



#	ARTICLE	IF	CITATIONS
1	The Drosophila RNA binding protein Hrp48 binds a specific RNA sequence of the msl-2 mRNA 3' UTR to regulate translation. <i>Biophysical Chemistry</i> , 2025, 316, 107346.	2.1	5
2	Computer Folding of Parallel DNA G-C Quadruplex: Hitchhiker's Guide to the Conformational Space. <i>Journal of Computational Chemistry</i> , 2025, 46, .	4.8	4
3	Refinement of the Sugar Puckering Torsion Potential in the AMBER DNA Force Field. <i>Journal of Chemical Theory and Computation</i> , 2025, 21, 833-846.	5.1	19
4	How Binding Site Flexibility Promotes RNA Scanning by TbRGG2 RRM: A Molecular Dynamics Simulation Study. <i>Journal of Chemical Information and Modeling</i> , 2025, 65, 896-907.	4.5	1
5	Can We Ever Develop an Ideal RNA Force Field? Lessons Learned from Simulations of the UUCG RNA Tetraloop and Other Systems. <i>Journal of Chemical Theory and Computation</i> , 2025, 21, 4183-4202.	5.1	23
6	Transcriptome-scale analysis uncovers conserved residues in the hydrophobic core of the bacterial RNA chaperone Hfq required for small regulatory RNA stability. <i>Nucleic Acids Research</i> , 2025, 53, .	15.5	3
7	The tautomer-specific excited state dynamics of 2,6-diaminopurine using resonance-enhanced multiphoton ionization and quantum chemical calculations. <i>Photochemistry and Photobiology</i> , 2024, 100, 404-418.	2.8	1
8	DNA Quadruplex Structure with a Unique Cation Dependency. <i>Angewandte Chemie - International Edition</i> , 2024, 63, .	14.4	10
9	DNA Quadruplex Structure with a Unique Cation Dependency. <i>Angewandte Chemie</i> , 2024, 136, .	1.4	0
10	Photoinduced charge separation and DNA self-repair depend on sequence directionality and stacking pattern. <i>Chemical Science</i> , 2024, 15, 2158-2166.	7.1	15
11	Molecular dynamics simulations reveal the parallel stranded d(GGGA)3GGG DNA quadruplex folds via multiple paths from a coil-like ensemble. <i>International Journal of Biological Macromolecules</i> , 2024, 261, 129712.	8.1	12
12	The tautomer-specific excited state dynamics of 2,6-diaminopurine using resonance-enhanced multiphoton ionization and quantum chemical calculations. <i>Photochemistry and Photobiology</i> , 2024, 100, 404-418.	2.8	0
13	Mechanical Stability and Unfolding Pathways of Parallel Tetrameric G-Quadruplexes Probed by Pulling Simulations. <i>Journal of Chemical Information and Modeling</i> , 2024, 64, 3896-3911.	4.5	4
14	Structure of an internal loop motif with three consecutive U-CU mismatches from stem-loop 1 in the 3'-UTR of the SARS-CoV-2 genomic RNA. <i>Nucleic Acids Research</i> , 2024, 52, 6687-6706.	15.5	12
15	Comprehensive Assessment of Force-Field Performance in Molecular Dynamics Simulations of DNA/RNA Hybrid Duplexes. <i>Journal of Chemical Theory and Computation</i> , 2024, 20, 6917-6929.	5.1	22
16	Phosphoric acid salts of amino acids as a source of oligopeptides on the early Earth. <i>Communications Chemistry</i> , 2024, 7, .	5.5	6
17	N-terminal domain of polypyrimidine-tract binding protein is a dynamic folding platform for adaptive RNA recognition. <i>Nucleic Acids Research</i> , 2024, 52, 10683-10704.	15.5	2
18	Molecular Simulations to Investigate the Impact of N6-Methylation in RNA Recognition: Improving Accuracy and Precision of Binding Free Energy Prediction. <i>Journal of Physical Chemistry B</i> , 2024, 128, 8896-8907.	2.7	2

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19	Structural and dynamic effects of pseudouridine modifications on noncanonical interactions in RNA. <i>Rna</i> , 2023, 29, 790-807.	3.8	17
20	Sensitivity of the RNA Structure to Ion Conditions as Probed by Molecular Dynamics Simulations of Common Canonical RNA Duplexes. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 2133-2146.	4.5	24
21	Atomistic Picture of Opening&#x2013;Closing Dynamics of DNA Holliday Junction Obtained by Molecular Simulations. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 2794-2809.	4.5	11
22	Influence of Silicate Rock Glass Compositions on the Efficacy of Prebiotic RNA Polymerization Reactions: The Case of 3&#x2013;5&#x2013;Cyclic Guanosine Monophosphate. <i>ChemSystemsChem</i> , 2023, 5, .	2.7	0
23	Assessing the Current State of Amber Force Field Modifications for DNA&#x2013;2023 Edition. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 4299-4307.	5.1	56
24	Complexity of Guanine Quadruplex Unfolding Pathways Revealed by Atomistic Pulling Simulations. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 4716-4731.	4.5	8
25	The Reactivity-Enhancing Role of Water Clusters in Ammonia Aqueous Solutions. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 7808-7813.	4.2	28
26	Prebiotic Synthesis of 3&#x2013;5&#x2013;Cyclic Adenosine and Guanosine Monophosphates through Carbodiimide&#x2013;Assisted Cyclization. <i>ChemBioChem</i> , 2023, 24, .	2.6	2
27	Topology of DNA G-Quadruplexes Can Be Harnessed in Holliday Junction-Based DNA Suprastructures to Control and Optimize Their Biocatalytic Properties. <i>ACS Catalysis</i> , 2023, 13, 10722-10733.	12.4	7
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29	Simple Adjustment of Intranucleotide Base-Phosphate Interaction in the OL3 AMBER Force Field Improves RNA Simulations. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 8423-8433.	5.1	23
30	Exploring Sequence Space to Design Controllable G-Quadruplex Topology Switches. <i>CCS Chemistry</i> , 2022, 4, 3036-3050.	8.6	18
31	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.	8.1	4
32	RNA kink-turns are highly anisotropic with respect to lateral displacement of the flanking stems. <i>Biophysical Journal</i> , 2022, 121, 705-714.	2.2	4
33	Photoinduced water&#x2013;chromophore electron transfer causes formation of guanosine photodamage. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 8217-8224.	2.7	7
34	Hydrolysis of Al3+ in Aqueous Solutions: Experiments and Ab Initio Simulations. <i>Liquids</i> , 2022, 2, 26-38.	2.1	18
35	Binding of Arsenic by Common Functional Groups: An Experimental and Quantum-Mechanical Study. <i>Applied Sciences (Switzerland)</i> , 2022, 12, 3210.	2.1	20
36	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.	5.1	56



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56	Electric Field and Temperature Effects on the Ab Initio Spectroscopy of Liquid Methanol. <i>Applied Sciences (Switzerland)</i> , 2021, 11, 5457.	2.1	4
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59	Ribose Alters the Photochemical Properties of the Nucleobase in Thionated Nucleosides. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6707-6713.	4.2	11
60	Nonenzymatic, Templateâ€Free Polymerization of 3â€™,5â€™ Cyclic Guanosine Monophosphate on Mineral Surfaces. <i>ChemSystemsChem</i> , 2021, 3, .	2.7	8
61	Ab Initio Molecular Dynamics Studies of the Electric-Field-Induced Catalytic Effects on Liquids. <i>Topics in Catalysis</i> , 2021, 65, 40-58.	2.5	31
62	Questions and Answers Related to the Prebiotic Production of Oligonucleotide Sequences from 3â€²,5â€² Cyclic Nucleotide Precursors. <i>Life</i> , 2021, 11, 800.	2.6	6
63	The beginning and the end: flanking nucleotides induce a parallel G-quadruplex topology. <i>Nucleic Acids Research</i> , 2021, 49, 9548-9559.	15.5	48
64	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.	5.1	78
65	MD simulations reveal the basis for dynamic assembly of Hfqâ€RNA complexes. <i>Journal of Biological Chemistry</i> , 2021, 296, 100656.	2.2	13
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74	UV-induced hydrogen transfer in DNA base pairs promoted by dark nI* states. Chemical Communications, 2020, 56, 201-204.	3.4	10
75	Short but Weak: The Z-DNA Lone-Pair...-Conundrum Challenges Standard Carbon Van der Waals Radii. Angewandte Chemie, 2020, 132, 16696-16703.	1.4	1
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92	Enhanced conductivity of water at the electrified airâ€“water interface: a DFT-MD characterization. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 10438-10446.	2.7	18
93	Prebiotic synthesis at impact craters: the role of Fe-clays and iron meteorites. <i>Chemical Communications</i> , 2019, 55, 10563-10566.	3.4	20
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95	<i>Ab initio</i> spectroscopy of water under electric fields. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21205-21212.	2.7	72
96	Interaction between As(III) and Simple Thioacids in Water: An Experimental and <i>ab Initio</i> Molecular Dynamics Investigation. <i>Journal of Physical Chemistry B</i> , 2019, 123, 6090-6098.	2.7	11
97	Role of Fine Structural Dynamics in Recognition of Histone H3 by HP1 <sup>3</sup> (CSD) Dimer and Ability of Force Fields to Describe Their Interaction Network. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5659-5673.	5.1	2
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103	Photodynamics of alternative DNA base isoguanine. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 13474-13485.	2.7	27
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105	Fitting Corrections to an RNA Force Field Using Experimental Data. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3425-3431.	5.1	73
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107	Catalyst-Free Hydrogen Synthesis from Liquid Ethanol: An <i>ab Initio</i> Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 9202-9208.	3.1	32
108	Interactions between cyclic nucleotides and common cations: an <i>ab initio</i> molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8121-8132.	2.7	18

#	ARTICLE	IF	CITATIONS
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