

# Pavel Banáš

## List of Publications by Year in descending order

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69  
papers

5,748  
citations

108046

37  
h-index

93651

72  
g-index

78  
all docs

78  
docs citations

78  
times ranked

6006  
citing authors

#	ARTICLE	IF	CITATIONS
1	Early steps of oxidative damage in DNA quadruplexes are position-dependent: Quantum mechanical and molecular dynamics analysis of human telomeric sequence containing ionized guanine. <i>International Journal of Biological Macromolecules</i> , 2022, 194, 882-894.	3.6	2
2	Toward Convergence in Folding Simulations of RNA Tetraloops: Comparison of Enhanced Sampling Techniques and Effects of Force Field Modifications. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2642-2656.	2.3	34
3	Automatic Learning of Hydrogen-Bond Fixes in the AMBER RNA Force Field. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4490-4502.	2.3	21
4	W-RESP: Well-Restrained Electrostatic Potential-Derived Charges. Revisiting the Charge Derivation Model. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3495-3509.	2.3	18
5	Molecular insights from theoretical calculations explain the differences in affinity and diffusion of airborne contaminants on surfaces of hBN and graphene. <i>Applied Surface Science</i> , 2021, 565, 150382.	3.1	2
6	UUCG RNA Tetraloop as a Formidable Force-Field Challenge for MD Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7601-7617.	2.3	29
7	Fine-Tuning of the AMBER RNA Force Field with a New Term Adjusting Interactions of Terminal Nucleotides. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3936-3946.	2.3	39
8	Parallel G-triplexes and G-hairpins as potential transitory ensembles in the folding of parallel-stranded DNA G-Quadruplexes. <i>Nucleic Acids Research</i> , 2019, 47, 7276-7293.	6.5	42
9	Variability of Câ€F Bonds Governs the Formation of Specific Structural Motifs in Fluorinated Graphenes. <i>Journal of Physical Chemistry C</i> , 2019, 123, 27896-27903.	1.5	22
10	Local-to-global signal transduction at the core of a Mn2+ sensing riboswitch. <i>Nature Communications</i> , 2019, 10, 4304.	5.8	24
11	Fitting Corrections to an RNA Force Field Using Experimental Data. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3425-3431.	2.3	54
12	Improving the Performance of the Amber RNA Force Field by Tuning the Hydrogen-Bonding Interactions. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3288-3305.	2.3	97
13	Ion Interactions across Graphene in Electrolyte Aqueous Solutions. <i>Journal of Physical Chemistry C</i> , 2019, 123, 9799-9806.	1.5	25
14	Investigations of Stacked DNA Base-Pair Steps: Highly Accurate Stacking Interaction Energies, Energy Decomposition, and Many-Body Stacking Effects. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 95-115.	2.3	55
15	RNA Structural Dynamics As Captured by Molecular Simulations: A Comprehensive Overview. <i>Chemical Reviews</i> , 2018, 118, 4177-4338.	23.0	408
16	Structural dynamics of propeller loop: towards folding of RNA G-quadruplex. <i>Nucleic Acids Research</i> , 2018, 46, 8754-8771.	6.5	29
17	Exploring the Dynamics of Propeller Loops in Human Telomeric DNA Quadruplexes Using Atomistic Simulations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2458-2480.	2.3	39
18	Noncanonical $\hat{\pm}/\hat{\beta}$ 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.	1.2	27

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19	Folding of guanine quadruplex moleculesâ€“funnel-like mechanism or kinetic partitioning? An overview from MD simulation studies. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2017, 1861, 1246-1263.	1.1	89
20	Mapping the Chemical Space of the RNA Cleavage and Its Implications for Ribozyme Catalysis. <i>Journal of Physical Chemistry B</i> , 2017, 121, 10828-10840.	1.2	4
21	How to understand atomistic molecular dynamics simulations of <sc>RNA</sc> and proteinâ€“<sc>RNA</sc> complexes?. <i>Wiley Interdisciplinary Reviews RNA</i> , 2017, 8, e1405.	3.2	54
22	Free Energy Landscape of GAGA and UUCG RNA Tetraloops. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4032-4038.	2.1	70
23	Exponential repulsion improves structural predictability of molecular docking. <i>Journal of Computational Chemistry</i> , 2016, 37, 2485-2494.	1.5	8
24	Computer Folding of RNA Tetraloops: Identification of Key Force Field Deficiencies. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4534-4548.	2.3	125
25	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, 15176-15190.	1.2	20
26	The role of an active site Mg <sup>2+</sup> in HDV ribozyme self-cleavage: insights from QM/MM calculations. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 670-679.	1.3	28
27	Insights into Stability and Folding of GNRA and UNCG Tetraloops Revealed by Microsecond Molecular Dynamics and Well-Tempered Metadynamics. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3866-3877.	2.3	60
28	Reactivity of Fluorographene: A Facile Way toward Graphene Derivatives. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 1430-1434.	2.1	90
29	Reactive Conformation of the Active Site in the Hairpin Ribozyme Achieved by Molecular Dynamics Simulations with $\mu/\tau$ Force Field Reparametrizations. <i>Journal of Physical Chemistry B</i> , 2015, 119, 4220-4229.	1.2	45
30	Chemical feasibility of the general acid/base mechanism of <i>glmS</i> ribozyme self-cleavage. <i>Biopolymers</i> , 2015, 103, 550-562.	1.2	9
31	Hairpins participating in folding of human telomeric sequence quadruplexes studied by standard and T-REMD simulations. <i>Nucleic Acids Research</i> , 2015, 43, gkv994.	6.5	47
32	Interplay between Ethanol Adsorption to High-Energy Sites and Clustering on Graphene and Graphite Alters the Measured Isosteric Adsorption Enthalpies. <i>Journal of Physical Chemistry C</i> , 2015, 119, 20535-20543.	1.5	31
33	Wobble pairs of the HDV ribozyme play specific roles in stabilization of active site dynamics. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 5887-5900.	1.3	6
34	Molecular dynamic simulations of protein/RNA complexes: CRISPR/Csy4 endoribonuclease. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2015, 1850, 1072-1090.	1.1	20
35	Anatomy of enzyme channels. <i>BMC Bioinformatics</i> , 2014, 15, 379.	1.2	89
36	The nature of high surface energy sites in graphene and graphite. <i>Carbon</i> , 2014, 73, 448-453.	5.4	38

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37	Molecular Dynamics Simulations of Nucleic Acids. From Tetranucleotides to the Ribosome. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1771-1782.	2.1	139
38	Comparison of ab Initio, DFT, and Semiempirical QM/MM Approaches for Description of Catalytic Mechanism of Hairpin Ribozyme. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1608-1622.	2.3	56
39	Energies and 2 <sup>+</sup> -Hydroxyl 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, 463-480.	2.3	24
40	Are Waters around RNA More than Just a Solvent? – An Insight from Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 401-411.	2.3	33
41	Disparate HDV ribozyme crystal structures represent intermediates on a rugged free-energy landscape. <i>Rna</i> , 2014, 20, 1112-1128.	1.6	15
42	Nature and magnitude of aromatic base stacking in DNA and RNA: Quantum chemistry, molecular mechanics, and experiment. <i>Biopolymers</i> , 2013, 99, 978-988.	1.2	106
43	MOLE 2.0: advanced approach for analysis of biomacromolecular channels. <i>Journal of Cheminformatics</i> , 2013, 5, 39.	2.8	262
44	Effect of Guanine to Inosine Substitution on Stability of Canonical DNA and RNA Duplexes: Molecular Dynamics Thermodynamics Integration Study. <i>Journal of Physical Chemistry B</i> , 2013, 117, 1872-1879.	1.2	42
45	Computer Folding of RNA Tetraloops? Are We There Yet?. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2115-2125.	2.3	84
46	Benchmark quantum-chemical calculations on a complete set of rotameric families of the DNA sugar-phosphate backbone and their comparison with modern density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 7295.	1.3	33
47	How to understand quantum chemical computations on DNA and RNA systems? A practical guide for non-specialists. <i>Methods</i> , 2013, 64, 3-11.	1.9	45
48	MOLEonline 2.0: interactive web-based analysis of biomacromolecular channels. <i>Nucleic Acids Research</i> , 2012, 40, W222-W227.	6.5	123
49	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.	2.3	231
50	The DNA and RNA sugar-phosphate backbone emerges as the key player. An overview of quantum-chemical, structural biology and simulation studies. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 15257.	1.3	76
51	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, 2448-2460.	2.3	67
52	Molecular Mechanism of preQ <sub>1</sub> Riboswitch Action: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2012, 116, 12721-12734.	1.2	43
53	Simulations of A-RNA Duplexes. The Effect of Sequence, Solute Force Field, Water Model, and Salt Concentration. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9899-9916.	1.2	64
54	Understanding RNA Flexibility Using Explicit Solvent Simulations: The Ribosomal and Group I Intron Reverse Kink-Turn Motifs. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2963-2980.	2.3	49

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55	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.	2.3	873
56	QM/MM Studies of Hairpin Ribozyme Self-Cleavage Suggest the Feasibility of Multiple Competing Reaction Mechanisms. <i>Journal of Physical Chemistry B</i> , 2011, 115, 13911-13924.	1.2	33
57	Theoretical Studies on the Intermolecular Interactions of Potentially Primordial Base-Pair Analogues. <i>Chemistry - A European Journal</i> , 2010, 16, 3057-3065.	1.7	13
58	Extensive Molecular Dynamics Simulations Showing That Canonical G8 and Protonated A38H <sup>+</sup> Forms Are Most Consistent with Crystal Structures of Hairpin Ribozyme. <i>Journal of Physical Chemistry B</i> , 2010, 114, 6642-6652.	1.2	81
59	Explicit Water Models Affect the Specific Solvation and Dynamics of Unfolded Peptides While the Conformational Behavior and Flexibility of Folded Peptides Remain Intact. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3569-3579.	2.3	108
60	Protonation States of the Key Active Site Residues and Structural Dynamics of the glmS Riboswitch As Revealed by Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8701-8712.	1.2	54
61	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.	2.3	339
62	Redesigning dehalogenase access tunnels as a strategy for degrading an anthropogenic substrate. <i>Nature Chemical Biology</i> , 2009, 5, 727-733.	3.9	238
63	Theoretical studies of RNA catalysis: Hybrid QM/MM methods and their comparison with MD and QM. <i>Methods</i> , 2009, 49, 202-216.	1.9	82
64	Two C-terminal ankyrin repeats form the minimal stable unit of the ankyrin repeat protein p18INK4c. <i>Journal of Molecular Modeling</i> , 2008, 14, 747-759.	0.8	6
65	Second step of hydrolytic dehalogenation in haloalkane dehalogenase investigated by QM/MM methods. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 70, 707-717.	1.5	24
66	General Base Catalysis for Cleavage by the Active-Site Cytosine of the Hepatitis Delta Virus Ribozyme: QM/MM Calculations Establish Chemical Feasibility. <i>Journal of Physical Chemistry B</i> , 2008, 112, 11177-11187.	1.2	46
67	Identification of tunnels in proteins, nucleic acids, inorganic materials and molecular ensembles. <i>Biotechnology Journal</i> , 2007, 2, 62-67.	1.8	53
68	Mechanism of enhanced conversion of 1,2,3-trichloropropane by mutant haloalkane dehalogenase revealed by molecular modeling. <i>Journal of Computer-Aided Molecular Design</i> , 2006, 20, 375-383.	1.3	25
69	CAVER: a new tool to explore routes from protein clefts, pockets and cavities. <i>BMC Bioinformatics</i> , 2006, 7, 316.	1.2	453