Scott D Kennedy

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Reparameterization of RNA χ Torsion Parameters for the AMBER Force Field and Comparison to NMR Spectra for Cytidine and Uridine. Journal of Chemical Theory and Computation, 2010, 6, 1520-1531.	2.3	155
2	Stacking in RNA: NMR of Four Tetramers Benchmark Molecular Dynamics. Journal of Chemical Theory and Computation, 2015, 11, 2729-2742.	2.3	99
3	Conformational ensembles of RNA oligonucleotides from integrating NMR and molecular simulations. Science Advances, 2018, 4, eaar8521.	4.7	99
4	Benchmarking AMBER Force Fields for RNA: Comparisons to NMR Spectra for Single-Stranded r(GACC) Are Improved by Revised χ Torsions. Journal of Physical Chemistry B, 2011, 115, 9261-9270.	1.2	95
5	Testing the Nearest Neighbor Model for Canonical RNA Base Pairs: Revision of GU Parameters. Biochemistry, 2012, 51, 3508-3522.	1.2	80
6	The Nuclear Magnetic Resonance of CCCC RNA Reveals a Right-Handed Helix, and Revised Parameters for AMBER Force Field Torsions Improve Structural Predictions from Molecular Dynamics. Biochemistry, 2013, 52, 996-1010.	1.2	78
7	Structure determination of noncanonical RNA motifs guided by 1H NMR chemical shifts. Nature Methods, 2014, 11, 413-416.	9.0	72
8	Structural effects of hydration: Studies of lysozyme by13C solids nmr. Biopolymers, 1990, 29, 1801-1806.	1.2	59
9	NMR-Assisted Prediction of RNA Secondary Structure: Identification of a Probable Pseudoknot in the Coding Region of an R2 Retrotransposon. Journal of the American Chemical Society, 2008, 130, 10233-10239.	6.6	45
10	Enhanced sensitivity to molecular diffusion with intermolecular double-quantum coherences: implications and potential applications. Magnetic Resonance Imaging, 2001, 19, 33-39.	1.0	37
11	NMR Structures of (rGCUGAGGCU)2and (rGCGGAUGCU)2:Â Probing the Structural Features That Shape the Thermodynamic Stability of GA Pairsâ€,‡. Biochemistry, 2007, 46, 1511-1522.	1.2	33
12	Amide linkages mimic phosphates in RNA interactions with proteins and are well tolerated in the guide strand of short interfering RNAs. Nucleic Acids Research, 2017, 45, 8142-8155.	6.5	33
13	Synthetic, Structural, and RNA Binding Studies on 2â€Aminopyridineâ€Modified Triplexâ€Forming Peptide Nucleic Acids. Chemistry - A European Journal, 2019, 25, 4367-4372.	1.7	33
14	Optimization of an AMBER Force Field for the Artificial Nucleic Acid, LNA, and Benchmarking with NMR of L(CAAU). Journal of Physical Chemistry B, 2014, 118, 1216-1228.	1.2	32
15	RNA Internal Loops with Tandem AG Pairs: The Structure of the 5′G <u>AG</u> U/3′U <u>GA</u> G Loop Can Be Dramatically Different from Others, Including 5′A <u>AG</u> U/3′U <u>GA</u> A. Biochemistry, 2010, 49, 5817-5827.	1.2	31
16	Diffusion measurements free of motion artifacts using intermolecular dipole-dipole interactions. Magnetic Resonance in Medicine, 2004, 52, 1-6.	1.9	28
17	Secondary structure prediction for RNA sequences including N6-methyladenosine. Nature Communications, 2022, 13, 1271.	5.8	27
18	Source of Transport Site Asymmetry in the Band 3 Anion Exchange Protein Determined by NMR Measurements of External Cl-Affinityâ€. Biochemistry, 1996, 35, 15228-15235.	1.2	25

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19	NMR structure of a 4 × 4 nucleotide RNA internal loop from an R2 retrotransposon: Identification of a three purine–purine sheared pair motif and comparison to MC-SYM predictions. Rna, 2011, 17, 1664-1677.	1.6	24
20	Secondary Structure of a Conserved Domain in an Intron of Influenza A M1 mRNA. Biochemistry, 2014, 53, 5236-5248.	1.2	24
21	A Single Amide Linkage in the Passenger Strand Suppresses Its Activity and Enhances Guide Strand Targeting of siRNAs. ACS Chemical Biology, 2018, 13, 533-536.	1.6	23
22	Nuclear Magnetic Resonance of Single-Stranded RNAs and DNAs of CAAU and UCAAUC as Benchmarks for Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 1968-1984.	2.3	22
23	Synthesis and RNA-Binding Properties of Extended Nucleobases for Triplex-Forming Peptide Nucleic Acids. Journal of Organic Chemistry, 2019, 84, 13276-13298.	1.7	20
24	Highâ€resolution MRS in the presence of field inhomogeneity via intermolecular doubleâ€quantum coherences on a 3â€T wholeâ€body scanner. Magnetic Resonance in Medicine, 2010, 63, 303-311.	1.9	18
25	Novel Conformation of an RNA Structural Switch. Biochemistry, 2012, 51, 9257-9259.	1.2	16
26	Disagreement Between the Structure of the dTpT Thymine Pair Determined by NMR and Molecular Dynamics Simulations Using Amber 14 Force Fields. Journal of Physical Chemistry B, 2016, 120, 1250-1258.	1.2	16
27	Structural Features of a 3′ Splice Site in Influenza A. Biochemistry, 2015, 54, 3269-3285.	1.2	15
28	Nuclear Magnetic Resonance-Assisted Prediction of Secondary Structure for RNA: Incorporation of Direction-Dependent Chemical Shift Constraints. Biochemistry, 2015, 54, 6769-6782.	1.2	13
29	Dynamic stacking of an expected branch point adenosine in duplexes containing pseudouridine-modified or unmodified U2 snRNA sites. Biochemical and Biophysical Research Communications, 2019, 511, 416-421.	1.0	12
30	Nuclear Magnetic Resonance Spectra and AMBER OL3 and ROC-RNA Simulations of UCUCGU Reveal Force Field Strengths and Weaknesses for Single-Stranded RNA. Journal of Chemical Theory and Computation, 2022, 18, 1241-1254.	2.3	11
31	Nuclear Magnetic Resonance Reveals That GU Base Pairs Flanking Internal Loops Can Adopt Diverse Structures. Biochemistry, 2019, 58, 1094-1108.	1.2	10
32	Quantitation of intermolecular dipolar effects in NMR spectroscopy and high order MSE MR imaging. Magnetic Resonance Materials in Physics, Biology, and Medicine, 2000, 11, 122-128.	1.1	9
33	Theoretical studies of the effect of the dipolar field in multiple spin-echo sequences with refocusing pulses of finite duration. Journal of Magnetic Resonance, 2007, 185, 247-258.	1.2	9
34	Molecular dynamics correctly models the unusual major conformation of the GAGU RNA internal loop and with NMR reveals an unusual minor conformation. Rna, 2018, 24, 656-672.	1.6	9
35	Hydration effects on dynamics of polyglycine and sodium poly(L-glutamate). Biopolymers, 1990, 30, 691-701.	1.2	7
36	Nuclear Magnetic Resonance Structure of an 8 × 8 Nucleotide RNA Internal Loop Flanked on Each Side by Three Watson–Crick Pairs and Comparison to Three-Dimensional Predictions. Biochemistry, 2017, 56, 3733-3744.	1.2	4

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37	Surprising Sequence Effects on GU Closure of Symmetric 2 × 2 Nucleotide RNA Internal Loops. Biochemistry, 2018, 57, 2121-2131.	1.2	4
38	NMR Methods for Characterization of RNA Secondary Structure. Methods in Molecular Biology, 2016, 1490, 253-264.	0.4	3
39	2â€Methoxypyridine as a Thymidine Mimic in Watson–Crick Base Pairs of DNA and PNA: Synthesis, Thermal Stability, and NMR Structural Studies. ChemBioChem, 2017, 18, 2165-2170.	1.3	3
40	Nuclear Magnetic Resonance reveals a two hairpin equilibrium near the 3'-splice site of Influenza A segment 7 mRNA that can be shifted by oligonucleotides. Rna, 2022, , rna.078951.121.	1.6	1