Miroslav Krepl

List of Publications by Year
in descending order

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36	1,837	394421	330143
papers	citations	19 h-index	37 g-index

41	41	41	1917
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	RNA Structural Dynamics As Captured by Molecular Simulations: A Comprehensive Overview. Chemical Reviews, 2018, 118, 4177-4338.	47.7	408
2	Reference Simulations of Noncanonical Nucleic Acids with Different Ï‡ Variants of the AMBER Force Field: Quadruplex DNA, Quadruplex RNA, and Z-DNA. Journal of Chemical Theory and Computation, 2012, 8, 2506-2520.	5.3	231
3	Molecular Dynamics Simulations of Nucleic Acids. From Tetranucleotides to the Ribosome. Journal of Physical Chemistry Letters, 2014, 5, 1771-1782.	4.6	139
4	Structural dynamics of possible late-stage intermediates in folding of quadruplex DNA studied by molecular simulations. Nucleic Acids Research, 2013, 41, 7128-7143.	14.5	111
5	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.	5.3	97
6	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.	7.1	69
7	Can We Execute Stable Microsecond-Scale Atomistic Simulations of Proteinâ€“RNA Complexes?. Journal of Chemical Theory and Computation, 2015, 11, 1220-1243.	5.3	67
8	How to understand atomistic molecular dynamics simulations of <scp>RNA</scp> and proteinâ€“<scp>RNA</scp> complexes?. Wiley Interdisciplinary Reviews RNA, 2017, 8, e1405.	6.4	54
9	Extended molecular dynamics of ac-kitpromoter quadruplex. Nucleic Acids Research, 2015, 43, 8673-8693.	14.5	49
10	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, 6452-6470.	14.5	48
11	Effect of Guanine to Inosine Substitution on Stability of Canonical DNA and RNA Duplexes: Molecular Dynamics Thermodynamics Integration Study. Journal of Physical Chemistry B, 2013, 117, 1872-1879.	2.6	42
12	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.	12.8	37
13	QM/MM Calculations on Proteinâ€“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.	5.3	34
14	Benchmark quantum-chemical calculations on a complete set of rotameric families of the DNA sugarâ€“phosphate backbone and their comparison with modern density functional theory. Physical Chemistry Chemical Physics, 2013, 15, 7295.	2.8	33
15	UUCG RNA Tetraloop as a Formidable Force-Field Challenge for MD Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7601-7617.	5.3	29
16	Coordination between the polymerase and RNase H activity of HIV-1 reverse transcriptase. Nucleic Acids Research, 2017, 45, gkx004.	14.5	28
17	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.	14.5	28
18	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.	5.3	28

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19	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.	14.5	26
20	The influence of Holliday junction sequence and dynamics on DNA crystal self-assembly. Nature Communications, 2022, 13, .	12.8	24
21	Aromatic side-chain conformational switch on the surface of the RNA Recognition Motif enables RNA discrimination. Nature Communications, 2017, 8, 654.	12.8	23
22	RuvC uses dynamic probing of the Holliday junction to achieve sequence specificity and efficient resolution. Nature Communications, 2019, 10, 4102.	12.8	23
23	Mechanism of polypurine tract primer generation by HIV-1 reverse transcriptase. Journal of Biological Chemistry, 2018, 293, 191-202.	3.4	21
24	Automatic Learning of Hydrogen-Bond Fixes in the AMBER RNA Force Field. Journal of Chemical Theory and Computation, 2022, 18, 4490-4502.	5.3	21
25	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, 15176-15190.	2.6	20
26	Molecular dynamic simulations of protein/RNA complexes: CRISPR/Csy4 endoribonuclease. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 1072-1090.	2.4	20
27	Bioinformatics and Molecular Dynamics Simulation Study of L1 Stalk Non-Canonical rRNA Elements: Kink-Turns, Loops, and Tetraloops. Journal of Physical Chemistry B, 2013, 117, 5540-5555.	2.6	17
28	MD and QM/MM Study of the Quaternary HutP Homohexamer Complex with mRNA, <scp>l</scp>-Histidine Ligand, and Mg²⁺. Journal of Chemical Theory and Computation, 2017, 13, 5658-5670.	5.3	17
29	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.	2.6	15
30	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.	3.2	14
31	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.	2.6	11
32	MD simulations reveal the basis for dynamic assembly of Hfqâ€“RNA complexes. Journal of Biological Chemistry, 2021, 296, 100656.	3.4	11
33	DNA Damage Changes Distribution Pattern and Levels of HP1 Protein Isoforms in the Nucleolus and Increases Phosphorylation of HP1Î²-Ser88. Cells, 2019, 8, 1097.	4.1	10
34	Combining NMR Spectroscopy and Molecular Dynamic Simulations to Solve and Analyze the Structure of Proteinâ€“RNA Complexes. Methods in Enzymology, 2019, 614, 393-422.	1.0	9
35	Role of Fine Structural Dynamics in Recognition of Histone H3 by HP1Î³(CSD) Dimer and Ability of Force Fields to Describe Their Interaction Network. Journal of Chemical Theory and Computation, 2019, 15, 5659-5673.	5.3	2
36	Residues flanking the ARKme3T/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.	2.4	2