Marie Zgarbova

List of Publications by Year in Descending Order

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	The Ad-MD method to calculate NMR shift including effects due to conformational dynamics: The P NMR shift in DNA. *Journal of Computational Chemistry*, **2022**, 43, 132-143	3.5	0
25	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	6.4	6
24	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	6.4	13
23	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	6.1	25
22	Noncanonical αIBackbone Conformations in RNA and the Accuracy of Their Description by the AMBER Force Field. *Journal of Physical Chemistry B*, **2017**, 121, 2420-2433	3.4	22
21	How to understand atomistic molecular dynamics simulations of RNA and protein-RNA complexes?. *Wiley Interdisciplinary Reviews RNA*, **2017**, 8, e1405	9.3	42
20	Assessing the Current State of Amber Force Field Modifications for DNA. *Journal of Chemical Theory and Computation*, **2016**, 12, 4114-27	6.4	203
19	On the Use of Molecular Dynamics Simulations for Probing Allostery through DNA. *Biophysical Journal*, **2016**, 110, 874-6	2.9	11
18	Reactive conformation of the active site in the hairpin ribozyme achieved by molecular dynamics simulations with αIforce field reparametrizations. *Journal of Physical Chemistry B*, **2015**, 119, 4220-9	3.4	31
17	Refinement of the Sugar-Phosphate Backbone Torsion Beta for AMBER Force Fields Improves the Description of Z- and B-DNA. *Journal of Chemical Theory and Computation*, **2015**, 11, 5723-36	6.4	243
16	Transferability and additivity of dihedral parameters in polarizable and nonpolarizable empirical force fields. *Journal of Computational Chemistry*, **2015**, 36, 1874-84	3.5	8
15	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, 15176-90	3.4	16
14	Molecular Dynamics Simulations of Nucleic Acids. From Tetranucleotides to the Ribosome. *Journal of Physical Chemistry Letters*, **2014**, 5, 1771-82	6.4	113
13	Mechanical Model of DNA Allostery. *Journal of Physical Chemistry Letters*, **2014**, 5, 3831-5	6.4	18
12	Base Pair Fraying in Molecular Dynamics Simulations of DNA and RNA. *Journal of Chemical Theory and Computation*, **2014**, 10, 3177-89	6.4	106
11	Energies and 2ŦHydroxyl 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, 463-80	6.4	20
10	Mechanical properties of symmetric and asymmetric DNA A-tracts: implications for looping and nucleosome positioning. *Nucleic Acids Research*, **2014**, 42, 7383-94	20.1	45

List of Publications

9	Toward Improved Description of DNA Backbone: Revisiting Epsilon and Zeta Torsion Force Field Parameters. *Journal of Chemical Theory and Computation*, **2013**, 9, 2339-2354	6.4	205
8	Reference simulations of noncanonical nucleic acids with different variants of the AMBER force field: quadruplex DNA, quadruplex RNA and Z-DNA. *Journal of Chemical Theory and Computation*, **2012**, 8, 2506-2520	6.4	184
7	A Novel Approach for Deriving Force Field Torsion Angle Parameters Accounting for Conformation-Dependent Solvation Effects. *Journal of Chemical Theory and Computation*, **2012**, 8, 3232-42	6.4	23
6	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, 2448-60	6.4	56
5	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. *Journal of Physical Chemistry A*, **2011**, 115, 11277-92	2.8	25
4	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	6.4	569
3	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	6.4	261
2	Reference Quantum Chemical Calculations on RNA Base Pairs Directly Involving the 2′OH Group of Ribose. *Journal of Chemical Theory and Computation*, **2009**, 5, 1166-79	6.4	26
1	Improving The Performance Of The Amber Rna Force Field By Tuning The Hydrogen-Bonding Interactions		1