Vojtech Mlynsky

List of Publications by Year
in descending order

16	598	687363 13	888059 17
papers	citations	h-index	g-index

24	24	24	420
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Toward Convergence in Folding Simulations of RNA Tetraloops: Comparison of Enhanced Sampling Techniques and Effects of Force Field Modifications. Journal of Chemical Theory and Computation, 2022, 18, 2642-2656.	5.3	34
2	Automatic Learning of Hydrogen-Bond Fixes in the AMBER RNA Force Field. Journal of Chemical Theory and Computation, 2022, 18, 4490-4502.	5.3	21
3	W-RESP: Well-Restrained Electrostatic Potential-Derived Charges. Revisiting the Charge Derivation Model. Journal of Chemical Theory and Computation, 2021, 17, 3495-3509.	5.3	18
4	Short-Range Imbalances in the AMBER Lennard-Jones Potential for (Deoxy)RiboseÂ·Â·Â·Nucleobase Lone-PairÂ·Â·Â·Ï€ Contacts in Nucleic Acids. Journal of Chemical Information and Modeling, 2021, 61, 5644-5657.	5.4	5
5	UUCG RNA Tetraloop as a Formidable Force-Field Challenge for MD Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7601-7617.	5.3	29
6	Fine-Tuning of the AMBER RNA Force Field with a New Term Adjusting Interactions of Terminal Nucleotides. Journal of Chemical Theory and Computation, 2020, 16, 3936-3946.	5.3	39
7	Improving the Performance of the Amber RNA Force Field by Tuning the Hydrogen-Bonding Interactions. Journal of Chemical Theory and Computation, 2019, 15, 3288-3305.	5.3	97
8	Exploring RNA structure and dynamics through enhanced sampling simulations. Current Opinion in Structural Biology, 2018, 49, 63-71.	5.7	47
9	Molecular Dynamics Simulations Reveal an Interplay between SHAPE Reagent Binding and RNA Flexibility. Journal of Physical Chemistry Letters, 2018, 9, 313-318.	4.6	30
10	Understanding in-line probing experiments by modeling cleavage of nonreactive RNA nucleotides. Rna, 2017, 23, 712-720.	3.5	10
11	Mapping the Chemical Space of the RNA Cleavage and Its Implications for Ribozyme Catalysis. Journal of Physical Chemistry B, 2017, 121, 10828-10840.	2.6	4
12	The role of an active site Mg²⁺ in HDV ribozyme self-cleavage: insights from QM/MM calculations. Physical Chemistry Chemical Physics, 2015, 17, 670-679.	2.8	28
13	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
14	Comparison of ab Initio, DFT, and Semiempirical QM/MM Approaches for Description of Catalytic Mechanism of Hairpin Ribozyme. Journal of Chemical Theory and Computation, 2014, 10, 1608-1622.	5.3	56
15	QM/MM Studies of Hairpin Ribozyme Self-Cleavage Suggest the Feasibility of Multiple Competing Reaction Mechanisms. Journal of Physical Chemistry B, 2011, 115, 13911-13924.	2.6	33
16	Extensive Molecular Dynamics Simulations Showing That Canonical G8 and Protonated A38H⁺ Forms Are Most Consistent with Crystal Structures of Hairpin Ribozyme. Journal of Physical Chemistry B, 2010, 114, 6642-6652.	2.6	81