Miroslav Krepl

List of Publications by Year
in descending order

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	The influence of Holliday junction sequence and dynamics on DNA crystal self-assembly. Nature Communications, 2022, 13, .	12.8	24
2	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
3	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
4	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
5	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
6	MD simulations reveal the basis for dynamic assembly of Hfqâ€“RNA complexes. Journal of Biological Chemistry, 2021, 296, 100656.	3.4	11
7	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
8	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
9	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
10	RuvC uses dynamic probing of the Holliday junction to achieve sequence specificity and efficient resolution. Nature Communications, 2019, 10, 4102.	12.8	23
11	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
12	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
13	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
14	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
15	RNA Structural Dynamics As Captured by Molecular Simulations: A Comprehensive Overview. Chemical Reviews, 2018, 118, 4177-4338.	47.7	408
16	Mechanism of polypurine tract primer generation by HIV-1 reverse transcriptase. Journal of Biological Chemistry, 2018, 293, 191-202.	3.4	21
17	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
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

#	Article	IF	Citations
19	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
20	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
21	Coordination between the polymerase and RNase H activity of HIV-1 reverse transcriptase. Nucleic Acids Research, 2017, 45, gkx004.	14.5	28
22	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
23	Aromatic side-chain conformational switch on the surface of the RNA Recognition Motif enables RNA discrimination. Nature Communications, 2017, 8, 654.	12.8	23
24	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
25	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
26	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
27	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
28	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
29	Extended molecular dynamics of ac-kitpromoter quadruplex. Nucleic Acids Research, 2015, 43, 8673-8693.	14.5	49
30	Molecular dynamic simulations of protein/RNA complexes: CRISPR/Csy4 endoribonuclease. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 1072-1090.	2.4	20
31	Molecular Dynamics Simulations of Nucleic Acids. From Tetranucleotides to the Ribosome. Journal of Physical Chemistry Letters, 2014, 5, 1771-1782.	4.6	139
32	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
33	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
34	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
35	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
36	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