Riccardo Capelli

List of Publications by Year
in descending order

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	Controlling the length of porphyrin supramolecular polymers via coupled equilibria and dilution-induced supramolecular polymerization. Nature Communications, 2022, 13, 248.	12.8	54
2	Automatic multi-objective optimization of coarse-grained lipid force fields using SwarmCG. Journal of Chemical Physics, 2022, 156, 024801.	3.0	11
3	Porous covalent organic nanotubes and their assembly in loops and toroids. Nature Chemistry, 2022, 14, 507-514.	13.6	46
4	Multiple Poses and Thermodynamics of Ligands Targeting Protein Surfaces: The Case of Furosemide Binding to mitoNEET in Aqueous Solution. Frontiers in Cell and Developmental Biology, 2022, 10, 886568.	3.7	3
5	Multiscale Molecular Modelling of ATPâ€Fueled Supramolecular Polymerisation and Depolymerisation**. ChemSystemsChem, 2021, 3, e2000038.	2.6	8
6	Evolution of frustrated and stabilising contacts in reconstructed ancient proteins. European Biophysics Journal, 2021, 50, 699-712.	2.2	1
7	A Data-Driven Dimensionality Reduction Approach to Compare and Classify Lipid Force Fields. Journal of Physical Chemistry B, 2021, 125, 7785-7796.	2.6	21
8	Enhanced Sampling Approach to the Induced-Fit Docking Problem in Proteinâ€“Ligand Binding: The Case of Mono-ADP-Ribosylation Hydrolase Inhibitors. Journal of Chemical Theory and Computation, 2021, 17, 7899-7911.	5.3	17
9	Accuracy of Molecular Simulation-Based Predictions of k_{off} Values: A Metadynamics Study. Journal of Physical Chemistry Letters, 2020, 11, 6373-6381.	4.6	41
10	Swarm-CG: Automatic Parametrization of Bonded Terms in MARTINI-Based Coarse-Grained Models of Simple to Complex Molecules via Fuzzy Self-Tuning Particle Swarm Optimization. ACS Omega, 2020, 5, 32823-32843.	3.5	49
11	Coevolutionary data-based interaction networks approach highlighting key residues across protein families: The case of the G-protein coupled receptors. Computational and Structural Biotechnology Journal, 2020, 18, 1153-1159.	4.1	8
12	Cooperative Supramolecular Block Copolymerization for the Synthesis of Functional Axial Organic Heterostructures. Journal of the American Chemical Society, 2020, 142, 11528-11539.	13.7	86
13	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	19.0	655
14	Exhaustive Search of Ligand Binding Pathways via Volume-Based Metadynamics. Journal of Physical Chemistry Letters, 2019, 10, 3495-3499.	4.6	59
15	Chasing the Full Free Energy Landscape of Neuroreceptor/Ligand Unbinding by Metadynamics Simulations. Journal of Chemical Theory and Computation, 2019, 15, 3354-3361.	5.3	53
16	The Subtle Trade-Off between Evolutionary and Energetic Constraints in Proteinâ€“Protein Interactions. Journal of Physical Chemistry Letters, 2019, 10, 1489-1497.	4.6	20
17	Enhancing Antibody Serodiagnosis Using a Controlled Peptide Coimmobilization Strategy. ACS Infectious Diseases, 2018, 4, 998-1006.	3.8	25
18	Exact value for the average optimal cost of the bipartite traveling salesman and two-factor problems in two dimensions. Physical Review E, 2018, 98, .	2.1	6

#	Article	IF	Citations
19	An implementation of the maximum-caliber principle by replica-averaged time-resolved restrained simulations. Journal of Chemical Physics, 2018, 148, 184114.	3.0	16
20	BPSL1626: Reverse and Structural Vaccinology Reveal a Novel Candidate for Vaccine Design Against Burkholderia pseudomallei. Antibodies, 2018, 7, 26.	2.5	11
21	SAGE: A Fast Computational Tool for Linear Epitope Grafting onto a Foreign Protein Scaffold. Journal of Chemical Information and Modeling, 2017, 57, 6-10.	5.4	10
22	Designing Probes for Immunodiagnostics: Structural Insights into an Epitope Targeting Burkholderia Infections. ACS Infectious Diseases, 2017, 3, 736-743.	3.8	8
23	Balancing Accuracy and Cost of Confinement Simulations by Interpolation and Extrapolation of Confinement Energies. Journal of Chemical Theory and Computation, 2016, 12, 2779-2789.	5.3	5
24	Assessment of Mutational Effects on Peptide Stability through Confinement Simulations. Journal of Physical Chemistry Letters, 2016, 7, 126-130.	4.6	9
25	MonteGrappa: An iterative Monte Carlo program to optimize biomolecular potentials in simplified models. Computer Physics Communications, 2015, 186, 93-104.	7.5	12
26	Iterative derivation of effective potentials to sample the conformational space of proteins at atomistic scale. Journal of Chemical Physics, 2014, 140, 195101.	3.0	6
27	Ephemeral Ice-Like Local Environments in Classical Rigid Models of Liquid Water. Journal of Chemical Physics, 0, , .	3.0	10
28	Enhanced-Sampling Simulations for the Estimation of Ligand Binding Kinetics: Current Status and Perspective. Frontiers in Molecular Biosciences, 0, 9, .	3.5	24