Marie Zgarbova

List of Publications by Year in descending order

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Version: 2024-02-01

25 papers	3,237 citations	361413 20 h-index	552781 26 g-index
29 all docs	29 docs citations	29 times ranked	2606 citing authors

#	Article	IF	Citations
1	The <scp>Adâ€MD</scp> method to calculate <scp>NMR</scp> shift including effects due to conformational dynamics: The <scp>³¹P NMR</scp> shift in <scp>DNA</scp>. Journal of Computational Chemistry, 2022, 43, 132-143.	3.3	5
2	Z-DNA as a Touchstone for Additive Empirical Force Fields and a Refinement of the Alpha/Gamma DNA Torsions for AMBER. Journal of Chemical Theory and Computation, 2021, 17, 6292-6301.	5.3	30
3	A- to B-DNA Transition in AMBER Force Fields and Its Coupling to Sugar Pucker. Journal of Chemical Theory and Computation, 2018, 14, 319-328.	5.3	22
4	Influence of BII Backbone Substates on DNA Twist: A Unified View and Comparison of Simulation and Experiment for All 136 Distinct Tetranucleotide Sequences. Journal of Chemical Information and Modeling, 2017, 57, 275-287.	5.4	31
5	Noncanonical Î±/Î³ Backbone Conformations in RNA and the Accuracy of Their Description by the AMBER Force Field. Journal of Physical Chemistry B, 2017, 121, 2420-2433.	2.6	27
6	How to understand atomistic molecular dynamics simulations of <scp>RNA</scp> and proteinâ€“<scp>RNA</scp> complexes?. Wiley Interdisciplinary Reviews RNA, 2017, 8, e1405.	6.4	54
7	Assessing the Current State of Amber Force Field Modifications for DNA. Journal of Chemical Theory and Computation, 2016, 12, 4114-4127.	5.3	351
8	On the Use of Molecular Dynamics Simulations for Probing Allostery through DNA. Biophysical Journal, 2016, 110, 874-876.	0.5	14
9	Transferability and additivity of dihedral parameters in polarizable and nonpolarizable empirical force fields. Journal of Computational Chemistry, 2015, 36, 1874-1884.	3.3	15
10	Microsecond-Scale MD Simulations of HIV-1 DIS Kissing-Loop Complexes Predict Bulged-In Conformation of the Bulged Bases and Reveal Interesting Differences between Available Variants of the AMBER RNA Force Fields. Journal of Physical Chemistry B, 2015, 119, 15176-15190.	2.6	20
11	Reactive Conformation of the Active Site in the Hairpin Ribozyme Achieved by Molecular Dynamics Simulations with Îµ/Î¶ Force Field Reparametrizations. Journal of Physical Chemistry B, 2015, 119, 4220-4229.	2.6	45
12	Refinement of the Sugarâ€“Phosphate Backbone Torsion Beta for AMBER Force Fields Improves the Description of Z- and B-DNA. Journal of Chemical Theory and Computation, 2015, 11, 5723-5736.	5.3	392
13	Mechanical properties of symmetric and asymmetric DNA A-tracts: implications for looping and nucleosome positioning. Nucleic Acids Research, 2014, 42, 7383-7394.	14.5	59
14	Molecular Dynamics Simulations of Nucleic Acids. From Tetranucleotides to the Ribosome. Journal of Physical Chemistry Letters, 2014, 5, 1771-1782.	4.6	139
15	Mechanical Model of DNA Allostery. Journal of Physical Chemistry Letters, 2014, 5, 3831-3835.	4.6	24
16	Base Pair Fraying in Molecular Dynamics Simulations of DNA and RNA. Journal of Chemical Theory and Computation, 2014, 10, 3177-3189.	5.3	135
17	Energies and 2â€²-Hydroxyl Group Orientations of RNA Backbone Conformations. Benchmark CCSD(T)/CBS Database, Electronic Analysis, and Assessment of DFT Methods and MD Simulations. Journal of Chemical Theory and Computation, 2014, 10, 463-480.	5.3	24
18	Toward Improved Description of DNA Backbone: Revisiting Epsilon and Zeta Torsion Force Field Parameters. Journal of Chemical Theory and Computation, 2013, 9, 2339-2354.	5.3	255

#	Article	IF	Citations
19	Reference Simulations of Noncanonical Nucleic Acids with Different Ï‡ Variants of the AMBER Force Field: Quadruplex DNA, Quadruplex RNA, and Z-DNA. Journal of Chemical Theory and Computation, 2012, 8, 2506-2520.	5.3	231
20	A Novel Approach for Deriving Force Field Torsion Angle Parameters Accounting for Conformation-Dependent Solvation Effects. Journal of Chemical Theory and Computation, 2012, 8, 3232-3242.	5.3	27
21	Can We Accurately Describe the Structure of Adenine Tracts in B-DNA? Reference Quantum-Chemical Computations Reveal Overstabilization of Stacking by Molecular Mechanics. Journal of Chemical Theory and Computation, 2012, 8, 2448-2460.	5.3	67
22	Refinement of the Cornell et al. Nucleic Acids Force Field Based on Reference Quantum Chemical Calculations of Glycosidic Torsion Profiles. Journal of Chemical Theory and Computation, 2011, 7, 2886-2902.	5.3	873
23	Noncanonical Hydrogen Bonding in Nucleic Acids. Benchmark Evaluation of Key Baseâ€“Phosphate Interactions in Folded RNA Molecules Using Quantum-Chemical Calculations and Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2011, 115, 11277-11292.	2.5	26
24	Performance of Molecular Mechanics Force Fields for RNA Simulations: Stability of UUCG and GNRA Hairpins. Journal of Chemical Theory and Computation, 2010, 6, 3836-3849.	5.3	339
25	Reference Quantum Chemical Calculations on RNA Base Pairs Directly Involving the 2â€²-OH Group of Ribose. Journal of Chemical Theory and Computation, 2009, 5, 1166-1179.	5.3	27