Jir Sponer

List of Publications by Year in Descending Order

396 papers	24,203 citations	76 h-index	141 g-index
432 ext. papers	26,609 ext. citations	6.7 avg, IF	7.01 L-index

#	Paper	IF	Citations
396	Hydrolysis of Al3+ in Aqueous Solutions: Experiments and Ab Initio Simulations. *Liquids*, **2022**, 2, 26-38		0
395	Binding of Arsenic by Common Functional Groups: An Experimental and Quantum-Mechanical Study. *Applied Sciences (Switzerland)*, **2022**, 12, 3210	2.6	1
394	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**,	6.4	4
393	Short-Range Imbalances in the AMBER Lennard-Jones Potential for (Deoxy)Ribose□Nucleobase Lone-Pair□Contacts in Nucleic Acids. *Journal of Chemical Information and Modeling*, **2021**, 61, 5644-5657	6.1	2
392	Acid-Catalyzed RNA-Oligomerization from 3',5'-cGMP. *Chemistry - A European Journal*, **2021**,	4.8	3
391	Early steps of oxidative damage in DNA quadruplexes are position-dependent: Quantum mechanical and molecular dynamics analysis of human telomeric sequence containing ionized guanine. *International Journal of Biological Macromolecules*, **2021**, 194, 882-882	7.9	1
390	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCEngine): Automation and interoperability among computational chemistry programs. *Journal of Chemical Physics*, **2021**, 155, 204801	3.9	3
389	molecular dynamics simulations and experimental speciation study of levofloxacin under different pH conditions. *Physical Chemistry Chemical Physics*, **2021**, 23, 24403-24412	3.6	1
388	Molecular dissociation and proton transfer in aqueous methane solution under an electric field. *Physical Chemistry Chemical Physics*, **2021**, 23, 25649-25657	3.6	1
387	Atomistic simulations of the free-energy landscapes of interstellar chemical reactions: the case of methyl isocyanate. *Monthly Notices of the Royal Astronomical Society*, **2021**, 504, 1565-1570	4.3	3
386	2,6-diaminopurine promotes repair of DNA lesions under prebiotic conditions. *Nature Communications*, **2021**, 12, 3018	17.4	4
385	Thermal Decomposition of Cocaine and Methamphetamine Investigated by Infrared Spectroscopy and Quantum Chemical Simulations. *ACS Omega*, **2021**, 6, 14447-14457	3.9	1
384	W-RESP: Well-Restrained Electrostatic Potential-Derived Charges. Revisiting the Charge Derivation Model. *Journal of Chemical Theory and Computation*, **2021**, 17, 3495-3509	6.4	6
383	Electric Field and Temperature Effects on the Ab Initio Spectroscopy of Liquid Methanol. *Applied Sciences (Switzerland)*, **2021**, 11, 5457	2.6	1
382	Recognition of N6-Methyladenosine by the YTHDC1 YTH Domain Studied by Molecular Dynamics and NMR Spectroscopy: The Role of Hydration. *Journal of Physical Chemistry B*, **2021**, 125, 7691-7705	3.4	3
381	G-Quadruplex Formation by DNA Sequences Deficient in Guanines: Two Tetrad Parallel Quadruplexes Do Not Fold Intramolecularly. *Chemistry - A European Journal*, **2021**, 27, 12115-12125	4.8	4
380	Ribose Alters the Photochemical Properties of the Nucleobase in Thionated Nucleosides. *Journal of Physical Chemistry Letters*, **2021**, 12, 6707-6713	6.4	1

379	Sustainability and Chaos in the Abiotic Polymerization of 3?,5? Cyclic Guanosine Monophosphate: The Role of Aggregation. *ChemSystemsChem*, **2021**, 3, e2000011	3.1	2
378	Residues flanking the ARKT/S motif allow binding of diverse targets to the HP1 chromodomain: Insights from molecular dynamics simulations. *Biochimica Et Biophysica Acta - General Subjects*, **2021**, 1865, 129771	4	
377	Phosphorothioate Substitutions in RNA Structure Studied by Molecular Dynamics Simulations, QM/MM Calculations, and NMR Experiments. *Journal of Physical Chemistry B*, **2021**, 125, 825-840	3.4	6
376	Insight into formation propensity of pseudocircular DNA G-hairpins. *Nucleic Acids Research*, **2021**, 49, 2317-2332	20.1	1
375	Insights into G-Quadruplex-Hemin Dynamics Using Atomistic Simulations: Implications for Reactivity and Folding. *Journal of Chemical Theory and Computation*, **2021**, 17, 1883-1899	6.4	4
374	Questions and Answers Related to the Prebiotic Production of Oligonucleotide Sequences from 3',5' Cyclic Nucleotide Precursors. *Life*, **2021**, 11,	3	1
373	The beginning and the end: flanking nucleotides induce a parallel G-quadruplex topology. *Nucleic Acids Research*, **2021**, 49, 9548-9559	20.1	5
372	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
371	Insoluble organic matter - an "organic" cradle of life: Comment on the paper "Insoluble organic matter in chondrites: Archetypal melanin-like PAH-based multifunctionality at the origin of life?" by Marco d'Ischia et al. *Physics of Life Reviews*, **2021**, 38, 135-136	2.1	
370	MD simulations reveal the basis for dynamic assembly of Hfq-RNA complexes. *Journal of Biological Chemistry*, **2021**, 296, 100656	5.4	4
369	Structure of SRSF1 RRM1 bound to RNA reveals an unexpected bimodal mode of interaction and explains its involvement in SMN1 exon7 splicing. *Nature Communications*, **2021**, 12, 428	17.4	9
368	Electric-Field-Induced Effects on the Dipole Moment and Vibrational Modes of the Centrosymmetric Indigo Molecule. *Journal of Physical Chemistry A*, **2020**, 124, 10856-10869	2.8	7
367	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	6.4	15
366	Composite 5-methylations of cytosines modulate i-motif stability in a sequence-specific manner: Implications for DNA nanotechnology and epigenetic regulation of plant telomeric DNA. *Biochimica Et Biophysica Acta - General Subjects*, **2020**, 1864, 129651	4	9
365	Short but Weak: The Z-DNA Lone-Pair???Conundrum Challenges Standard Carbon Van der Waals Radii. *Angewandte Chemie - International Edition*, **2020**, 59, 16553-16560	16.4	11
364	Surprisingly broad applicability of the cc-pVnZ-F12 basis set for ground and excited states. *Journal of Chemical Physics*, **2020**, 152, 214104	3.9	3
363	Compensatory Mechanisms in Temperature Dependence of DNA Double Helical Structure: Bending and Elongation. *Journal of Chemical Theory and Computation*, **2020**, 16, 2857-2863	6.4	7
362	Removal of As(III) from Biological Fluids: Mono- versus Dithiolic Ligands. *Chemical Research in Toxicology*, **2020**, 33, 967-974	4	10

361	Stability of Two-Quartet G-Quadruplexes and Their Dimers in Atomistic Simulations. *Journal of Chemical Theory and Computation*, **2020**, 16, 3447-3463	6.4	7
360	Arsenic-nucleotides interactions: an experimental and computational investigation. *Dalton Transactions*, **2020**, 49, 6302-6311	4.3	5
359	Enhanced conductivity of water at the electrified air-water interface: a DFT-MD characterization. *Physical Chemistry Chemical Physics*, **2020**, 22, 10438-10446	3.6	6
358	Meteorite-Assisted Phosphorylation of Adenosine Under Proton Irradiation Conditions. *ChemSystemsChem*, **2020**, 2, e1900039	3.1	4
357	Short but Weak: The Z-DNA Lone-Pair???Conundrum Challenges Standard Carbon Van der Waals Radii. *Angewandte Chemie*, **2020**, 132, 16696	3.6	
356	UUCG RNA Tetraloop as a Formidable Force-Field Challenge for MD Simulations. *Journal of Chemical Theory and Computation*, **2020**, 16, 7601-7617	6.4	9
355	Ariel a window to the origin of life on early earth?. *Experimental Astronomy*, **2020**, 1	1.3	1
354	Molecular dynamics simulations of G-quadruplexes: The basic principles and their application to folding and ligand binding. *Annual Reports in Medicinal Chemistry*, **2020**, 197-241	1.6	3
353	Formic acid, the precursor of formamide, from serpentinization: Comment on the paper: "Mineral self-organization on a lifeless planet" by Juan Manuel Garc-Ruiz, Mark A. van Zuilen and Wolfgang Bach. *Physics of Life Reviews*, **2020**, 34-35, 94-95	2.1	1
352	One-Pot Hydrogen Cyanide-Based Prebiotic Synthesis of Canonical Nucleobases and Glycine Initiated by High-Velocity Impacts on Early Earth. *Astrobiology*, **2020**, 20, 1476-1488	3.7	7
351	High-Energy Proton-Beam-Induced Polymerization/Oxygenation of Hydroxynaphthalenes on Meteorites and Nitrogen Transfer from Urea: Modeling Insoluble Organic Matter?. *Chemistry - A European Journal*, **2020**, 26, 14919-14928	4.8	5
350	Molecular Dynamics Study of Methanol-Water Mixtures under External Electric Fields. *Molecules*, **2020**, 25,	4.8	7
349	Formic Acid, a Ubiquitous but Overlooked Component of the Early Earth Atmosphere. *Chemistry - A European Journal*, **2020**, 26, 12075-12080	4.8	6
348	Stereocontrolled Synthesis of (-)-Bactobolin A. *Journal of the American Chemical Society*, **2020**, 142, 7306-7311	16.4	9
347	Role of Fine Structural Dynamics in Recognition of Histone H3 by HP1 (CSD) Dimer and Ability of Force Fields to Describe Their Interaction Network. *Journal of Chemical Theory and Computation*, **2019**, 15, 5659-5673	6.4	1
346	RuvC uses dynamic probing of the Holliday junction to achieve sequence specificity and efficient resolution. *Nature Communications*, **2019**, 10, 4102	17.4	10
345	Local-to-global signal transduction at the core of a Mn sensing riboswitch. *Nature Communications*, **2019**, 10, 4304	17.4	9
344	Revisiting the Potential Energy Surface of the Stacked Cytosine Dimer: FNO-CCSD(T) Interaction Energies, SAPT Decompositions, and Benchmarking. *Journal of Physical Chemistry A*, **2019**, 123, 9209-9222	2.8	5

343	Photodynamics of alternative DNA base isoguanine. *Physical Chemistry Chemical Physics*, **2019**, 21, 13474-13485	3.6	3
342	Structural and Energetic Compatibility: The Driving Principles of Molecular Evolution. *Astrobiology*, **2019**, 19, 1117-1122	3.7	3
341	Fitting Corrections to an RNA Force Field Using Experimental Data. *Journal of Chemical Theory and Computation*, **2019**, 15, 3425-3431	6.4	31
340	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	6.4	56
339	Catalyst-Free Hydrogen Synthesis from Liquid Ethanol: An ab Initio Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2019**, 123, 9202-9208	3.8	14
338	Interactions between cyclic nucleotides and common cations: an ab initio molecular dynamics study. *Physical Chemistry Chemical Physics*, **2019**, 21, 8121-8132	3.6	7
337	Stabilization of Short Oligonucleotides in the Prebiotic Mix: The Potential Role of Amino Alcohols. *ChemSystemsChem*, **2019**, 1, e1900006	3.1	1
336	Molecular basis for AU-rich element recognition and dimerization by the HuR C-terminal RRM. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 2935-2944	11.5	36
335	Comment on "Evaluating Unexpectedly Short Non-covalent Distances in X-ray Crystal Structures of Proteins with Electronic Structure Analysis". *Journal of Chemical Information and Modeling*, **2019**, 59, 3605-3608	6.1	9
334	Prebiotic synthesis at impact craters: the role of Fe-clays and iron meteorites. *Chemical Communications*, **2019**, 55, 10563-10566	5.8	9
333	Parallel G-triplexes and G-hairpins as potential transitory ensembles in the folding of parallel-stranded DNA G-Quadruplexes. *Nucleic Acids Research*, **2019**, 47, 7276-7293	20.1	24
332	Ab initio spectroscopy of water under electric fields. *Physical Chemistry Chemical Physics*, **2019**, 21, 21205-21212	3.6	5
331	Interaction between As(III) and Simple Thioacids in Water: An Experimental and ab Initio Molecular Dynamics Investigation. *Journal of Physical Chemistry B*, **2019**, 123, 6090-6098	3.4	9
330	UV-induced hydrogen transfer in DNA base pairs promoted by dark nπ* states. *Chemical Communications*, **2019**, 56, 201-204	5.8	4
329	Combining NMR Spectroscopy and Molecular Dynamic Simulations to Solve and Analyze the Structure of Protein-RNA Complexes. *Methods in Enzymology*, **2019**, 614, 393-422	1.7	6
328	Investigations of Stacked DNA Base-Pair Steps: Highly Accurate Stacking Interaction Energies, Energy Decomposition, and Many-Body Stacking Effects. *Journal of Chemical Theory and Computation*, **2019**, 15, 95-115	6.4	39
327	Sequential electron transfer governs the UV-induced self-repair of DNA photolesions. *Chemical Science*, **2018**, 9, 3131-3140	9.4	16
326	Highly accurate equilibrium structure of the C2h symmetric N1-to-O2 hydrogen-bonded uracil-dimer. *International Journal of Quantum Chemistry*, **2018**, 118, e25624	2.1	8

325	Mobilities of iodide anions in aqueous solutions for applications in natural dye-sensitized solar cells. *Physical Chemistry Chemical Physics*, **2018**, 20, 13038-13046	3.6	20
324	Synthesis of (d)-erythrose from glycolaldehyde aqueous solutions under electric field. *Chemical Communications*, **2018**, 54, 3211-3214	5.8	39
323	RNA Structural Dynamics As Captured by Molecular Simulations: A Comprehensive Overview. *Chemical Reviews*, **2018**, 118, 4177-4338	68.1	235
322	Rewarming the Primordial Soup: Revisitations and Rediscoveries in Prebiotic Chemistry. *ChemBioChem*, **2018**, 19, 22-25	3.8	7
321	Chemomimesis and Molecular Darwinism in Action: From Abiotic Generation of Nucleobases to Nucleosides and RNA. *Life*, **2018**, 8,	3	9
320	An intricate balance of hydrogen bonding, ion atmosphere and dynamics facilitates a seamless uracil to cytosine substitution in the U-turn of the neomycin-sensing riboswitch. *Nucleic Acids Research*, **2018**, 46, 6528-6543	20.1	16
319	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
318	Mechanism of polypurine tract primer generation by HIV-1 reverse transcriptase. *Journal of Biological Chemistry*, **2018**, 293, 191-202	5.4	12
317	Molecular basis for the increased affinity of an RNA recognition motif with re-engineered specificity: A molecular dynamics and enhanced sampling simulations study. *PLoS Computational Biology*, **2018**, 14, e1006642	5	8
316	Photostability of oxazoline RNA-precursors in UV-rich prebiotic environments. *Chemical Communications*, **2018**, 54, 13407-13410	5.8	9
315	Selective prebiotic conversion of pyrimidine and purine anhydronucleosides into Watson-Crick base-pairing arabino-furanosyl nucleosides in water. *Nature Communications*, **2018**, 9, 4073	17.4	29
314	How Proximal Nucleobases Regulate the Catalytic Activity of G-Quadruplex/Hemin DNAzymes. *ACS Catalysis*, **2018**, 8, 11352-11361	13.1	33
313	Dust Motions in Magnetized Turbulence: Source of Chemical Complexity. *Astrophysical Journal Letters*, **2018**, 866, L23	7.9	11
312	Structural Dynamics of Lateral and Diagonal Loops of Human Telomeric G-Quadruplexes in Extended MD Simulations. *Journal of Chemical Theory and Computation*, **2018**, 14, 5011-5026	6.4	23
311	QM/MM Calculations on Protein-RNA Complexes: Understanding Limitations of Classical MD Simulations and Search for Reliable Cost-Effective QM Methods. *Journal of Chemical Theory and Computation*, **2018**, 14, 5419-5433	6.4	22
310	Stability of hydrolytic arsenic species in aqueous solutions: Asvs. As. *Physical Chemistry Chemical Physics*, **2018**, 20, 23272-23280	3.6	26
309	Structural dynamics of propeller loop: towards folding of RNA G-quadruplex. *Nucleic Acids Research* , **2018**, 46, 8754-8771	20.1	18
308	Electron-driven proton transfer enables nonradiative photodeactivation in microhydrated 2-aminoimidazole. *Faraday Discussions*, **2018**, 212, 345-358	3.6	3

307	Solvation effects alter the photochemistry of 2-thiocytosine. *Chemical Physics*, **2018**, 515, 502-508	2.3	8
306	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
305	Computational Modeling of DNA and RNA Fragments **2017**, 1803-1826		1
304	Metal Interactions with Nucleobases, Base Pairs, and Oligomer Sequences; Computational Approach **2017**, 1827-1874		1
303	Structure of a Stable G-Hairpin. *Journal of the American Chemical Society*, **2017**, 139, 3591-3594	16.4	36
302	Coordination between the polymerase and RNase H activity of HIV-1 reverse transcriptase. *Nucleic Acids Research*, **2017**, 45, 3341-3352	20.1	23
301	Selectivity of major isoquinoline alkaloids from Chelidonium majus towards telomeric G-quadruplex: A study using a transition-FRET (t-FRET) assay. *Biochimica Et Biophysica Acta - General Subjects*, **2017**, 1861, 2020-2030	4	25
300	Nonenzymatic Oligomerization of 3',5'-Cyclic CMP Induced by Proton and UV Irradiation Hints at a Nonfastidious Origin of RNA. *ChemBioChem*, **2017**, 18, 1535-1543	3.8	12
299	Exploring the Dynamics of Propeller Loops in Human Telomeric DNA Quadruplexes Using Atomistic Simulations. *Journal of Chemical Theory and Computation*, **2017**, 13, 2458-2480	6.4	30
298	rRNA C-Loops: Mechanical Properties of a Recurrent Structural Motif. *Journal of Chemical Theory and Computation*, **2017**, 13, 3359-3371	6.4	5
297	Water-chromophore electron transfer determines the photochemistry of cytosine and cytidine. *Physical Chemistry Chemical Physics*, **2017**, 19, 17531-17537	3.6	16
296	Channeling through Two Stacked Guanine Quartets of One and Two Alkali Cations in the Li, Na, K, and Rb Series. Assessment of the Accuracy of the SIBFA Anisotropic Polarizable Molecular Mechanics Potential. *Journal of Physical Chemistry B*, **2017**, 121, 3997-4014	3.4	18
295	Noncanonical αBackbone 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
294	Stability of 2',3' and 3',5' cyclic nucleotides in formamide and in water: a theoretical insight into the factors controlling the accumulation of nucleic acid building blocks in a prebiotic pool. *Physical Chemistry Chemical Physics*, **2017**, 19, 1817-1825	3.6	14
293	Folding of guanine quadruplex molecules-funnel-like mechanism or kinetic partitioning? An overview from MD simulation studies. *Biochimica Et Biophysica Acta - General Subjects*, **2017**, 1861, 1246-1263	4	66
292	MD and QM/MM Study of the Quaternary HutP Homohexamer Complex with mRNA, l-Histidine Ligand, and Mg. *Journal of Chemical Theory and Computation*, **2017**, 13, 5658-5670	6.4	13
291	Aromatic side-chain conformational switch on the surface of the RNA Recognition Motif enables RNA discrimination. *Nature Communications*, **2017**, 8, 654	17.4	15
290	Ionic diffusion and proton transfer in aqueous solutions of alkali metal salts. *Physical Chemistry Chemical Physics*, **2017**, 19, 20420-20429	3.6	36

289	Structural study of the Fox-1 RRM protein hydration reveals a role for key water molecules in RRM-RNA recognition. *Nucleic Acids Research*, **2017**, 45, 8046-8063	20.1	24
288	Novel electrochemical route to cleaner fuel dimethyl ether. *Scientific Reports*, **2017**, 7, 6901	4.9	21
287	Multifunctional energy landscape for a DNA G-quadruplex: An evolved molecular switch. *Journal of Chemical Physics*, **2017**, 147, 152715	3.9	22
286	Mapping the Chemical Space of the RNA Cleavage and Its Implications for Ribozyme Catalysis. *Journal of Physical Chemistry B*, **2017**, 121, 10828-10840	3.4	4
285	Proton irradiation: a key to the challenge of N-glycosidic bond formation in a prebiotic context. *Scientific Reports*, **2017**, 7, 14709	4.9	24
284	Effect of Monovalent Ion Parameters on Molecular Dynamics Simulations of G-Quadruplexes. *Journal of Chemical Theory and Computation*, **2017**, 13, 3911-3926	6.4	42
283	How to understand atomistic molecular dynamics simulations of RNA and protein-RNA complexes?. *Wiley Interdisciplinary Reviews RNA*, **2017**, 8, e1405	9.3	42
282	New evolutionary insights into the non-enzymatic origin of RNA oligomers. *Wiley Interdisciplinary Reviews RNA*, **2017**, 8, e1400	9.3	11
281	A prebiotically plausible synthesis of pyrimidine β-ribonucleosides and their phosphate derivatives involving photoanomerization. *Nature Chemistry*, **2017**, 9, 303-309	17.6	81
280	Computer Folding of RNA Tetraloops: Identification of Key Force Field Deficiencies. *Journal of Chemical Theory and Computation*, **2016**, 12, 4534-48	6.4	77
279	Coarse-Grained Simulations Complemented by Atomistic Molecular Dynamics Provide New Insights into Folding and Unfolding of Human Telomeric G-Quadruplexes. *Journal of Chemical Theory and Computation*, **2016**, 12, 6077-6097	6.4	35
278	Ultrafast excited-state dynamics of isocytosine. *Physical Chemistry Chemical Physics*, **2016**, 18, 20208-18	3.6	27
277	Synergy between NMR measurements and MD simulations of protein/RNA complexes: application to the RRMs, the most common RNA recognition motifs. *Nucleic Acids Research*, **2016**, 44, 6452-70	20.1	43
276	Assessing the Current State of Amber Force Field Modifications for DNA. *Journal of Chemical Theory and Computation*, **2016**, 12, 4114-27	6.4	203
275	Photorelaxation of imidazole and adenine via electron-driven proton transfer along HO wires. *Faraday Discussions*, **2016**, 195, 237-251	3.6	11
274	On the Use of Molecular Dynamics Simulations for Probing Allostery through DNA. *Biophysical Journal*, **2016**, 110, 874-6	2.9	11
273	Derivation of Reliable Geometries in QM Calculations of DNA Structures: Explicit Solvent QM/MM and Restrained Implicit Solvent QM Optimizations of G-Quadruplexes. *Journal of Chemical Theory and Computation*, **2016**, 12, 2000-16	6.4	20
272	Can We Execute Reliable MM-PBSA Free Energy Computations of Relative Stabilities of Different Guanine Quadruplex Folds?. *Journal of Physical Chemistry B*, **2016**, 120, 2899-912	3.4	25

271	Non-Enzymatic Oligomerization of 3', 5' Cyclic AMP. *PLoS ONE*, **2016**, 11, e0165723	3.7	10
270	TiO2-catalyzed synthesis of sugars from formaldehyde in extraterrestrial impacts on the early Earth. *Scientific Reports*, **2016**, 6, 23199	4.9	22
269	Computational Modeling of DNA and RNA Fragments **2016**, 1-24		
268	Molecular Dynamics Simulation Study of Parallel Telomeric DNA Quadruplexes at Different Ionic Strengths: Evaluation of Water and Ion Models. *Journal of Physical Chemistry B*, **2016**, 120, 7380-91	3.4	26
267	Four Ways to Oligonucleotides Without Phosphoimidazolides. *Journal of Molecular Evolution*, **2016**, 82, 5-10	3.1	7
266	Emergence of the First Catalytic Oligonucleotides in a Formamide-Based Origin Scenario. *Chemistry - A European Journal*, **2016**, 22, 3572-86	4.8	52
265	Prebiotic synthesis of nucleic acids and their building blocks at the atomic level - merging models and mechanisms from advanced computations and experiments. *Physical Chemistry Chemical Physics*, **2016**, 18, 20047-66	3.6	40
264	Conformations of Human Telomeric G-Quadruplex Studied Using a Nucleotide-Independent Nitroxide Label. *Biochemistry*, **2016**, 55, 360-72	3.2	18
263	Free Energy Landscape of GAGA and UUCG RNA Tetraloops. *Journal of Physical Chemistry Letters*, **2016**, 7, 4032-4038	6.4	49
262	Comparative Assessment of Different RNA Tetranucleotides from the DFT-D3 and Force Field Perspective. *Journal of Physical Chemistry B*, **2016**, 120, 10635-10648	3.4	14
261	The role of an active site Mg(2+) in HDV ribozyme self-cleavage: insights from QM/MM calculations. *Physical Chemistry Chemical Physics*, **2015**, 17, 670-9	3.6	22
260	Insights into Stability and Folding of GNRA and UNCG Tetraloops Revealed by Microsecond Molecular Dynamics and Well-Tempered Metadynamics. *Journal of Chemical Theory and Computation*, **2015**, 11, 3866-77	6.4	39
259	Stacked and H-Bonded Cytosine Dimers. Analysis of the Intermolecular Interaction Energies by Parallel Quantum Chemistry and Polarizable Molecular Mechanics. *Journal of Physical Chemistry B*, **2015**, 119, 9477-95	3.4	17
258	A G-quadruplex-binding compound showing anti-tumour activity in an in vivo model for pancreatic cancer. *Scientific Reports*, **2015**, 5, 11385	4.9	77
257	Conformational dynamics of bacterial and human cytoplasmic models of the ribosomal A-site. *Biochimie*, **2015**, 112, 96-110	4.6	8
256	Reactive conformation of the active site in the hairpin ribozyme achieved by molecular dynamics simulations with □ force field reparametrizations. *Journal of Physical Chemistry B*, **2015**, 119, 4220-9	3.4	31
255	Electron-Driven Proton Transfer Along H2O Wires Enables Photorelaxation of □ States in Chromophore-Water Clusters. *Journal of Physical Chemistry Letters*, **2015**, 6, 1467-71	6.4	29
254	Extended molecular dynamics of a c-kit promoter quadruplex. *Nucleic Acids Research*, **2015**, 43, 8673-93	20.1	40

253	Chemical feasibility of the general acid/base mechanism of glmS ribozyme self-cleavage. *Biopolymers*, **2015**, 103, 550-62	2.2	8
252	Hairpins participating in folding of human telomeric sequence quadruplexes studied by standard and T-REMD simulations. *Nucleic Acids Research*, **2015**, 43, 9626-44	20.1	37
251	Wobble pairs of the HDV ribozyme play specific roles in stabilization of active site dynamics. *Physical Chemistry Chemical Physics*, **2015**, 17, 5887-900	3.6	3
250	Quantum chemical benchmark study on 46 RNA backbone families using a dinucleotide unit. *Journal of Chemical Theory and Computation*, **2015**, 11, 4972-91	6.4	74
249	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
248	Towards biochemically relevant QM computations on nucleic acids: controlled electronic structure geometry optimization of nucleic acid structural motifs using penalty restraint functions. *Physical Chemistry Chemical Physics*, **2015**, 17, 1399-410	3.6	22
247	High-energy chemistry of formamide: a unified mechanism of nucleobase formation. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 657-62	11.5	132
246	Molecular dynamic simulations of protein/RNA complexes: CRISPR/Csy4 endoribonuclease. *Biochimica Et Biophysica Acta - General Subjects*, **2015**, 1850, 1072-1090	4	17
245	Tetraloop-like geometries could form the basis of the catalytic activity of the most ancient ribooligonucleotides. *Chemistry - A European Journal*, **2015**, 21, 3596-604	4.8	8
244	Excited-state hydrogen atom abstraction initiates the photochemistry of 2′-deoxycytidine. *Chemical Science*, **2015**, 6, 2035-2043	9.4	14
243	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
242	Untemplated nonenzymatic polymerization of 3′,5′cGMP: a plausible route to 3′,5′-linked oligonucleotides in primordia. *Journal of Physical Chemistry B*, **2015**, 119, 2979-89	3.4	23
241	Molecular Dynamics Simulations of Nucleic Acids. From Tetranucleotides to the Ribosome. *Journal of Physical Chemistry Letters*, **2014**, 5, 1771-82	6.4	113
240	Mechanical Model of DNA Allostery. *Journal of Physical Chemistry Letters*, **2014**, 5, 3831-5	6.4	18
239	Ion Binding to Quadruplex DNA Stems. Comparison of MM and QM Descriptions Reveals Sizable Polarization Effects Not Included in Contemporary Simulations. *Journal of Chemical Theory and Computation*, **2014**, 10, 1326-40	6.4	60
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