

Marie Zgarbova

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

26

papers

2,273

citations

18

h-index

29

g-index

29

ext. papers

2,846

ext. citations

5.9

avg, IF

4.63

L-index

#	Paper	IF	Citations
26	Refinement of the Cornell et al. Nucleic Acids Force Field Based on Reference Quantum Chemical Calculations of Glycosidic Torsion Profiles. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 2886-2902	6.4	569
25	Performance of Molecular Mechanics Force Fields for RNA Simulations: Stability of UUCG and GNRA Hairpins.. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 3836-3849	6.4	261
24	Refinement of the Sugar-Phosphate Backbone Torsion Beta for AMBER Force Fields Improves the Description of Z- and B-DNA. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5723-36	6.4	243
23	Toward Improved Description of DNA Backbone: Revisiting Epsilon and Zeta Torsion Force Field Parameters. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 2339-2354	6.4	205
22	Assessing the Current State of Amber Force Field Modifications for DNA. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 4114-27	6.4	203
21	Reference simulations of noncanonical nucleic acids with different variants of the AMBER force field: quadruplex DNA, quadruplex RNA and Z-DNA. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 2506-2520	6.4	184
20	Molecular Dynamics Simulations of Nucleic Acids. From Tetranucleotides to the Ribosome. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 1771-82	6.4	113
19	Base Pair Fraying in Molecular Dynamics Simulations of DNA and RNA. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3177-89	6.4	106
18	Can We Accurately Describe the Structure of Adenine Tracts in B-DNA? Reference Quantum-Chemical Computations Reveal Overstabilization of Stacking by Molecular Mechanics. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 2448-60	6.4	56
17	Mechanical properties of symmetric and asymmetric DNA A-tracts: implications for looping and nucleosome positioning. <i>Nucleic Acids Research</i> , 2014 , 42, 7383-94	20.1	45
16	How to understand atomistic molecular dynamics simulations of RNA and protein-RNA complexes?. <i>Wiley Interdisciplinary Reviews RNA</i> , 2017 , 8, e1405	9.3	42
15	Reactive conformation of the active site in the hairpin ribozyme achieved by molecular dynamics simulations with force field reparametrizations. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 4220-9	3.4	31
14	Reference Quantum Chemical Calculations on RNA Base Pairs Directly Involving the 2'OH Group of Ribose. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 1166-79	6.4	26
13	Influence of BII Backbone Substates on DNA Twist: A Unified View and Comparison of Simulation and Experiment for All 136 Distinct Tetranucleotide Sequences. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 275-287	6.1	25
12	Noncanonical hydrogen bonding in nucleic acids. Benchmark evaluation of key base-phosphate interactions in folded RNA molecules using quantum-chemical calculations and molecular dynamics simulations. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 11277-92	2.8	25
11	A Novel Approach for Deriving Force Field Torsion Angle Parameters Accounting for Conformation-Dependent Solvation Effects. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 3232-42	6.4	23
10	Noncanonical Backbone Conformations in RNA and the Accuracy of Their Description by the AMBER Force Field. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 2420-2433	3.4	22

9	Energies and 2THydroxyl Group Orientations of RNA Backbone Conformations. Benchmark CCSD(T)/CBS Database, Electronic Analysis, and Assessment of DFT Methods and MD Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 463-80	6.4	20
8	Mechanical Model of DNA Allostery. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 3831-5	6.4	18
7	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. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 15176-90	3.4	16
6	A- to B-DNA Transition in AMBER Force Fields and Its Coupling to Sugar Pucker. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 319-328	6.4	13
5	On the Use of Molecular Dynamics Simulations for Probing Allostery through DNA. <i>Biophysical Journal</i> , 2016 , 110, 874-6	2.9	11
4	Transferability and additivity of dihedral parameters in polarizable and nonpolarizable empirical force fields. <i>Journal of Computational Chemistry</i> , 2015 , 36, 1874-84	3.5	8
3	Z-DNA as a Touchstone for Additive Empirical Force Fields and a Refinement of the Alpha/Gamma DNA Torsions for AMBER. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 6292-6301	6.4	6
2	Improving The Performance Of The Amber Rna Force Field By Tuning The Hydrogen-Bonding Interactions		1
1	The Ad-MD method to calculate NMR shift including effects due to conformational dynamics: The P NMR shift in DNA. <i>Journal of Computational Chemistry</i> , 2022 , 43, 132-143	3.5	0