Walter Rocchia

List of Publications by Year
in descending order

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Version: 2024-02-01

75 papers	3,834 citations	186209 28 h-index	128225 60 g-index
83 all docs	83 docs citations	83 times ranked	4797 citing authors

#	Article	IF	Citations
1	A Fast and Interpretable Deep Learning Approach for Accurate Electrostatics-Driven pK_a Predictions in Proteins. Journal of Chemical Theory and Computation, 2022, 18, 5068-5078.	2.3	11
2	SHREC 2022: Proteinâ€“ligand binding site recognition. Computers and Graphics, 2022, 107, 20-31.	1.4	10
3	Tuning Local Hydration Enables a Deeper Understanding of Proteinâ€“Ligand Binding: The PP1-Src Kinase Case. Journal of Physical Chemistry Letters, 2021, 12, 49-58.	2.1	5
4	Adaptive nanopores: A bioinspired label-free approach for protein sequencing and identification. Nano Research, 2021, 14, 328-333.	5.8	9
5	Molecular Recognition by Gold Nanoparticle-Based Receptors as Defined through Surface Morphology and Pockets Fingerprint. Journal of Physical Chemistry Letters, 2021, 12, 5616-5622.	2.1	5
6	Charged dielectric spheres interacting in electrolytic solution: A linearized Poissonâ€“Boltzmann equation model. Journal of Chemical Physics, 2021, 155, 114114.	1.2	11
7	SHREC 2021: Retrieval and classification of protein surfaces equipped with physical and chemical properties. Computers and Graphics, 2021, 99, 1-21.	1.4	10
8	Enhanced Molecular Dynamics Method to Efficiently Increase the Discrimination Capability of Computational Proteinâ€“Protein Docking. Journal of Chemical Theory and Computation, 2021, 17, 7271-7280.	2.3	6
9	Pandemic drugs at pandemic speed: infrastructure for accelerating COVID-19 drug discovery with hybrid machine learning- and physics-based simulations on high-performance computers. Interface Focus, 2021, 11, 20210018.	1.5	23
10	The role of histone tails in nucleosome stability: An electrostatic perspective. Computational and Structural Biotechnology Journal, 2020, 18, 2799-2809.	1.9	11
11	PypKa: A Flexible Python Module for Poissonâ€“Boltzmann-Based pK_a Calculations. Journal of Chemical Information and Modeling, 2020, 60, 4442-4448.	2.5	33
12	Chromatin Compaction Multiscale Modeling: A Complex Synergy Between Theory, Simulation, and Experiment. Frontiers in Molecular Biosciences, 2020, 7, 15.	1.6	21
13	Multiplexed Discrimination of Single Amino Acid Residues in Polypeptides in a Single SERS Hot Spot. Angewandte Chemie - International Edition, 2020, 59, 11423-11431.	7.2	71
14	Cognitive Insights into Sentic Spaces Using Principal Paths. Cognitive Computation, 2019, 11, 656-675.	3.6	8
15	Kinetics of Drug Binding and Residence Time. Annual Review of Physical Chemistry, 2019, 70, 143-171.	4.8	105
16	Binding and Internalization in Receptorâ€Targeted Carriers: The Complex Role of CD44 in the Uptake of Hyaluronic Acidâ€Based Nanoparticles (siRNA Delivery). Advanced Healthcare Materials, 2019, 8, e1901182.	3.9	37
17	NanoShaperâ€“VMD interface: computing and visualizing surfaces, pockets and channels in molecular systems. Bioinformatics, 2019, 35, 1241-1243.	1.8	23
18	Finding Principal Paths in Data Space. IEEE Transactions on Neural Networks and Learning Systems, 2019, 30, 2449-2462.	7.2	15

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19	BiKi Life Sciences: A New Suite for Molecular Dynamics and Related Methods in Drug Discovery. Journal of Chemical Information and Modeling, 2018, 58, 219-224.	2.5	48
20	Fast Dynamic Docking Guided by Adaptive Electrostatic Bias: The MD-Binding Approach. Journal of Chemical Theory and Computation, 2018, 14, 1727-1736.	2.3	40
21	Force Field Parametrization of Metal Ions from Statistical Learning Techniques. Journal of Chemical Theory and Computation, 2018, 14, 255-273.	2.3	39
22	Specific Residue Interactions Regulate the Binding of Dengue Antigens to Broadly Neutralizing EDE Antibodies. ChemistryOpen, 2018, 7, 604-610.	0.9	1
23	Including diverging electrostatic potential in 3D-RISM theory: The charged wall case. Journal of Chemical Physics, 2018, 148, 114106.	1.2	2
24	Import Vector Domain Description: A Kernel Logistic One-Class Learning Algorithm. IEEE Transactions on Neural Networks and Learning Systems, 2017, 28, 1722-1729.	7.2	11
25	Allosteric Communication Networks in Proteins Revealed through Pocket Crosstalk Analysis. ACS Central Science, 2017, 3, 949-960.	5.3	60
26	Distributed Kernel K-Means for Large Scale Clustering. , 2017, , .		3
27	dMM-PBSA: A New HADDOCK Scoring Function for Protein-Peptide Docking. Frontiers in Molecular Biosciences, 2016, 3, 46.	1.6	67
28	A simple and accurate protocol for absolute polar metabolite quantification in cell cultures using quantitative nuclear magnetic resonance. Analytical Biochemistry, 2016, 501, 26-34.	1.1	12
29	Absolute nutrient concentration measurements in cell culture media: 1H q-NMR spectra and data to compare the efficiency of pH-controlled protein precipitation versus CPMG or post-processing filtering approaches. Data in Brief, 2016, 8, 387-393.	0.5	3
30	Probing Hydration Patterns in Class-A GPCRs via Biased MD: The A_{2A} Receptor. Journal of Chemical Theory and Computation, 2016, 12, 6049-6061.	2.3	18
31	Kinetic and Structural Insights into the Mechanism of Binding of Sulfonamides to Human Carbonic Anhydrase by Computational and Experimental Studies. Journal of Medicinal Chemistry, 2016, 59, 4245-4256.	2.9	60
32	Kinetics of protein-ligand unbinding via smoothed potential molecular dynamics simulations. Scientific Reports, 2015, 5, 11539.	1.6	132
33	Implicit solvent methods for free energy estimation. European Journal of Medicinal Chemistry, 2015, 91, 27-42.	2.6	46
34	The ligand binding mechanism to purine nucleoside phosphorylase elucidated via molecular dynamics and machine learning. Nature Communications, 2015, 6, 6155.	5.8	98
35	A Pipeline To Enhance Ligand Virtual Screening: Integrating Molecular Dynamics and Fingerprints for Ligand and Proteins. Journal of Chemical Information and Modeling, 2015, 55, 2256-2274.	2.5	65
36	Building and Analyzing Molecular Surfaces: A Tutorial on NanoShaper. , 2015, , 199-213.		1

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37	Molecular mechanics and dynamics: numerical tools to sample the configuration space. Frontiers in Bioscience - Landmark, 2014, 19, 578.	3.0	13
38	A Combined MPI-CUDA Parallel Solution of Linear and Nonlinear Poisson-Boltzmann Equation. BioMed Research International, 2014, 2014, 1-12.	0.9	9
39	CUDA accelerated molecular surface generation. Concurrency Computation Practice and Experience, 2014, 26, 1819-1831.	1.4	4
40	GPU linear and non-linear Poissonâ€“Boltzmann solver module for DelPhi. Bioinformatics, 2014, 30, 569-570.	1.8	9
41	Describing the Conformational Landscape of Small Organic Molecules through Gaussian Mixtures in Dihedral Space. Journal of Chemical Theory and Computation, 2014, 10, 2557-2568.	2.3	10
42	Steered Molecular Dynamics Simulations for Studying Proteinâ€“Ligand Interaction in Cyclin-Dependent Kinase 5. Journal of Chemical Information and Modeling, 2014, 54, 470-480.	2.5	138
43	Solving the Linearized Poisson-Boltzmann Equation on GPUs Using CUDA. , 2013, , .		2
44	Between Algorithm and Model: Different Molecular Surface Definitions for the Poisson-Boltzmann Based Electrostatic Characterization of Biomolecules in Solution. Communications in Computational Physics, 2013, 13, 61-89.	0.7	46
45	Using DelPhi Capabilities to Mimic Proteinâ€™s Conformational Reorganization with Amino Acid Specific Dielectric Constants. Communications in Computational Physics, 2013, 13, 13-30.	0.7	23
46	A general and Robust Ray-Casting-Based Algorithm for Triangulating Surfaces at the Nanoscale. PLoS ONE, 2013, 8, e59744.	1.1	98
47	A statistical mechanics handbook for protein-ligand binding simulation. Frontiers in Bioscience - Scholar, 2013, S5, 478-495.	0.8	0
48	DelPhi Web Server: A Comprehensive Online Suite for Electrostatic Calculations of Biological Macromolecules and Their Complexes. Communications in Computational Physics, 2013, 13, 269-284.	0.7	52
49	A catalytically silent FAAH-1 variant drives anandamide transport in neurons. Nature Neuroscience, 2012, 15, 64-69.	7.1	150
50	Application of Conformational Clustering in Proteinâ€“Ligand Docking. Methods in Molecular Biology, 2012, 819, 169-186.	0.4	7
51	CUDA Accelerated Blobby Molecular Surface Generation. Lecture Notes in Computer Science, 2012, , 347-356.	1.0	5
52	Enhanced Sampling Methods in Drug Design. RSC Drug Discovery Series, 2012, , 273-301.	0.2	11
53	Insights into Ligandâ€“Protein Binding from Local Mechanical Response. Journal of Chemical Theory and Computation, 2011, 7, 3368-3378.	2.3	14
54	Systematic Exploitation of Multiple Receptor Conformations for Virtual Ligand Screening. PLoS ONE, 2011, 6, e18845.	1.1	82

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55	SDPhound, a Mutual Information-Based Method to Investigate Specificity-Determining Positions. Algorithms, 2009, 2, 764-789.	1.2	2
56	Complexes of HIVâ€1 integrase with HAT proteins: Multiscale models, dynamics, and hypotheses on allosteric sites of inhibition. Proteins: Structure, Function and Bioinformatics, 2009, 76, 946-958.	1.5	29
57	Electroactive carbon nanotube actuators: Soft-lithographic fabrication and electro-chemical modelling. Materials Science and Engineering C, 2008, 28, 1057-1064.	3.8	11
58	Green Fluorescent Protein Ground States:â€‰ The Influence of a Second Protonation Site near the Chromophore,. Biochemistry, 2007, 46, 5494-5504.	1.2	60
59	Mapping All-Atom Models onto One-Bead Coarse-Grained Models:Â General Properties and Applications to a Minimal Polypeptide Model. Journal of Chemical Theory and Computation, 2006, 2, 667-673.	2.3	64
60	AClAP, Autonomous hierarchical agglomerative Cluster Analysis based protocol to partition conformational datasets. Bioinformatics, 2006, 22, e58-e65.	1.8	41
61	Predicting the dielectric nonlinearity of anisotropic composite materials via tensorial analysis. Journal of Physics Condensed Matter, 2006, 18, 10585-10599.	0.7	12
62	Analytical electrostatics for biomolecules: Beyond the generalizedâ€‡ Born approximation. Journal of Chemical Physics, 2006, 124, 124902.	1.2	113
63	Poisson-boltzmann equation boundary conditions for biological applications. Mathematical and Computer Modelling, 2005, 41, 1109-1118.	2.0	15
64	Shape-dependent effects of dielectrically nonlinear inclusions in heterogeneous media. Journal of Applied Physics, 2005, 98, 104101.	1.1	27
65	JavaProtein Dossier: a novel web-based data visualization tool for comprehensive analysis of protein structure. Nucleic Acids Research, 2004, 32, W595-W601.	6.5	30
66	Wearable, Redundant Fabric-Based Sensor Arrays for Reconstruction of Body Segment Posture. IEEE Sensors Journal, 2004, 4, 807-818.	2.4	221
67	Combined atomistic and continuum methods to map electric properties of nanostructured carbon films. Computational Materials Science, 2004, 30, 150-154.	1.4	0
68	FACE: facial automaton for conveying emotions. Applied Bionics and Biomechanics, 2004, 1, 91-100.	0.5	16
69	Exploiting conducting polymer fiber radial expansion for bio-inspired actuation. , 2003, , .		1
70	Rapid grid-based construction of the molecular surface and the use of induced surface charge to calculate reaction field energies: Applications to the molecular systems and geometric objects. Journal of Computational Chemistry, 2002, 23, 128-137.	1.5	631
71	Extending the Applicability of the Nonlinear Poissonâ^'Boltzmann Equation:Â Multiple Dielectric Constants and Multivalent Ionsâ€. Journal of Physical Chemistry B, 2001, 105, 6507-6514.	1.2	747
72	Strain-amplified electroactive polymer actuator for haptic interfaces. , 2001, , .		5

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73	ASSEMBLING GOLD NANOPARTICLE PATTERNS FOR MOLECULAR ELECTRONICS APPLICATIONS. , 2000, , .		0
74	The State of the Science for the Langevin-Lorentz Model. , 1999, , 375-378.		2
75	Antibody-Antigen Binding Interface Analysis in the Big Data Era. Frontiers in Molecular Biosciences, 0, 9, .	1.6	8