Serdal Kirmizialtin

List of Publications by Year
in descending order

44 papers	1,359 citations	331670 21 h-index	361022 35 g-index
48 all docs	48 docs citations	48 times ranked	1521 citing authors

#	Article	IF	Citations
1	How Conformational Dynamics of DNA Polymerase Select Correct Substrates: Experiments and Simulations. Structure, 2012, 20, 618-627.	3.3	107
2	RNA and Its Ionic Cloud: Solution Scattering Experiments and Atomically Detailed Simulations. Biophysical Journal, 2012, 102, 819-828.	0.5	89
3	Single-Molecule Electrophoresis of Î²-Hairpin Peptides by Electrical Recordings and Langevin Dynamics Simulations. Journal of Physical Chemistry B, 2007, 111, 3332-3335.	2.6	82
4	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
5	Revisiting and Computing Reaction Coordinates with Directional Milestoning. Journal of Physical Chemistry A, 2011, 115, 6137-6148.	2.5	74
6	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
7	The Ionic Atmosphere around A-RNA: Poisson-Boltzmann and Molecular Dynamics Simulations. Biophysical Journal, 2012, 102, 829-838.	0.5	68
8	Topography of the free-energy landscape probed via mechanical unfolding of proteins. Journal of Chemical Physics, 2005, 122, 234915.	3.0	67
9	Computational Exploration of Mobile Ion Distributions around RNA Duplex. Journal of Physical Chemistry B, 2010, 114, 8207-8220.	2.6	64
10	Translocation of a Î²-hairpin-forming peptide through a cylindrical tunnel. Journal of Chemical Physics, 2004, 121, 10268-10277.	3.0	50
11	Designed Cell-Penetrating Peptide Inhibitors of Amyloid-beta Aggregation and Cytotoxicity. Cell Reports Physical Science, 2020, 1, 100014.	5.6	47
12	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
13	The in vitro selection world. Methods, 2016, 106, 3-13.	3.8	41
14	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
15	Calix[4]arene-Based Porous Organic Nanosheets. ACS Applied Materials & Interfaces, 2018, 10, 17359-17365.	8.0	39
16	Revealing the distinct folding phases of an RNA three-helix junction. Nucleic Acids Research, 2018, 46, 7354-7365.	14.5	38
17	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
18	Cryo_fit: Democratization of flexible fitting for cryo-EM. Journal of Structural Biology, 2019, 208, 1-6.	2.8	30

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19	A polyrotaxanated covalent organic network based on viologen and cucurbit[7]uril. Communications Chemistry, 2019, 2, .	4.5	29
20	Enzyme Selectivity of HIV Reverse Transcriptase: Conformations, Ligands, and Free Energy Partition. Journal of Physical Chemistry B, 2015, 119, 11513-11526.	2.6	28
21	The structural plasticity of nucleic acid duplexes revealed by WAXS and MD. Science Advances, 2021, 7, .	10.3	25
22	Computer simulations of protein translocation. Physica Status Solidi (B): Basic Research, 2006, 243, 2038-2047.	1.5	24
23	Structure-guided DNAâ€“DNA attraction mediated by divalent cations. Nucleic Acids Research, 2020, 48, 7018-7026.	14.5	24
24	Using Molecular Simulation to Model High-Resolution Cryo-EM Reconstructions. Methods in Enzymology, 2015, 558, 497-514.	1.0	21
25	Tracking fluctuation hotspots on the yeast ribosome through the elongation cycle. Nucleic Acids Research, 2017, 45, 4958-4971.	14.5	17
26	Integrating Molecular Dynamics Simulations with Chemical Probing Experiments Using SHAPE-FIT. Methods in Enzymology, 2015, 553, 215-234.	1.0	14
27	A Chemical Template for Synthesis of Molecular Sheets of Calcium Carbonate. Scientific Reports, 2016, 6, 25393.	3.3	12
28	Visualizing RNA Structures by SAXS-Driven MD Simulations. Frontiers in Bioinformatics, 2022, 2, .	2.1	12
29	Simulations of the untying of molecular friction knots between individual polymer strands. Journal of Chemical Physics, 2008, 128, 094901.	3.0	11
30	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
31	Comparative Computational Approach To Study Enzyme Reactions Using QM and QM-MM Methods. ACS Omega, 2018, 3, 14689-14703.	3.5	10
32	New surfactants design for CO2 applications: Molecular dynamics simulations of fluorocarbonâ€“hydrocarbon oligomers. Journal of Chemical Physics, 2003, 119, 4953-4961.	3.0	9
33	Substrate specificity and proposed structure of the proofreading complex of T7 DNA polymerase. Journal of Biological Chemistry, 2022, 298, 101627.	3.4	8
34	A DFT-based mechanistic study on the formation of oximes. Journal of Physical Organic Chemistry, 2017, 30, e3711.	1.9	7
35	Refining the RNA Force Field with Small-Angle X-ray Scattering of Helixâ€“Junctionâ€“Helix RNA. Journal of Physical Chemistry Letters, 2022, 13, 3400-3408.	4.6	7
36	Exploring Cation Mediated DNA Interactions Using Computer Simulations. Lecture Notes in Bioengineering, 2020, , 51-63.	0.4	6

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37	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
38	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
39	Conformational Properties of the Bacterial Polyester Poly(3-hydroxy-5,8-decadienoate). Macromolecules, 2003, 36, 1132-1137.	4.8	4
40	Dramatic Shape Changes Occur as Cytochrome c Folds. Journal of Physical Chemistry B, 2020, 124, 8240-8248.	2.6	4
41	Molecular Dynamics Simulations of Ribosomes: Integrating Theory and Experiment. Biophysical Journal, 2014, 106, 39a.	0.5	2
42	Vibrational spectroscopy of structural defects in oligothiophenes. Molecular Physics, 2003, 101, 2725-2729.	1.7	1
43	Nanoscale Biological Materials. Journal of Nanomaterials, 2016, 2016, 1-2.	2.7	0
44	Dynamics of inducedâ€fit in HIV reverse transcriptase specificity and resistance. FASEB Journal, 2012, 26, 964.5.	0.5	0