Sereina Riniker

List of Publications by Year
in descending order

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95 papers	5,446 citations	147566 31 h-index	85405 71 g-index
97 all docs	97 docs citations	97 times ranked	6868 citing authors

#	Article	IF	Citations
1	Definition and testing of the GROMOS force-field versions 54A7 and 54B7. European Biophysics Journal, 2011, 40, 843-856.	1.2	1,902
2	Better Informed Distance Geometry: Using What We Know To Improve Conformation Generation. Journal of Chemical Information and Modeling, 2015, 55, 2562-2574.	2.5	327
3	Open-source platform to benchmark fingerprints for ligand-based virtual screening. Journal of Cheminformatics, 2013, 5, 26.	2.8	243
4	On developing coarse-grained models for biomolecular simulation: a review. Physical Chemistry Chemical Physics, 2012, 14, 12423.	1.3	216
5	The impact of molecular dynamics on drug design: applications for the characterization of ligandâ€“macromolecule complexes. Drug Discovery Today, 2015, 20, 686-702.	3.2	171
6	Fixed-Charge Atomistic Force Fields for Molecular Dynamics Simulations in the Condensed Phase: An Overview. Journal of Chemical Information and Modeling, 2018, 58, 565-578.	2.5	144
7	A simple, efficient polarizable coarse-grained water model for molecular dynamics simulations. Journal of Chemical Physics, 2011, 134, 084110.	1.2	121
8	A GROMOS-Compatible Force Field for Small Organic Molecules in the Condensed Phase: The 2016H66 Parameter Set. Journal of Chemical Theory and Computation, 2016, 12, 3825-3850.	2.3	118
9	Machine Learning of Partial Charges Derived from High-Quality Quantum-Mechanical Calculations. Journal of Chemical Information and Modeling, 2018, 58, 579-590.	2.5	117
10	Validation of Molecular Simulation: An Overview of Issues. Angewandte Chemie - International Edition, 2018, 57, 884-902.	7.2	101
11	New functionalities in the GROMOS biomolecular simulation software. Journal of Computational Chemistry, 2012, 33, 340-353.	1.5	98
12	Kinetic Models of Cyclosporin A in Polar and Apolar Environments Reveal Multiple Congruent Conformational States. Journal of Chemical Information and Modeling, 2016, 56, 1547-1562.	2.5	95
13	Improving Conformer Generation for Small Rings and Macrocycles Based on Distance Geometry and Experimental Torsional-Angle Preferences. Journal of Chemical Information and Modeling, 2020, 60, 2044-2058.	2.5	82
14	Using Information from Historical High-Throughput Screens to Predict Active Compounds. Journal of Chemical Information and Modeling, 2014, 54, 1880-1891.	2.5	79
15	Machine Learning in QM/MM Molecular Dynamics Simulations of Condensed-Phase Systems. Journal of Chemical Theory and Computation, 2021, 17, 2641-2658.	2.3	76
16	Molecular Dynamics Fingerprints (MDFP): Machine Learning from MD Data To Predict Free-Energy Differences. Journal of Chemical Information and Modeling, 2017, 57, 726-741.	2.5	73
17	Multiâ€Resolution Simulation of Biomolecular Systems: A Review of Methodological Issues. Angewandte Chemie - International Edition, 2013, 52, 2820-2834.	7.2	72
18	Calculation of Relative Free Energies for Ligand-Protein Binding, Solvation, and Conformational Transitions Using the GROMOS Software. Journal of Physical Chemistry B, 2011, 115, 13570-13577.	1.2	71

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19	GHOST: Adjusting the Decision Threshold to Handle Imbalanced Data in Machine Learning. Journal of Chemical Information and Modeling, 2021, 61, 2623-2640.	2.5	62
20	Rationalization of the Membrane Permeability Differences in a Series of Analogue Cyclic Decapeptides. Journal of Chemical Information and Modeling, 2019, 59, 294-308.	2.5	55
21	Interconversion Rates between Conformational States as Rationale for the Membrane Permeability of Cyclosporines. ChemPhysChem, 2017, 18, 3309-3314.	1.0	53
22	On the Calculation of the Dielectric Permittivity and Relaxation of Molecular Models in the Liquid Phase. Journal of Chemical Theory and Computation, 2011, 7, 1469-1475.	2.3	52
23	Cross-Linked Collagen Triple Helices by Oxime Ligation. Journal of the American Chemical Society, 2017, 139, 12815-12820.	6.6	50
24	A molecular mechanism for the enzymatic methylation of nitrogen atoms within peptide bonds. Science Advances, 2018, 4, eaat2720.	4.7	48
25	Solvating atomic level fine-grained proteins in supra-molecular level coarse-grained water for molecular dynamics simulations. European Biophysics Journal, 2012, 41, 647-661.	1.2	45
26	Comparison of enveloping distribution sampling and thermodynamic integration to calculate binding free energies of phenylethanolamine N-methyltransferase inhibitors. Journal of Chemical Physics, 2011, 135, 024105.	1.2	41
27	Mixing coarse-grained and fine-grained water in molecular dynamics simulations of a single system. Journal of Chemical Physics, 2012, 137, 044120.	1.2	38
28	Heterogeneous Classifier Fusion for Ligand-Based Virtual Screening: Or, How Decision Making by Committee Can Be a Good Thing. Journal of Chemical Information and Modeling, 2013, 53, 2829-2836.	2.5	38
29	Novel Directions in Free Energy Methods and Applications. Journal of Chemical Information and Modeling, 2020, 60, 1-5.	2.5	36
30	Structural Effects of an Atomic-Level Layer of Water Molecules around Proteins Solvated in Supra-Molecular Coarse-Grained Water. Journal of Physical Chemistry B, 2012, 116, 8873-8879.	1.2	35
31	A Lanthipeptideâ€like Nâ€Terminal Leader Region Guides Peptide Epimerization by Radical SAM Epimerases: Implications for RiPP Evolution. Angewandte Chemie - International Edition, 2016, 55, 12330-12333.	7.2	34
32	Combining Molecular Dynamics and Machine Learning to Predict Self-Solvation Free Energies and Limiting Activity Coefficients. Journal of Chemical Information and Modeling, 2020, 60, 5319-5330.	2.5	31
33	Combining Machine Learning and Molecular Dynamics to Predict P-Glycoprotein Substrates. Journal of Chemical Information and Modeling, 2020, 60, 4730-4749.	2.5	30
34	Efficient Round-Trip Time Optimization for Replica-Exchange Enveloping Distribution Sampling (RE-EDS). Journal of Chemical Theory and Computation, 2017, 13, 3020-3030.	2.3	25
35	Localized and Collective Motions in HETâ€s(218â€289) Fibrils from Combined NMR Relaxation and MD Simulation. Angewandte Chemie - International Edition, 2019, 58, 9383-9388.	7.2	25
36	Influence of Lipidation on the Folding and Stability of Collagen Triple Helicesâ€”An Experimental and Theoretical Study. Journal of the American Chemical Society, 2021, 143, 5937-5942.	6.6	25

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37	Free enthalpies of replacing water molecules in protein binding pockets. Journal of Computer-Aided Molecular Design, 2012, 26, 1293-1309.	1.3	23
38	Replica exchange enveloping distribution sampling (RE-EDS): A robust method to estimate multiple free-energy differences from a single simulation. Journal of Chemical Physics, 2016, 145, 154114.	1.2	23
39	Effect of Flexibility, Lipophilicity, and the Location of Polar Residues on the Passive Membrane Permeability of a Series of Cyclic Decapeptides. Journal of Medicinal Chemistry, 2021, 64, 12761-12773.	2.9	22
40	Enhanced sampling without borders: on global biasing functions and how to reweight them. Physical Chemistry Chemical Physics, 2022, 24, 1225-1236.	1.3	22
41	Assessment of enveloping distribution sampling to calculate relative free enthalpies of binding for eight netropsinâ€“DNA duplex complexes in aqueous solution. Journal of Computational Chemistry, 2012, 33, 640-651.	1.5	21
42	Systematic Optimization of a Fragment-Based Force Field against Experimental Pure-Liquid Properties Considering Large Compound Families: Application to Saturated Haloalkanes. Journal of Chemical Theory and Computation, 2020, 16, 7525-7555.	2.3	21
43	Temperature Dependence of the Dielectric Permittivity of Acetic Acid, Propionic Acid and Their Methyl Esters: A Molecular Dynamics Simulation Study. ChemPhysChem, 2012, 13, 1182-1190.	1.0	19
44	Use of molecular dynamics fingerprints (MDFPs) in SAMPL6 octanolâ€“water log P blind challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 393-403.	1.3	19
45	On the Use of Enveloping Distribution Sampling (EDS) to Compute Free Enthalpy Differences between Different Conformational States of Molecules: Application to 3₁₀-, Î±-, and Ï€-Helices. Journal of Chemical Theory and Computation, 2011, 7, 3884-3897.	2.3	18
46	An Alternative to Conventional Î»-Intermediate States in Alchemical Free Energy Calculations: Î»-Enveloping Distribution Sampling. Journal of Chemical Information and Modeling, 2020, 60, 5407-5423.	2.5	18
47	Reaction-field electrostatics in molecular dynamics simulations: development of a conservative scheme compatible with an atomic cutoff. Physical Chemistry Chemical Physics, 2020, 22, 26419-26437.	1.3	16
48	Glycanâ€“protein interactions determine kinetics of N-glycan remodeling. RSC Chemical Biology, 2021, 2, 917-931.	2.0	16
49	Mutanobactin D from the Human Microbiome: Total Synthesis, Configurational Assignment, and Biological Evaluation. Journal of the American Chemical Society, 2021, 143, 10389-10402.	6.6	16
50	N-Glycosylation Enhances Conformational Flexibility of Protein Disulfide Isomerase Revealed by Microsecond Molecular Dynamics and Markov State Modeling. Journal of Physical Chemistry B, 2021, 125, 9467-9479.	1.2	16
51	Rapid Sampling of Folding Equilibria of Î²-Peptides in Methanol Using a Supramolecular Solvent Model. Journal of Chemical Theory and Computation, 2014, 10, 2213-2223.	2.3	15
52	The importance of N-methylations for the stability of the $$eta ^{6.3}$$ Î² 6.3 -helical conformation of polytheonamide B. European Biophysics Journal, 2017, 46, 363-374.	1.2	14
53	Reoptimized interaction parameters for the peptideâ€backbone model compound Nâ€methylacetamide in the GROMOS force field: Influence on the folding properties of two betaâ€peptides in methanol. Journal of Computational Chemistry, 2012, 33, 1907-1917.	1.5	13
54	Free Enthalpy Differences between Î±-, Ï€-, and 3₁₀-Helices of an Atomic Level Fine-Grained Alanine Deca-Peptide Solvated in Supramolecular Coarse-Grained Water. Journal of Chemical Theory and Computation, 2013, 9, 1328-1333.	2.3	13

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55	Determination of Absolute Stereochemistry of Flexible Molecules Using a Vibrational Circular Dichroism Spectra Alignment Algorithm. Journal of Chemical Information and Modeling, 2019, 59, 1826-1838.	2.5	13
56	On the faithfulness of molecular mechanics representations of proteins towards quantum-mechanical energy surfaces. Interface Focus, 2020, 10, 20190121.	1.5	13
57	Toward the elucidation of the mechanism for passive membrane permeability of cyclic peptides. Future Medicinal Chemistry, 2019, 11, 637-639.	1.1	12
58	Matched Molecular Series Analysis for ADME Property Prediction. Journal of Chemical Information and Modeling, 2020, 60, 2903-2914.	2.5	12
59	On the Effect of the Various Assumptions and Approximations used in Molecular Simulations on the Properties of Bioâ€Molecular Systems: Overview and Perspective on Issues. ChemPhysChem, 2021, 22, 264-282.	1.0	12
60	Learning Atomic Multipoles: Prediction of the Electrostatic Potential with Equivariant Graph Neural Networks. Journal of Chemical Theory and Computation, 2022, 18, 1701-1710.	2.3	12
61	The Playbooks of Medicinal Chemistry Design Moves. Journal of Chemical Information and Modeling, 2021, 61, 729-742.	2.5	11
62	Modulation of the Passive Permeability of Semipeptidic Macrocycles: N- and C-Methylations Fine-Tune Conformation and Properties. Journal of Medicinal Chemistry, 2021, 64, 5365-5383.	2.9	11
63	Determining the Regiochemistry and Relative Stereochemistry of Small and Druglike Molecules Using an Alignment Algorithm for Infrared Spectra. Analytical Chemistry, 2020, 92, 9124-9131.	3.2	10
64	Relative free-energy calculations for scaffold hopping-type transformations with an automated RE-EDS sampling procedure. Journal of Computer-Aided Molecular Design, 2022, 36, 117-130.	1.3	10
65	Polar/apolar interfaces modulate the conformational behavior of cyclic peptides with impact on their passive membrane permeability. RSC Advances, 2022, 12, 5782-5796.	1.7	10
66	A Lanthipeptideâ€like Nâ€Terminal Leader Region Guides Peptide Epimerization by Radical SAM Epimerases: Implications for RiPP Evolution. Angewandte Chemie, 2016, 128, 12518-12521.	1.6	9
67	Improved accuracy of hybrid atomistic/coarse-grained simulations using reparametrised interactions. Journal of Chemical Physics, 2017, 146, 124131.	1.2	9
68	Localized and Collective Motions in HETâ€s(218â€289) Fibrils from Combined NMR Relaxation and MD Simulation. Angewandte Chemie, 2019, 131, 9483-9488.	1.6	9
69	Fast NosÃ©â€“Hoover thermostat: molecular dynamics in quasi-thermodynamic equilibrium. Physical Chemistry Chemical Physics, 2019, 21, 6059-6070.	1.3	9
70	Exploring Novel Directions in Free Energy Calculations. Journal of Chemical Information and Modeling, 2020, 60, 5283-5286.	2.5	9
71	Connecting the conformational behavior of cyclic octadepsipeptides with their ionophoric property and membrane permeability. Organic and Biomolecular Chemistry, 2020, 18, 7110-7126.	1.5	9
72	Anisotropic reaction field correction for long-range electrostatic interactions in molecular dynamics simulations. Journal of Chemical Physics, 2018, 148, 234105.	1.2	8

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73	A New Family of Rigid Dienone Musks Challenges the Perceptive Range of the Human Olfactory Receptor OR5AN1. Synlett, 2020, 31, 972-976.	1.0	8
74	Volume-scaled common nearest neighbor clustering algorithm with free-energy hierarchy. Journal of Chemical Physics, 2021, 154, 084106.	1.2	8
75	Efficient Alchemical Intermediate States in Free Energy Calculations Using Î»-Enveloping Distribution Sampling. Journal of Chemical Theory and Computation, 2021, 17, 5805-5815.	2.3	8
76	Virtual-screening workflow tutorials and prospective results from the Teach-Discover-Treat competition 2014 against malaria. F1000Research, 2017, 6, 1136.	0.8	7
77	Incorporating NOE-Derived Distances in Conformer Generation of Cyclic Peptides with Distance Geometry. Journal of Chemical Information and Modeling, 2022, , .	2.5	7
78	Virtual-screening workflow tutorials and prospective results from the Teach-Discover-Treat competition 2014 against malaria. F1000Research, 2018, 6, 1136.	0.8	6
79	Beyond the Rosenfeld Equation: Computation of Vibrational Circular Dichroism Spectra for Anisotropic Solutions. Journal of Chemical Theory and Computation, 2019, 15, 2492-2503.	2.3	6
80	Benchmarking Hybrid Atomistic/Coarse-Grained Schemes for Proteins with an Atomistic Water Layer. Journal of Physical Chemistry B, 2019, 123, 3033-3042.	1.2	5
81	Machine Learning with and for Molecular Dynamics Simulations. Chimia, 2019, 73, 1024.	0.3	5
82	Recent developments in multiscale free energy simulations. Current Opinion in Structural Biology, 2022, 72, 55-62.	2.6	5
83	Connecting dynamic reweighting Algorithms: Derivation of the dynamic reweighting family tree. Journal of Chemical Physics, 2020, 153, 234106.	1.2	5
84	RestraintMaker: a graph-based approach to select distance restraints in free-energy calculations with dual topology. Journal of Computer-Aided Molecular Design, 2022, 36, 175-192.	1.3	5
85	Replica-Exchange Enveloping Distribution Sampling Using Generalized AMBER Force-Field Topologies: Application to Relative Hydration Free-Energy Calculations for Large Sets of Molecules. Journal of Chemical Information and Modeling, 2022, 62, 3043-3056.	2.5	5
86	Ensembler: A Simple Package for Fast Prototyping and Teaching Molecular Simulations. Journal of Chemical Information and Modeling, 2021, 61, 560-564.	2.5	4
87	Passing the Barrier â€“ How Computer Simulations Can Help to Understand and Improve the Passive Membrane Permeability of Cyclic Peptides. Chimia, 2021, 75, 518-521.	0.3	4
88	Validierung von molekularen Simulationen: eine Ãœbersicht verschiedener Aspekte. Angewandte Chemie, 2018, 130, 894-915.	1.6	3
89	Transition from Academia to Industry and Back. Journal of Chemical Information and Modeling, 2018, 58, 1469-1472.	2.5	2
90	Solvent-scaling as an alternative to coarse-graining in adaptive-resolution simulations: The adaptive solvent-scaling (AdSoS) scheme. Journal of Chemical Physics, 2021, 155, 094107.	1.2	2

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91	Density artefacts at interfaces caused by multiple time-step effects in molecular dynamics simulations. F1000Research, 2018, 7, 1745.	0.8	2
92	Density artefacts at interfaces caused by multiple time-step effects in molecular dynamics simulations. F1000Research, 2018, 7, 1745.	0.8	2
93	Density artefacts at interfaces caused by multiple time-step effects in molecular dynamics simulations. F1000Research, 0, 7, 1745.	0.8	1
94	Crossing the Boundaries within Computational Chemistry: From Molecular Dynamics to Cheminformatics and back. Chimia, 2014, 68, 620-623.	0.3	0
95	11th Young Faculty Meeting, 5th June 2018. Chimia, 2018, 72, 550.	0.3	0