

# Riccardo Capelli

## List of Publications by Year in descending order

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Version: 2024-02-01

28  
papers

1,281  
citations

687363

13  
h-index

526287

27  
g-index

36  
all docs

36  
docs citations

36  
times ranked

1496  
citing authors

#	ARTICLE	IF	CITATIONS
1	Promoting transparency and reproducibility in enhanced molecular simulations. <i>Nature Methods</i> , 2019, 16, 670-673.	19.0	655
2	Cooperative Supramolecular Block Copolymerization for the Synthesis of Functional Axial Organic Heterostructures. <i>Journal of the American Chemical Society</i> , 2020, 142, 11528-11539.	13.7	86
3	Exhaustive Search of Ligand Binding Pathways via Volume-Based Metadynamics. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3495-3499.	4.6	59
4	Controlling the length of porphyrin supramolecular polymers via coupled equilibria and dilution-induced supramolecular polymerization. <i>Nature Communications</i> , 2022, 13, 248.	12.8	54
5	Chasing the Full Free Energy Landscape of Neuroreceptor/Ligand Unbinding by Metadynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3354-3361.	5.3	53
6	<i>Swarm-CG</i>: Automatic Parametrization of Bonded Terms in MARTINI-Based Coarse-Grained Models of Simple to Complex Molecules <i>via</i> Fuzzy Self-Tuning Particle Swarm Optimization. <i>ACS Omega</i> , 2020, 5, 32823-32843.	3.5	49
7	Porous covalent organic nanotubes and their assembly in loops and toroids. <i>Nature Chemistry</i> , 2022, 14, 507-514.	13.6	46
8	Accuracy of Molecular Simulation-Based Predictions of <i>k</i><sub>off</sub> Values: A Metadynamics Study. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 6373-6381.	4.6	41
9	Enhancing Antibody Serodiagnosis Using a Controlled Peptide Coimmobilization Strategy. <i>ACS Infectious Diseases</i> , 2018, 4, 998-1006.	3.8	25
10	Enhanced-Sampling Simulations for the Estimation of Ligand Binding Kinetics: Current Status and Perspective. <i>Frontiers in Molecular Biosciences</i> , 0, 9, .	3.5	24
11	A Data-Driven Dimensionality Reduction Approach to Compare and Classify Lipid Force Fields. <i>Journal of Physical Chemistry B</i> , 2021, 125, 7785-7796.	2.6	21
12	The Subtle Trade-Off between Evolutionary and Energetic Constraints in Protein-Protein Interactions. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 1489-1497.	4.6	20
13	Enhanced Sampling Approach to the Induced-Fit Docking Problem in Protein-Ligand Binding: The Case of Mono-ADP-Ribosylation Hydrolase Inhibitors. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7899-7911.	5.3	17
14	An implementation of the maximum-caliber principle by replica-averaged time-resolved restrained simulations. <i>Journal of Chemical Physics</i> , 2018, 148, 184114.	3.0	16
15	MonteGrappa: An iterative Monte Carlo program to optimize biomolecular potentials in simplified models. <i>Computer Physics Communications</i> , 2015, 186, 93-104.	7.5	12
16	BPSL1626: Reverse and Structural Vaccinology Reveal a Novel Candidate for Vaccine Design Against <i>Burkholderia pseudomallei</i> . <i>Antibodies</i> , 2018, 7, 26.	2.5	11
17	Automatic multi-objective optimization of coarse-grained lipid force fields using <i>SwarmCG</i>. <i>Journal of Chemical Physics</i> , 2022, 156, 024801.	3.0	11
18	SAGE: A Fast Computational Tool for Linear Epitope Grafting onto a Foreign Protein Scaffold. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 6-10.	5.4	10

#	ARTICLE	IF	CITATIONS
19	Ephemeral Ice-Like Local Environments in Classical Rigid Models of Liquid Water. <i>Journal of Chemical Physics</i> , 0, , .	3.0	10
20	Assessment of Mutational Effects on Peptide Stability through Confinement Simulations. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 126-130.	4.6	9
21	Designing Probes for Immunodiagnostics: Structural Insights into an Epitope Targeting <i>Burkholderia</i> Infections. <i>ACS Infectious Diseases</i> , 2017, 3, 736-743.	3.8	8
22	Coevolutionary data-based interaction networks approach highlighting key residues across protein families: The case of the G-protein coupled receptors. <i>Computational and Structural Biotechnology Journal</i> , 2020, 18, 1153-1159.	4.1	8
23	Multiscale Molecular Modelling of ATP-Fueled Supramolecular Polymerisation and Depolymerisation**. <i>ChemSystemsChem</i> , 2021, 3, e2000038.	2.6	8
24	Iterative derivation of effective potentials to sample the conformational space of proteins at atomistic scale. <i>Journal of Chemical Physics</i> , 2014, 140, 195101.	3.0	6
25	Exact value for the average optimal cost of the bipartite traveling salesman and two-factor problems in two dimensions. <i>Physical Review E</i> , 2018, 98, .	2.1	6
26	Balancing Accuracy and Cost of Confinement Simulations by Interpolation and Extrapolation of Confinement Energies. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2779-2789.	5.3	5
27	Multiple Poses and Thermodynamics of Ligands Targeting Protein Surfaces: The Case of Furosemide Binding to mitoNEET in Aqueous Solution. <i>Frontiers in Cell and Developmental Biology</i> , 2022, 10, 886568.	3.7	3
28	Evolution of frustrated and stabilising contacts in reconstructed ancient proteins. <i>European Biophysics Journal</i> , 2021, 50, 699-712.	2.2	1