Serdal Kirmizialtin

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Conformational dynamics during misincorporation andÂmismatch extension defined using a DNA polymerase with a fluorescent artificial amino acid. Journal of Biological Chemistry, 2022, 298, 101451.	3.4	5
2	Substrate specificity and proposed structure of the proofreading complex of T7 DNA polymerase. Journal of Biological Chemistry, 2022, 298, 101627.	3.4	8
3	Visualizing RNA Structures by SAXS-Driven MD Simulations. Frontiers in Bioinformatics, 2022, 2, .	2.1	12
4	Refining the RNA Force Field with Small-Angle X-ray Scattering of Helix–Junction–Helix RNA. Journal of Physical Chemistry Letters, 2022, 13, 3400-3408.	4.6	7
5	Insights into the structural stability of major groove RNA triplexes by WAXS-guided MD simulations. Cell Reports Physical Science, 2022, 3, 100971.	5.6	5
6	Kinetic and thermodynamic analysis defines roles for two metal ions in DNA polymerase specificity and catalysis. Journal of Biological Chemistry, 2021, 296, 100184.	3.4	11
7	Taming the Topology of Calix[4]arene-Based 2D-Covalent Organic Frameworks: Interpenetrated vs Noninterpenetrated Frameworks and Their Selective Removal of Cationic Dyes. Journal of the American Chemical Society, 2021, 143, 3407-3415.	13.7	80
8	The structural plasticity of nucleic acid duplexes revealed by WAXS and MD. Science Advances, 2021, 7,	10.3	25
9	Rapid and Efficient Removal of Perfluorooctanoic Acid from Water with Fluorine-Rich Calixarene-Based Porous Polymers. ACS Applied Materials & Interfaces, 2020, 12, 43160-43166.	8.0	40
10	Dramatic Shape Changes Occur as Cytochrome <i>c</i> Folds. Journal of Physical Chemistry B, 2020, 124, 8240-8248.	2.6	4
11	Structure-guided DNA–DNA attraction mediated by divalent cations. Nucleic Acids Research, 2020, 48, 7018-7026.	14.5	24
12	Designed Cell-Penetrating Peptide Inhibitors of Amyloid-beta Aggregation and Cytotoxicity. Cell Reports Physical Science, 2020, 1, 100014.	5.6	47
13	Exploring Cation Mediated DNA Interactions Using Computer Simulations. Lecture Notes in Bioengineering, 2020, , 51-63.	0.4	6
14	Cryo_fit: Democratization of flexible fitting for cryo-EM. Journal of Structural Biology, 2019, 208, 1-6.	2.8	30
15	A polyrotaxanated covalent organic network based on viologen and cucurbit[7]uril. Communications Chemistry, 2019, 2, .	4.5	29
16	Calix[4]arene-Based Porous Organic Nanosheets. ACS Applied Materials & Interfaces, 2018, 10, 17359-17365.	8.0	39
17	Redoxâ€Responsive Covalent Organic Nanosheets from Viologens and Calix[4]arene for Iodine and Toxic Dye Capture. Chemistry - A European Journal, 2018, 24, 8648-8655.	3.3	43
18	Comparative Computational Approach To Study Enzyme Reactions Using QM and QM-MM Methods. ACS Omega, 2018, 3, 14689-14703.	3.5	10

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19	Revealing the distinct folding phases of an RNA three-helix junction. Nucleic Acids Research, 2018, 46, 7354-7365.	14.5	38
20	A DFT-based mechanistic study on the formation of oximes. Journal of Physical Organic Chemistry, 2017, 30, e3711.	1.9	7
21	Tracking fluctuation hotspots on the yeast ribosome through the elongation cycle. Nucleic Acids Research, 2017, 45, 4958-4971.	14.5	17
22	Nanoscale Biological Materials. Journal of Nanomaterials, 2016, 2016, 1-2.	2.7	0
23	A Chemical Template for Synthesis of Molecular Sheets of Calcium Carbonate. Scientific Reports, 2016, 6, 25393.	3.3	12
24	The in vitro selection world. Methods, 2016, 106, 3-13.	3.8	41
25	Using Molecular Simulation to Model High-Resolution Cryo-EM Reconstructions. Methods in Enzymology, 2015, 558, 497-514.	1.0	21
26	Integrating Molecular Dynamics Simulations with Chemical Probing Experiments Using SHAPE-FIT. Methods in Enzymology, 2015, 553, 215-234.	1.0	14
27	Enzyme Selectivity of HIV Reverse Transcriptase: Conformations, Ligands, and Free Energy Partition. Journal of Physical Chemistry B, 2015, 119, 11513-11526.	2.6	28
28	Molecular Dynamics Simulations of Ribosomes: Integrating Theory and Experiment. Biophysical Journal, 2014, 106, 39a.	0.5	2
29	Polyelectrolyte properties of single stranded DNA measured using SAXS and singleâ€molecule FRET: Beyond the wormlike chain model. Biopolymers, 2013, 99, 1032-1045.	2.4	34
30	The Ionic Atmosphere around A-RNA: Poisson-Boltzmann and Molecular Dynamics Simulations. Biophysical Journal, 2012, 102, 829-838.	0.5	68
31	RNA and Its Ionic Cloud: Solution Scattering Experiments and Atomically Detailed Simulations. Biophysical Journal, 2012, 102, 819-828.	0.5	89
32	How Conformational Dynamics of DNA Polymerase Select Correct Substrates: Experiments and Simulations. Structure, 2012, 20, 618-627.	3.3	107
33	Dynamics of inducedâ€fit in HIV reverse transcriptase specificity and resistance. FASEB Journal, 2012, 26, 964.5.	0.5	0
34	Revisiting and Computing Reaction Coordinates with Directional Milestoning. Journal of Physical Chemistry A, 2011, 115, 6137-6148.	2.5	74
35	Computational Exploration of Mobile Ion Distributions around RNA Duplex. Journal of Physical Chemistry B, 2010, 114, 8207-8220.	2.6	64
36	Simulations of the untying of molecular friction knots between individual polymer strands. Journal of Chemical Physics, 2008, 128, 094901.	3.0	11

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37	Single-Molecule Electrophoresis of β-Hairpin Peptides by Electrical Recordings and Langevin Dynamics Simulations. Journal of Physical Chemistry B, 2007, 111, 3332-3335.	2.6	82
38	Computer simulations of protein translocation. Physica Status Solidi (B): Basic Research, 2006, 243, 2038-2047.	1.5	24
39	Topography of the free-energy landscape probed via mechanical unfolding of proteins. Journal of Chemical Physics, 2005, 122, 234915.	3.0	67
40	Computer simulations of the translocation and unfolding of a protein pulled mechanically through a pore. Journal of Chemical Physics, 2005, 123, 124903.	3.0	70
41	Translocation of a \hat{l}^2 -hairpin-forming peptide through a cylindrical tunnel. Journal of Chemical Physics, 2004, 121, 10268-10277.	3.0	50
42	Vibrational spectroscopy of structural defects in oligothiophenes. Molecular Physics, 2003, 101, 2725-2729.	1.7	1
43	Conformational Properties of the Bacterial Polyester Poly(3-hydroxy-5,8-decadienoate). Macromolecules, 2003, 36, 1132-1137.	4.8	4
44	New surfactants design for CO2 applications: Molecular dynamics simulations of	3.0	9

fluorocarbon–hydrocarbon oligomers. Journal of Chemical Physics, 2003, 119, 4953-4961. 14