

Marco Agostino Deriu

List of Publications by Year in descending order

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Version: 2024-02-01

93
papers

1,970
citations

236833

25
h-index

289141

40
g-index

101
all docs

101
docs citations

101
times ranked

2592
citing authors

#	ARTICLE	IF	CITATIONS
1	Machine learning-based prediction of adverse events following an acute coronary syndrome (PRAISE): a modelling study of pooled datasets. <i>Lancet, The</i> , 2021, 397, 199-207.	6.3	164
2	On the Use of In Vivo Measured Flow Rates as Boundary Conditions for Image-Based Hemodynamic Models of the Human Aorta: Implications for Indicators of Abnormal Flow. <i>Annals of Biomedical Engineering</i> , 2012, 40, 729-741.	1.3	126
3	On the importance of blood rheology for bulk flow in hemodynamic models of the carotid bifurcation. <i>Journal of Biomechanics</i> , 2011, 44, 2427-2438.	0.9	93
4	Anisotropic Elastic Network Modeling of Entire Microtubules. <i>Biophysical Journal</i> , 2010, 99, 2190-2199.	0.2	91
5	Outflow Conditions for Image-Based Hemodynamic Models of the Carotid Bifurcation: Implications for Indicators of Abnormal Flow. <i>Journal of Biomechanical Engineering</i> , 2010, 132, 091005.	0.6	80
6	A Survey of Methods for the Evaluation of Tissue Engineering Scaffold Permeability. <i>Annals of Biomedical Engineering</i> , 2013, 41, 2027-2041.	1.3	74
7	A rational approach to defining principal axes of multidirectional wall shear stress in realistic vascular geometries, with application to the study of the influence of helical flow on wall shear stress directionality in aorta. <i>Journal of Biomechanics</i> , 2015, 48, 899-906.	0.9	71
8	When Stiffness Matters: Mechanosensing in Heart Development and Disease. <i>Frontiers in Cell and Developmental Biology</i> , 2020, 8, 334.	1.8	50
9	Tubulin: from atomistic structure to supramolecular mechanical properties. <i>Journal of Materials Science</i> , 2007, 42, 8864-8872.	1.7	45
10	A Versatile Bioreactor for Dynamic Suspension Cell Culture. Application to the Culture of Cancer Cell Spheroids. <i>PLoS ONE</i> , 2016, 11, e0154610.	1.1	45
11	The Extent of Human Apolipoprotein A-I Lipidation Strongly Affects the β -Amyloid Efflux Across the Blood-Brain Barrier in vitro. <i>Frontiers in Neuroscience</i> , 2019, 13, 419.	1.4	42
12	Cell penetrating peptide modulation of membrane biomechanics by Molecular dynamics. <i>Journal of Biomechanics</i> , 2018, 73, 137-144.	0.9	40
13	Bioreactors as Engineering Support to Treat Cardiac Muscle and Vascular Disease. <i>Journal of Healthcare Engineering</i> , 2013, 4, 329-370.	1.1	38
14	A Machine Learning Approach for Mortality Prediction in COVID-19 Pneumonia: Development and Evaluation of the Piacenza Score. <i>Journal of Medical Internet Research</i> , 2021, 23, e29058.	2.1	36
15	Biomechanics of actin filaments: A computational multi-level study. <i>Journal of Biomechanics</i> , 2011, 44, 630-636.	0.9	33
16	Cell Penetrating Peptide Adsorption on Magnetite and Silica Surfaces: A Computational Investigation. <i>Journal of Physical Chemistry B</i> , 2015, 119, 8239-8246.	1.2	33
17	Multiscale impact of nucleotides and cations on the conformational equilibrium, elasticity and rheology of actin filaments and crosslinked networks. <i>Biomechanics and Modeling in Mechanobiology</i> , 2015, 14, 1143-1155.	1.4	31
18	Genetic, cellular, and structural characterization of the membrane potential-dependent cell-penetrating peptide translocation pore. <i>ELife</i> , 2021, 10, .	2.8	31

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19	Multiscale modeling of cellular actin filaments: From atomistic molecular to coarse-grained dynamics. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012, 80, 1598-1609.	1.5	30
20	Conformational fluctuations of the AXH monomer of Ataxin-1. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 52-59.	1.5	30
21	Conformational Dynamics and Stability of U-Shaped and S-Shaped Amyloid β Assemblies. <i>International Journal of Molecular Sciences</i> , 2018, 19, 571.	1.8	30
22	Investigation of the Josephin Domain Protein-Protein Interaction by Molecular Dynamics. <i>PLoS ONE</i> , 2014, 9, e108677.	1.1	28
23	Electro-Acoustic Behavior of the Mitotic Spindle: A Semi-Classical Coarse-Grained Model. <i>PLoS ONE</i> , 2014, 9, e86501.	1.1	28
24	Structure Based Modeling of Small Molecules Binding to the TLR7 by Atomistic Level Simulations. <i>Molecules</i> , 2015, 20, 8316-8340.	1.7	27
25	Multivalent interacting glycodendrimer to prevent amyloid-peptide fibril formation induced by Cu(II): A multidisciplinary approach. <i>Nano Research</i> , 2018, 11, 1204-1226.	5.8	27
26	Mechanical Model of the Tubulin Dimer Based on Molecular Dynamics Simulations. <i>Journal of Biomechanical Engineering</i> , 2008, 130, 041008.	0.6	26
27	Mechanical response and conformational changes of alpha-actinin domains during unfolding: a molecular dynamics study. <i>Biomechanics and Modeling in Mechanobiology</i> , 2007, 6, 399-407.	1.4	25
28	Numerical and experimental characterization of a novel modular passive micromixer. <i>Biomedical Microdevices</i> , 2012, 14, 849-862.	1.4	25
29	Free energy landscape of siRNA-polycation complexation: Elucidating the effect of molecular geometry, polymer flexibility, and charge neutralization. <i>PLoS ONE</i> , 2017, 12, e0186816.	1.1	25
30	A Hydrophobic Gold Surface Triggers Misfolding and Aggregation of the Amyloidogenic Josephin Domain in Monomeric Form, While Leaving the Oligomers Unaffected. <i>PLoS ONE</i> , 2013, 8, e58794.	1.1	24
31	Insights into the Effect of the G245S Single Point Mutation on the Structure of p53 and the Binding of the Protein to DNA. <i>Molecules</i> , 2017, 22, 1358.	1.7	23
32	Josephin Domain Structural Conformations Explored by Metadynamics in Essential Coordinates. <i>PLoS Computational Biology</i> , 2016, 12, e1004699.	1.5	22
33	Deformation pattern in vibrating microtubule: Structural mechanics study based on an atomistic approach. <i>Scientific Reports</i> , 2017, 7, 4227.	1.6	22
34	Characterization of the <sc>AXH</sc> domain of Ataxin-1 using enhanced sampling and functional mode analysis. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 666-673.	1.5	21
35	The Role of Structural Polymorphism in Driving the Mechanical Performance of the Alzheimer's Beta Amyloid Fibrils. <i>Frontiers in Bioengineering and Biotechnology</i> , 2019, 7, 83.	2.0	21
36	Cardiovascular Risk Prediction in Ankylosing Spondylitis: From Traditional Scores to Machine Learning Assessment. <i>Rheumatology and Therapy</i> , 2020, 7, 867-882.	1.1	21

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37	Elucidating the role of surface chemistry on cationic phosphorus dendrimer-siRNA complexation. <i>Nanoscale</i> , 2018, 10, 10952-10962.	2.8	20
38	The synergistic effect of chlorotoxin-mApoE in boosting drug-loaded liposomes across the BBB. <i>Journal of Nanobiotechnology</i> , 2019, 17, 115.	4.2	20
39	Iron oxide/PAMAM nanostructured hybrids: combined computational and experimental studies. <i>Journal of Materials Science</i> , 2016, 51, 1996-2007.	1.7	18
40	The Impact of Natural Compounds on S-Shaped A β 242 Fibril: From Molecular Docking to Biophysical Characterization. <i>International Journal of Molecular Sciences</i> , 2020, 21, 2017.	1.8	18
41	On the human taste perception: Molecular-level understanding empowered by computational methods. <i>Trends in Food Science and Technology</i> , 2021, 116, 445-459.	7.8	17
42	Fludarabine-Specific Molecular Interactions with Maltose-Modified Poly(propyleneimine) Dendrimer Enable Effective Cell Entry of the Active Drug Form: Comparison with Clofarabine. <i>Biomacromolecules</i> , 2019, 20, 1429-1442.	2.6	16
43	A machine-learning approach to cardiovascular risk prediction in psoriatic arthritis. <i>Rheumatology</i> , 2020, 59, 1767-1769.	0.9	16
44	Exploration of Spanish Olive Oil Quality with a Miniaturized Low-Cost Fluorescence Sensor and Machine Learning Techniques. <i>Foods</i> , 2021, 10, 1010.	1.9	16
45	A molecular dynamics study of a miRNA:mRNA interaction. <i>Journal of Molecular Modeling</i> , 2011, 17, 2895-2906.	0.8	15
46	Identification of a model of non-esterified fatty acids dynamics through genetic algorithms: The case of women with a history of gestational diabetes. <i>Computers in Biology and Medicine</i> , 2011, 41, 146-153.	3.9	15
47	Thermodynamic and kinetic stability of the Josephin Domain closed arrangement: evidences from replica exchange molecular dynamics. <i>Biology Direct</i> , 2017, 12, 2.	1.9	15
48	Biofunctionalization of Silica Nanoparticles with Cell-Penetrating Peptides: Adsorption Mechanism and Binding Energy Estimation. <i>Journal of Physical Chemistry B</i> , 2019, 123, 10622-10630.	1.2	15
49	In silico Investigations of the Mode of Action of Novel Colchicine Derivatives Targeting β -Tubulin Isotypes: A Search for a Selective and Specific β -III Tubulin Ligand. <i>Frontiers in Chemistry</i> , 2020, 8, 108.	1.8	15
50	Destabilizing the AXH Tetramer by Mutations: Mechanisms and Potential Antiaggregation Strategies. <i>Biophysical Journal</i> , 2018, 114, 323-330.	0.2	14
51	Virtual screening using covalent docking to find activators for G245S mutant p53. <i>PLoS ONE</i> , 2018, 13, e0200769.	1.1	12
52	Noncovalent Interactions with PAMAM and PPI Dendrimers Promote the Cellular Uptake and Photodynamic Activity of Rose Bengal: The Role of the Dendrimer Structure. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 15758-15771.	2.9	11
53	In Silico Analysis of the Multi-Targeted Mode of Action of Ivermectin and Related Compounds. <i>Computation</i> , 2022, 10, 51.	1.0	9
54	A survey on computational taste predictors. <i>European Food Research and Technology</i> , 2022, 248, 2215-2235.	1.6	9

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55	Aminoacid substitutions in the glycine zipper affect the conformational stability of amyloid beta fibrils. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 3908-3915.	2.0	8
56	Ultrasonic waves effect on S-shaped β -amyloids conformational dynamics by non-equilibrium molecular dynamics. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 96, 107518.	1.3	8
57	Fragmented blind docking: a novel protein-ligand binding prediction protocol. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 13472-13481.	2.0	8
58	MICROTUBULE-KINESIN MECHANICS BY MOLECULAR MODELING. <i>Biophysical Reviews and Letters</i> , 2009, 04, 45-61.	0.9	7
59	Electric field generated by longitudinal axial microtubule vibration modes with high spatial resolution microtubule model. <i>Journal of Physics: Conference Series</i> , 2011, 329, 012013.	0.3	7
60	Explaining the Microtubule Energy Balance: Contributions Due to Dipole Moments, Charges, van der Waals and Solvation Energy. <i>International Journal of Molecular Sciences</i> , 2017, 18, 2042.	1.8	7
61	Enhancing the activity of platinum-based drugs by improved inhibitors of ERCC1-XPF-mediated DNA repair. <i>Cancer Chemotherapy and Pharmacology</i> , 2021, 87, 259-267.	1.1	7
62	Alteration of lipid bilayer mechanics by volatile anesthetics: Insights from μ s-long molecular dynamics simulations. <i>IScience</i> , 2022, 25, 103946.	1.9	7
63	Computational Study of Potential Galectin-3 Inhibitors in the Treatment of COVID-19. <i>Biomedicines</i> , 2021, 9, 1208.	1.4	6
64	ALS2-Related Motor Neuron Diseases: From Symptoms to Molecules. <i>Biology</i> , 2022, 11, 77.	1.3	6
65	Self-Assembled Ligands Targeting TLR7: A Molecular Level Investigation. <i>Langmuir</i> , 2017, 33, 14460-14471.	1.6	5
66	Using the Gibbs Function as a Measure of Human Brain Development Trends from Fetal Stage to Advanced Age. <i>International Journal of Molecular Sciences</i> , 2020, 21, 1116.	1.8	5
67	Prediction of Protein-Protein Interactions Between Alsin DH/PH and Rac1 and Resulting Protein Dynamics. <i>Frontiers in Molecular Neuroscience</i> , 2021, 14, 772122.	1.4	5
68	Modeling methodology for defining a priori the hydrodynamics of a dynamic suspension bioreactor. Application to human induced pluripotent stem cell culture. <i>Journal of Biomechanics</i> , 2019, 94, 99-106.	0.9	4
69	Insights into the interaction dynamics between volatile anesthetics and tubulin through computational molecular modelling. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 7324-7338.	2.0	4
70	Coarse Grain Modeling for Microtubule Mechanics. <i>Materials Science Forum</i> , 2010, 638-642, 629-634.	0.3	3
71	A Novel Interaction Between the TLR7 and a Colchicine Derivative Revealed Through a Computational and Experimental Study. <i>Pharmaceuticals</i> , 2018, 11, 22.	1.7	3
72	Protein Environment: A Crucial Triggering Factor in Josephin Domain Aggregation: The Role of 2,2,2-Trifluoroethanol. <i>International Journal of Molecular Sciences</i> , 2018, 19, 2151.	1.8	3

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73	A Survey of Quantitative Descriptors of Arterial Flows. Lecture Notes in Computational Vision and Biomechanics, 2014, , 1-24.	0.5	3
74	Microtubule Electrodynamics Associated with Vibrational Normal Modes. Biophysical Journal, 2015, 108, 449a.	0.2	2
75	A Survey of Microchannel Geometries for Mixing of Species in Biomicrofluidics. , 2012, , 548-578.		2
76	In silico investigation of Alsin RLD conformational dynamics and phosphoinositides binding mechanism. PLoS ONE, 2022, 17, e0270955.	1.1	2
77	Multiscale Modeling of Microtubules and Actin Filaments. IFAC Postprint Volumes IPPV / International Federation of Automatic Control, 2012, 45, 1023-1028.	0.4	1
78	A Model-Agnostic Algorithm for Bayes Error Determination in Binary Classification. Algorithms, 2021, 14, 301.	1.2	1
79	On the Use of In Vivo Measured Flow Rates as Boundary Conditions for Image-Based Hemodynamic Models of the Human Aorta. , 2011, , .		1
80	Cardiovascular risk prediction: from classical statistical methods to machine learning approaches. Minerva Cardiology and Angiology, 2022, 70, 102-122.	0.4	1
81	Alteration of Consciousness by Anaesthetics: A Multiscale Modulation from the Molecular to the Systems Level. Journal of Consciousness Studies, 2022, 29, 21-49.	0.4	1
82	Mechanical Properties of Tubulin Molecules by Molecular Dynamics Simulations. , 2006, , 587.		0
83	Bottom-Up Mesoscale Model of Microtubule. , 2007, , 345.		0
84	Identification of Atheroprone Morphological Features in Wall Shear Stress Waveforms in Carotid Bifurcations: A CFD-Based Integrated Approach. , 2010, , .		0
85	Insights Into the Molecular Mechanisms of Actin Dynamics: A Multiscale Modeling Approach. , 2011, , .		0
86	Scale/Physics/Time Properties and Functions in Bioartificial Systems. Materials Science Forum, 0, 706-709, 121-126.	0.3	0
87	A Virtual Test Bench to Study Transport Phenomena in 3D Porous Scaffolds Using Lattice Boltzmann Simulations. , 2013, , .		0
88	Deformability of Microtubules: An Atomistic Computational Study. Biophysical Journal, 2016, 110, 131a.	0.2	0
89	Computational molecular modelling as a platform for a deeper understanding of protein dynamics and rational drug design. Biomedical Science and Engineering, 2020, , .	0.0	0
90	Elastic Network Normal Mode Analysis for Microtubule Mechanics. , 2009, , .		0

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91	Elastic Network Modeling of Actin Filaments. , 2010, , .		0
92	On the Importance of Assumptions for Bulk Flow in Hemodynamic Models of the Carotid Bifurcation. , 2011, , .		0
93	Multiscale Biomechanics of Actin Filaments and Crosslinked Networks. , 2012, , .		0