

# Petr Stadlbauer

## List of Publications by Year in descending order

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Version: 2024-02-01

25  
papers

1,180  
citations

471509

17  
h-index

610901

24  
g-index

29  
all docs

29  
docs citations

29  
times ranked

1078  
citing authors

#	ARTICLE	IF	CITATIONS
1	Reference Simulations of Noncanonical Nucleic Acids with Different İ± 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.	5.3	231
2	Molecular Dynamics Simulations of Nucleic Acids. From Tetranucleotides to the Ribosome. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1771-1782.	4.6	139
3	Structural dynamics of possible late-stage intermediates in folding of quadruplex DNA studied by molecular simulations. <i>Nucleic Acids Research</i> , 2013, 41, 7128-7143.	14.5	111
4	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.	2.4	89
5	Triplex intermediates in folding of human telomeric quadruplexes probed by microsecond-scale molecular dynamics simulations. <i>Biochimie</i> , 2014, 105, 22-35.	2.6	72
6	Structure of a Stable G-Hairpin. <i>Journal of the American Chemical Society</i> , 2017, 139, 3591-3594.	13.7	51
7	Coarse-Grained Simulations Complemented by Atomistic Molecular Dynamics Provide New Insights into Folding and Unfolding of Human Telomeric G-Quadruplexes. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 6077-6097.	5.3	50
8	Effect of Monovalent Ion Parameters on Molecular Dynamics Simulations of G-Quadruplexes. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3911-3926.	5.3	50
9	Extended molecular dynamics of a c-kit promoter quadruplex. <i>Nucleic Acids Research</i> , 2015, 43, 8673-8693.	14.5	49
10	Hairpins participating in folding of human telomeric sequence quadruplexes studied by standard and T-REMD simulations. <i>Nucleic Acids Research</i> , 2015, 43, gkv994.	14.5	47
11	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.	14.5	42
12	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.	5.3	39
13	Can We Execute Reliable MM-PBSA Free Energy Computations of Relative Stabilities of Different Guanine Quadruplex Folds?. <i>Journal of Physical Chemistry B</i> , 2016, 120, 2899-2912.	2.6	32
14	Structural dynamics of propeller loop: towards folding of RNA G-quadruplex. <i>Nucleic Acids Research</i> , 2018, 46, 8754-8771.	14.5	29
15	Structural Dynamics of Lateral and Diagonal Loops of Human Telomeric G-Quadruplexes in Extended MD Simulations. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5011-5026.	5.3	28
16	The beginning and the end: flanking nucleotides induce a parallel G-quadruplex topology. <i>Nucleic Acids Research</i> , 2021, 49, 9548-9559.	14.5	27
17	Conformations of Human Telomeric G-Quadruplex Studied Using a Nucleotide-Independent Nitroxide Label. <i>Biochemistry</i> , 2016, 55, 360-372.	2.5	19
18	Insights into G-Quadruplexâ€“Hemin Dynamics Using Atomistic Simulations: Implications for Reactivity and Folding. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1883-1899.	5.3	19

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19	Stability of Two-Quartet G-Quadruplexes and Their Dimers in Atomistic Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3447-3463.	5.3	16
20	G-Quadruplex Formation by DNA Sequences Deficient in Guanines: Two Tetrad Parallel Quadruplexes Do Not Fold Intramolecularly. <i>Chemistry - A European Journal</i> , 2021, 27, 12115-12125.	3.3	15
21	Tetraloop-like Geometries Could Form the Basis of the Catalytic Activity of the Most Ancient Ribooligonucleotides. <i>Chemistry - A European Journal</i> , 2015, 21, 3596-3604.	3.3	9
22	Molecular dynamics simulations of G-quadruplexes: The basic principles and their application to folding and ligand binding. <i>Annual Reports in Medicinal Chemistry</i> , 2020, , 197-241.	0.9	6
23	Exploring Sequence Space to Design Controllable G-Quadruplex Topology Switches. <i>CCS Chemistry</i> , 2022, 4, 3036-3050.	7.8	6
24	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.	7.5	2
25	Frontispiece: Tetraloop-like Geometries Could Form the Basis of the Catalytic Activity of the Most Ancient Ribooligonucleotides. <i>Chemistry - A European Journal</i> , 2015, 21, n/a-n/a.	3.3	0