2	33
7	Temperature-dependent structure-property modeling of viscosity for ionic liquids. Fluid Phase Equilibria, 2016, 427, 9-17.	1.4	32
8	3-[2-(8-Quinoliny)benzoxazol-5-yl]alanine derivativeâ€œ”a specific fluorophore for transition and rare-earth metal ion detection. Tetrahedron, 2004, 60, 11889-11894.	1.0	27
9	Prediction of protein structure with the coarseâ€œgrained UNRES force field assisted by small Xâ€œray scattering data and knowledgeâ€œbased information. Proteins: Structure, Function and Bioinformatics, 2018, 86, 228-239.	1.5	26
10	Theoretical Study of Polymerization Mechanism of <i>p</i>-Xylylene Based Polymers. Journal of Physical Chemistry A, 2010, 114, 4296-4303.	1.1	25
11	Crystal structure of a low molecular weight activator Blm-pep with yeast 20S proteasome â€œ” insights into the enzyme activation mechanism. Scientific Reports, 2017, 7, 6177.	1.6	23
12	Molecular modeling of interactions of the non-peptide antagonist YM087 with the human vasopressin V1a, V2 receptors and with oxytocin receptors. Journal of Computer-Aided Molecular Design, 2001, 15, 1085-1104.	1.3	22
13	The LA Loop as an Important Regulatory Element of the HtrA (DegP) Protease from Escherichia coli. Journal of Biological Chemistry, 2014, 289, 15880-15893.	1.6	22
14	Structure-based design and in vivo anti-arthritis activity evaluation of a potent dipeptidyl cyclopropyl nitrile inhibitor of cathepsin C. Biochemical Pharmacology, 2019, 164, 349-367.	2.0	21
15	Scale-consistent approach to the derivation of coarse-grained force fields for simulating structure, dynamics, and thermodynamics of biopolymers. Progress in Molecular Biology and Translational Science, 2020, 170, 73-122.	0.9	20
16	Temperature-induced conformational changes within the regulatory loops L1â€œ”L2â€œ”LA of the HtrA heat-shock protease from Escherichia coli. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2009, 1794, 1573-1582.	1.1	19
17	Use of the UNRES force field in template-assisted prediction of protein structures and the refinement of server models: Test with CASP12 targets. Journal of Molecular Graphics and Modelling, 2018, 83, 92-99.	1.3	19
18	An analysis and evaluation of the WeFold collaborative for protein structure prediction and its pipelines in CASP11 and CASP12. Scientific Reports, 2018, 8, 9939.	1.6	19

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19	Evaluation of the scale-consistent UNRES force field in template-free prediction of protein structures in the CASP13 experiment. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 92, 154-166.	1.3	19
20	An enormously active and selective azapeptide inhibitor of cathepsin B. <i>Journal of Peptide Science</i> , 2007, 13, 536-543.	0.8	18
21	Anti-inflammatory effect of novel analogs of natural enkephalinase inhibitors in a mouse model of experimental colitis. <i>Future Medicinal Chemistry</i> , 2016, 8, 2231-2243.	1.1	17
22	Theoretical calculation of the physico-chemical properties of 1-butyl-4-methylpyridinium based ionic liquids. <i>Journal of Molecular Liquids</i> , 2017, 225, 467-474.	2.3	17
23	Modeling protein structures with the coarse-grained UNRES force field in the CASP14 experiment. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 108, 108008.	1.3	17
24	Cathepsin C inhibition as a potential treatment strategy in cancer. <i>Biochemical Pharmacology</i> , 2021, 194, 114803.	2.0	17
25	A new protein nucleic acid coarse-grained force field based on the UNRES and NARES2P force fields. <i>Journal of Computational Chemistry</i> , 2018, 39, 2360-2370.	1.5	16
26	Theoretical Calculations of Heteroconjugation Equilibrium Constants in Systems Modeling Acid-Base Interactions in Side Chains of Biomolecules Using the Potential of Mean Force. <i>Journal of Physical Chemistry B</i> , 2004, 108, 12222-12230.	1.2	15
27	RASMOL AB - New functionalities in the program for structure analysis. <i>Acta Biochimica Polonica</i> , 2015, 62, 629-631.	0.3	14
28	Distinct 3D Architecture and Dynamics of the Human HtrA2(Omi) Protease and Its Mutated Variants. <i>PLoS ONE</i> , 2016, 11, e0161526.	1.1	14
29	Study of New Oxytocin Antagonist Barusiban (Fe200 440) Affinity Toward Human Oxytocin Receptor Versus Vasopressin V1a and V2 Receptors - Molecular Dynamics Simulation in POPC Bilayer. <i>QSAR and Combinatorial Science</i> , 2005, 24, 603-610.	1.5	12
30	Biochemical properties of the HtrA homolog from bacterium <i>Stenotrophomonas maltophilia</i> . <i>International Journal of Biological Macromolecules</i> , 2018, 109, 992-1005.	3.6	12
31	Processing and Maturation of Cathepsin C Zymogen: A Biochemical and Molecular Modeling Analysis. <i>International Journal of Molecular Sciences</i> , 2019, 20, 4747.	1.8	12
32	Improved Consensus-Fragment Selection in Template-Assisted Prediction of Protein Structures with the UNRES Force Field in CASP13. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1844-1864.	2.5	11
33	Theoretical Study of the Human Bradykinin-Bradykinin B2 Receptor Complex. <i>ChemBioChem</i> , 2008, 9, 2487-2497.	1.3	10
34	Molecular dynamics of protein A and a WW domain with a united-residue model including hydrodynamic interaction. <i>Journal of Chemical Physics</i> , 2016, 144, 184110.	1.2	10
35	PEGylated substrates of NSP4 protease: A tool to study protease specificity. <i>Scientific Reports</i> , 2016, 6, 22856.	1.6	10
36	Introduction of Phosphorylated Residues into the UNRES Coarse-Grained Model: Toward Modeling of Signaling Processes. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5721-5729.	1.2	10

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37	Alanine scan of sialorphin and its hybrids with opiorphin: synthesis, molecular modelling and effect on enkephalins degradation. <i>Amino Acids</i> , 2018, 50, 1083-1088.	1.2	9
38	The <sc>LD</sc> loop as an important structural element required for transmission of the allosteric signal in the HtrA (DegP) protease from <i>Escherichia coli</i> . <i>FEBS Journal</i> , 2016, 283, 3471-3487.	2.2	8
39	Molecular dynamics study of 4-OH-phenylacetyl- D -Y(Me)FQNRPR-NH 2 selectivity to V1a receptor. <i>Journal of Molecular Modeling</i> , 2003, 9, 372-378.	0.8	7
40	Theoretical study on binding of S100B protein. <i>Journal of Molecular Modeling</i> , 2007, 13, 1123-1131.	0.8	7
41	1-Substituted sialorphin analogues synthesis, molecular modelling and in vitro effect on enkephalins degradation by NEP. <i>Amino Acids</i> , 2019, 51, 1201-1207.	1.2	6
42	The role of the L2 loop in the regulation and maintaining the proteolytic activity of HtrA (DegP) protein from <i>Escherichia coli</i> . <i>Archives of Biochemistry and Biophysics</i> , 2010, 500, 123-130.	1.4	5
43	Impact of selected amino acids of HP0377 (<i>Helicobacter pylori</i> thiol oxidoreductase) on its functioning as a CcmG (cytochrome c maturation) protein and Dsb (disulfide bond) isomerase. <i>PLoS ONE</i> , 2018, 13, e0195358.	1.1	5
44	Molecular dynamics simulations of the growth of poly(chloro-para-xylylene) films. <i>Journal of Molecular Modeling</i> , 2011, 17, 2725-2733.	0.8	4
45	A Peptidomimetic Fluorescent Probe to Detect the Trypsin β 2 Subunit of the Human 20S Proteasome. <i>International Journal of Molecular Sciences</i> , 2020, 21, 2396.	1.8	4
46	Polymerization of chloro-p-xylylenes, quantum-chemical study. <i>Journal of Molecular Modeling</i> , 2017, 23, 40.	0.8	2
47	Influence of Temperature and Salt Concentration on the Hydrophobic Interactions of Adamantane and Hexane. <i>Journal of Physical Chemistry B</i> , 2022, 126, 634-642.	1.2	2
48	Theoretical Investigation of the Coronavirus SARS-CoV-2 (COVID-19) Infection Mechanism and Selectivity. <i>Molecules</i> , 2022, 27, 2080.	1.7	2
49	Low-Molecular Pyrazine-Based DNA Binders: Physicochemical and Antimicrobial Properties. <i>Molecules</i> , 2022, 27, 3704.	1.7	2
50	Molecular dynamics simulation of polymerization of p-xylylene. , 2012, , .		1
51	Selection of Effective HTRA3 Activators Using Combinatorial Chemistry. <i>ACS Combinatorial Science</i> , 2017, 19, 565-573.	3.8	1
52	Peptidomimetics Based on C-Terminus of Blm10 Stimulate Human 20S Proteasome Activity and Promote Degradation of Proteins. <i>Biomolecules</i> , 2022, 12, 777.	1.8	1
53	Determination of the Binding Sites of Activators within the Proteasome Structure. <i>Proceedings (mdpi)</i> , 2019, 22, .	0.2	0