Marco Agostino Deriu

List of Publications by Year
in descending order

93 papers	1,970 citations	236925 25 h-index	289244 40 g-index
101 all docs	101 docs citations	101 times ranked	2592 citing authors

#	Article	IF	Citations
1	Insights into the interaction dynamics between volatile anesthetics and tubulin through computational molecular modelling. Journal of Biomolecular Structure and Dynamics, 2022, 40, 7324-7338.	3.5	4
2	Fragmented blind docking: a novel proteinâ€“ligand binding prediction protocol. Journal of Biomolecular Structure and Dynamics, 2022, 40, 13472-13481.	3.5	8
3	ALS2-Related Motor Neuron Diseases: From Symptoms to Molecules. Biology, 2022, 11, 77.	2.8	6
4	Alteration of lipid bilayer mechanics by volatile anesthetics: Insights from Î¼s-long molecular dynamics simulations. IScience, 2022, 25, 103946.	4.1	7
5	Cardiovascular risk prediction: from classical statistical methods to machine learning approaches. Minerva Cardiology and Angiology, 2022, 70, 102-122.	0.7	1
6	In Silico Analysis of the Multi-Targeted Mode of Action of Ivermectin and Related Compounds. Computation, 2022, 10, 51.	2.0	9
7	A survey on computational taste predictors. European Food Research and Technology, 2022, 248, 2215-2235.	3.3	9
8	Alteration of Consciousness by Anaesthetics: A Multiscale Modulation from the Molecular to the Systems Level. Journal of Consciousness Studies, 2022, 29, 21-49.	0.7	1
9	In silico investigation of Alsin RLD conformational dynamics and phosphoinositides binding mechanism. PLoS ONE, 2022, 17, e0270955.	2.5	2
10	Enhancing the activity of platinum-based drugs by improved inhibitors of ERCC1â€“XPF-mediated DNA repair. Cancer Chemotherapy and Pharmacology, 2021, 87, 259-267.	2.3	7
11	Machine learning-based prediction of adverse events following an acute coronary syndrome (PRAISE): a modelling study of pooled datasets. Lancet, The, 2021, 397, 199-207.	13.7	164
12	Exploration of Spanish Olive Oil Quality with a Miniaturized Low-Cost Fluorescence Sensor and Machine Learning Techniques. Foods, 2021, 10, 1010.	4.3	16
13	A Machine Learning Approach for Mortality Prediction in COVID-19 Pneumonia: Development and Evaluation of the Piacenza Score. Journal of Medical Internet Research, 2021, 23, e29058.	4.3	36
14	Computational Study of Potential Galectin-3 Inhibitors in the Treatment of COVID-19. Biomedicines, 2021, 9, 1208.	3.2	6
15	Noncovalent Interactions with PAMAM and PPI Dendrimers Promote the Cellular Uptake and Photodynamic Activity of Rose Bengal: The Role of the Dendrimer Structure. Journal of Medicinal Chemistry, 2021, 64, 15758-15771.	6.4	11
16	On the human taste perception: Molecular-level understanding empowered by computational methods. Trends in Food Science and Technology, 2021, 116, 445-459.	15.1	17
17	A Model-Agnostic Algorithm for Bayes Error Determination in Binary Classification. Algorithms, 2021, 14, 301.	2.1	1
18	Genetic, cellular, and structural characterization of the membrane potential-dependent cell-penetrating peptide translocation pore. ELife, 2021, 10, .	6.0	31

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19	Prediction of Proteinâ€“Protein Interactions Between Alsin DH/PH and Rac1 and Resulting Protein Dynamics. Frontiers in Molecular Neuroscience, 2021, 14, 772122.	2.9	5
20	Aminoacid substitutions in the glycine zipper affect the conformational stability of amyloid beta fibrils. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3908-3915.	3.5	8
21	Ultrasonic waves effect on S-shaped Î²-amyloids conformational dynamics by non-equilibrium molecular dynamics. Journal of Molecular Graphics and Modelling, 2020, 96, 107518.	2.4	8
22	Cardiovascular Risk Prediction in Ankylosing Spondylitis: From Traditional Scores to Machine Learning Assessment. Rheumatology and Therapy, 2020, 7, 867-882.	2.3	21
23	The Impact of Natural Compounds on S-Shaped AÎ²42 Fibril: From Molecular Docking to Biophysical Characterization. International Journal of Molecular Sciences, 2020, 21, 2017.	4.1	18
24	In silico Investigations of the Mode of Action of Novel Colchicine Derivatives Targeting Î²-Tubulin Isotypes: A Search for a Selective and Specific Î²-III Tubulin Ligand. Frontiers in Chemistry, 2020, 8, 108.	3.6	15
25	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
26	Using the Gibbs Function as a Measure of Human Brain Development Trends from Fetal Stage to Advanced Age. International Journal of Molecular Sciences, 2020, 21, 1116.	4.1	5
27	A machine-learning approach to cardiovascular risk prediction in psoriatic arthritis. Rheumatology, 2020, 59, 1767-1769.	1.9	16
28	When Stiffness Matters: Mechanosensing in Heart Development and Disease. Frontiers in Cell and Developmental Biology, 2020, 8, 334.	3.7	50
29	Modeling methodology for defining a priori the hydrodynamics of a dynamic suspension bioreactor. Application to human induced pluripotent stem cell culture. Journal of Biomechanics, 2019, 94, 99-106.	2.1	4
30	The Extent of Human Apolipoprotein A-I Lipidation Strongly Affects the Î²-Amyloid Efflux Across the Blood-Brain Barrier in vitro. Frontiers in Neuroscience, 2019, 13, 419.	2.8	42
31	Fludarabine-Specific Molecular Interactions with Maltose-Modified Poly(propyleneimine) Dendrimer Enable Effective Cell Entry of the Active Drug Form: Comparison with Clofarabine. Biomacromolecules, 2019, 20, 1429-1442.	5.4	16
32	The Role of Structural Polymorphism in Driving the Mechanical Performance of the Alzheimer's Beta Amyloid Fibrils. Frontiers in Bioengineering and Biotechnology, 2019, 7, 83.	4.1	21
33	The synergistic effect of chlorotoxin-mApoE in boosting drug-loaded liposomes across the BBB. Journal of Nanobiotechnology, 2019, 17, 115.	9.1	20
34	Biofunctionalization of Silica Nanoparticles with Cell-Penetrating Peptides: Adsorption Mechanism and Binding Energy Estimation. Journal of Physical Chemistry B, 2019, 123, 10622-10630.	2.6	15
35	Cell penetrating peptide modulation of membrane biomechanics by Molecular dynamics. Journal of Biomechanics, 2018, 73, 137-144.	2.1	40
36	Destabilizing the AXH Tetramer by Mutations: Mechanisms and Potential Antiaggregation Strategies. Biophysical Journal, 2018, 114, 323-330.	0.5	14

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37	Multivalent interacting glycodendrimer to prevent amyloid-peptide fibril formation induced by Cu(II): A multidisciplinary approach. Nano Research, 2018, 11, 1204-1226.	10.4	27
38	Virtual screening using covalent docking to find activators for G245S mutant p53. PLoS ONE, 2018, 13, e0200769.	2.5	12
39	Elucidating the role of surface chemistry on cationic phosphorus dendrimerâ€“siRNA complexation. Nanoscale, 2018, 10, 10952-10962.	5.6	20
40	Conformational Dynamics and Stability of U-Shaped and S-Shaped Amyloid Î² Assemblies. International Journal of Molecular Sciences, 2018, 19, 571.	4.1	30
41	A Novel Interaction Between the TLR7 and a Colchicine Derivative Revealed Through a Computational and Experimental Study. Pharmaceuticals, 2018, 11, 22.	3.8	3
42	Protein Environment: A Crucial Triggering Factor in Josephin Domain Aggregation: The Role of 2,2,2-Trifluoroethanol. International Journal of Molecular Sciences, 2018, 19, 2151.	4.1	3
43	Self-Assembled Ligands Targeting TLR7: A Molecular Level Investigation. Langmuir, 2017, 33, 14460-14471.	3.5	5
44	Deformation pattern in vibrating microtubule: Structural mechanics study based on an atomistic approach. Scientific Reports, 2017, 7, 4227.	3.3	22
45	Thermodynamic and kinetic stability of the Josephin Domain closed arrangement: evidences from replica exchange molecular dynamics. Biology Direct, 2017, 12, 2.	4.6	15
46	Explaining the Microtubule Energy Balance: Contributions Due to Dipole Moments, Charges, van der Waals and Solvation Energy. International Journal of Molecular Sciences, 2017, 18, 2042.	4.1	7
47	Insights into the Effect of the G245S Single Point Mutation on the Structure of p53 and the Binding of the Protein to DNA. Molecules, 2017, 22, 1358.	3.8	23
48	Free energy landscape of siRNA-polycation complexation: Elucidating the effect of molecular geometry, polymer flexibility, and charge neutralization. PLoS ONE, 2017, 12, e0186816.	2.5	25
49	Josephin Domain Structural Conformations Explored by Metadynamics in Essential Coordinates. PLoS Computational Biology, 2016, 12, e1004699.	3.2	22
50	A Versatile Bioreactor for Dynamic Suspension Cell Culture. Application to the Culture of Cancer Cell Spheroids. PLoS ONE, 2016, 11, e0154610.	2.5	45
51	Characterization of the <scp>AXH</scp> domain of Ataxinâ€1 using enhanced sampling and functional mode analysis. Proteins: Structure, Function and Bioinformatics, 2016, 84, 666-673.	2.6	21
52	Conformational fluctuations of the AXH monomer of Ataxin-1. Proteins: Structure, Function and Bioinformatics, 2016, 84, 52-59.	2.6	30
53	Iron oxide/PAMAM nanostructured hybrids: combined computational and experimental studies. Journal of Materials Science, 2016, 51, 1996-2007.	3.7	18
54	Deformability of Microtubules: An Atomistic Computational Study. Biophysical Journal, 2016, 110, 131a.	0.5	0

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55	Structure Based Modeling of Small Molecules Binding to the TLR7 by Atomistic Level Simulations. Molecules, 2015, 20, 8316-8340.	3.8	27
56	Microtubule Electrodynamics Associated with Vibrational Normal Modes. Biophysical Journal, 2015, 108, 449a.	0.5	2
57	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. Journal of Biomechanics, 2015, 48, 899-906.	2.1	71
58	Cell Penetrating Peptide Adsorption on Magnetite and Silica Surfaces: A Computational Investigation. Journal of Physical Chemistry B, 2015, 119, 8239-8246.	2.6	33
59	Multiscale impact of nucleotides and cations on the conformational equilibrium, elasticity and rheology of actin filaments and crosslinked networks. Biomechanics and Modeling in Mechanobiology, 2015, 14, 1143-1155.	2.8	31
60	Investigation of the Josephin Domain Protein-Protein Interaction by Molecular Dynamics. PLoS ONE, 2014, 9, e108677.	2.5	28
61	A Survey of Quantitative Descriptors of Arterial Flows. Lecture Notes in Computational Vision and Biomechanics, 2014, , 1-24.	0.5	3
62	Electro-Acoustic Behavior of the Mitotic Spindle: A Semi-Classical Coarse-Grained Model. PLoS ONE, 2014, 9, e86501.	2.5	28
63	Bioreactors as Engineering Support to Treat Cardiac Muscle and Vascular Disease. Journal of Healthcare Engineering, 2013, 4, 329-370.	1.9	38
64	A Hydrophobic Gold Surface Triggers Misfolding and Aggregation of the Amyloidogenic Josephin Domain in Monomeric Form, While Leaving the Oligomers Unaffected. PLoS ONE, 2013, 8, e58794.	2.5	24
65	A Survey of Methods for the Evaluation of Tissue Engineering Scaffold Permeability. Annals of Biomedical Engineering, 2013, 41, 2027-2041.	2.5	74
66	A Virtual Test Bench to Study Transport Phenomena in 3D Porous Scaffolds Using Lattice Boltzmann Simulations. , 2013, , .		0
67	Multiscale Modeling of Microtubules and Actin Filaments. IFAC Postprint Volumes IPPV / International Federation of Automatic Control, 2012, 45, 1023-1028.	0.4	1
68	Numerical and experimental characterization of a novel modular passive micromixer. Biomedical Microdevices, 2012, 14, 849-862.	2.8	25
69	Multiscale modeling of cellular actin filaments: From atomistic molecular to coarseâ€grained dynamics. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1598-1609.	2.6	30
70	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. Annals of Biomedical Engineering, 2012, 40, 729-741.	2.5	126
71	A Survey of Microchannel Geometries for Mixing of Species in Biomicrofluidics. , 2012, , 548-578.		2
72	Multiscale Biomechanics of Actin Filaments and Crosslinked Networks. , 2012, , .		0

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73	On the importance of blood rheology for bulk flow in hemodynamic models of the carotid bifurcation. Journal of Biomechanics, 2011, 44, 2427-2438.	2.1	93
74	A molecular dynamics study of a miRNA:mRNA interaction. Journal of Molecular Modeling, 2011, 17, 2895-2906.	1.8	15
75	Identification of a model of non-esterified fatty acids dynamics through genetic algorithms: The case of women with a history of gestational diabetes. Computers in Biology and Medicine, 2011, 41, 146-153.	7.0	15
76	Biomechanics of actin filaments: A computational multi-level study. Journal of Biomechanics, 2011, 44, 630-636.	2.1	33
77	Insights Into the Molecular Mechanisms of Actin Dynamics: A Multiscale Modeling Approach. , 2011, , .		0
78	Electric field generated by longitudinal axial microtubule vibration modes with high spatial resolution microtubule model. Journal of Physics: Conference Series, 2011, 329, 012013.	0.4	7
79	On the Importance of Assumptions for Bulk Flow in Hemodynamic Models of the Carotid Bifurcation. , 2011, , .		0
80	On the Use of In Vivo Measured Flow Rates as Boundary Conditions for Image-Based Hemodynamic Models of the Human Aorta. , 2011, , .		1
81	Identification of Atheroprone Morphological Features in Wall Shear Stress Waveforms in Carotid Bifurcations: A CFD-Based Integrated Approach. , 2010, , .		0
82	Coarse Grain Modeling for Microtubule Mechanics. Materials Science Forum, 2010, 638-642, 629-634.	0.3	3
83	Outflow Conditions for Image-Based Hemodynamic Models of the Carotid Bifurcation: Implications for Indicators of Abnormal Flow. Journal of Biomechanical Engineering, 2010, 132, 091005.	1.3	80
84	Anisotropic Elastic Network Modeling of Entire Microtubules. Biophysical Journal, 2010, 99, 2190-2199.	0.5	91
85	Elastic Network Modeling of Actin Filaments. , 2010, , .		0
86	MICROTUBULE-KINESIN MECHANICS BY MOLECULAR MODELING. Biophysical Reviews and Letters, 2009, 04, 45-61.	0.8	7
87	Elastic Network Normal Mode Analysis for Microtubule Mechanics. , 2009, , .		0
88	Mechanical Model of the Tubulin Dimer Based on Molecular Dynamics Simulations. Journal of Biomechanical Engineering, 2008, 130, 041008.	1.3	26
89	Bottom-Up Mesoscale Model of Microtubule. , 2007, , 345.		0
90	Tubulin: from atomistic structure to supramolecular mechanical properties. Journal of Materials Science, 2007, 42, 8864-8872.	3.7	45

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91	Mechanical response and conformational changes of alpha-actinin domains during unfolding: a molecular dynamics study. Biomechanics and Modeling in Mechanobiology, 2007, 6, 399-407.	2.8	25
92	Mechanical Properties of Tubulin Molecules by Molecular Dynamics Simulations. , 2006, , 587.		0
93	Scale/Physics/Time Properties and Functions in Bioartificial Systems. Materials Science Forum, 0, 706-709, 121-126.	0.3	0