Lennart Nilsson

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4821720/publications.pdf

Version: 2024-02-01

181	17,442	36303	14759
papers	citations	51 h-index	127 g-index

186	186	186	19033
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	CHARMM: The biomolecular simulation program. Journal of Computational Chemistry, 2009, 30, 1545-1614.	3.3	7,077
2	Structure and Dynamics of the TIP3P, SPC, and SPC/E Water Models at 298 K. Journal of Physical Chemistry A, 2001, 105, 9954-9960.	2.5	2,458
3	Optimization of the CHARMM Additive Force Field for DNA: Improved Treatment of the BI/BII Conformational Equilibrium. Journal of Chemical Theory and Computation, 2012, 8, 348-362.	5.3	464
4	Impact of 2â€²â€hydroxyl sampling on the conformational properties of RNA: Update of the CHARMM allâ€atom additive force field for RNA. Journal of Computational Chemistry, 2011, 32, 1929-1943.	3.3	341
5	Magnesium Ionâ€“Water Coordination and Exchange in Biomolecular Simulations. Journal of Chemical Theory and Computation, 2012, 8, 1493-1502.	5.3	325
6	Empirical energy functions for energy minimization and dynamics of nucleic acids. Journal of Computational Chemistry, 1986, 7, 591-616.	3.3	254
7	On the Truncation of Long-Range Electrostatic Interactions in DNA. Biophysical Journal, 2000, 79, 1537-1553.	0.5	225
8	Rigidity versus flexibility: the dilemma of understanding protein thermal stability. FEBS Journal, 2015, 282, 3899-3917.	4.7	206
9	Molecular origin of time-dependent fluorescence shifts in proteins. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 13867-13872.	7.1	192
10	Molecular dynamics simulations of nucleic acidâ€“protein complexes. Current Opinion in Structural Biology, 2008, 18, 194-199.	5.7	157
11	Structure refinement of oligonucleotides by molecular dynamics with nuclear overhauser effect interproton distance restraints: Application to 5â€² d(C-G-T-A-C-G)2. Journal of Molecular Biology, 1986, 188, 455-475.	4.2	152
12	Molecular dynamics simulation of galanin in aqueous and nonaqueous solution. Journal of the American Chemical Society, 1992, 114, 4028-4035.	13.7	140
13	Characterization of two novel mutations in the glucocorticoid receptor gene in patients with primary cortisol resistance. Clinical Endocrinology, 2001, 55, 363-371.	2.4	138
14	Effect of Urea on Peptide Conformation in Water: Molecular Dynamics and Experimental Characterization. Biophysical Journal, 2005, 89, 842-857.	0.5	136
15	Structure and dynamics of liquid water with different long-range interaction truncation and temperature control methods in molecular dynamics simulations. Journal of Computational Chemistry, 2002, 23, 1211-1219.	3.3	134
16	Advances in biomolecular simulations: methodology and recent applications. Quarterly Reviews of Biophysics, 2003, 36, 257-306.	5.7	125
17	Does the Dynamic Stokes Shift Report on Slow Protein Hydration Dynamics?. Journal of Physical Chemistry B, 2009, 113, 8210-8213.	2.6	113
18	Aromatic interactions define the binding of the alphavirus spike to its nucleocapsid. Structure, 1996, 4, 519-529.	3.3	112

#	Article	IF	Citations
19	Intrinsic Conformational Energetics Associated with the Glycosyl Torsion in DNA: A Quantum Mechanical Study. Biophysical Journal, 2002, 82, 1554-1569.	0.5	111
20	Stacking Free Energy Profiles for All 16 Natural Ribodinucleoside Monophosphates in Aqueous Solution. Journal of the American Chemical Society, 1995, 117, 10832-10840.	13.7	103
21	Tec homology (TH) adjacent to the PH domain. FEBS Letters, 1994, 350, 263-265.	2.8	99
22	Molecular Dynamics Applied to Nucleic Acids. Accounts of Chemical Research, 2002, 35, 465-472.	15.6	99
23	Deletion within the Src homology domain 3 of Bruton's tyrosine kinase resulting in X-linked agammaglobulinemia (XLA).. Journal of Experimental Medicine, 1994, 180, 461-470.	8.5	87
24	Mycoredoxinâ€1 is one of the missing links in the oxidative stress defence mechanism of <scp>M</scp>ycobacteria. Molecular Microbiology, 2012, 86, 787-804.	2.5	86
25	Structural basis for chromosome X-linked agammaglobulinemia: a tyrosine kinase disease.. Proceedings of the National Academy of Sciences of the United States of America, 1994, 91, 12803-12807.	7.1	85
26	How Consistent are Molecular Dynamics Simulations?. Journal of Molecular Biology, 1993, 233, 766-780.	4.2	84
27	Structure, dynamics and electrostatics of the active site of glutaredoxin 3 from Escherichia coli: comparison with functionally related proteins. Journal of Molecular Biology, 2001, 310, 449-470.	4.2	84
28	MD Simulations of Homomorphous PNA, DNA, and RNA Single Strands:Â Characterization and Comparison of Conformations and Dynamics. Journal of the American Chemical Society, 2001, 123, 7414-7422.	13.7	80
29	DNA-based mutation analysis of Bruton's tyrosine kinase gene in patients with X-linked agammaglobulinaemia. Human Molecular Genetics, 1995, 4, 51-58.	2.9	79
30	Molecular Dynamics of Duplex Systems Involving PNA:Â Structural and Dynamical Consequences of the Nucleic Acid Backbone. Journal of the American Chemical Society, 1998, 120, 619-631.	13.7	78
31	Refinement of the solution structure of the DNA hexamer 5'd(GCATGC)2: combined use of nuclear magnetic resonance and restrained molecular dynamics. Biochemistry, 1987, 26, 3718-3733.	2.5	74
32	Solvent Influence on Base Stacking. Biophysical Journal, 1998, 74, 394-402.	0.5	73
33	The role of positively charged amino acids and electrostatic interactions in the complex of U1A protein and U1 hairpin II RNA. Nucleic Acids Research, 2006, 34, 275-285.	14.5	73
34	Ab initio conformational analysis of nucleic acid components: Intrinsic energetic contributions to nucleic acid structure and dynamics. Biopolymers, 2001, 61, 61-76.	2.4	70
35	Unbinding of Retinoic Acid from the Retinoic Acid Receptor by Random Expulsion Molecular Dynamics. Biophysical Journal, 2006, 91, 3151-3161.	0.5	68
36	Effect of Zn2+ on DNA Recognition and Stability of the p53 DNA-Binding Domain. Biochemistry, 2006, 45, 7483-7492.	2.5	68

#	Article	IF	Citations
37	Structural Basis for Pleckstrin Homology Domain Mutations in X-Linked Agammaglobulinemia. Biochemistry, 1995, 34, 1475-1481.	2.5	67
38	How Thioredoxin Dissociates Its Mixed Disulfide. PLoS Computational Biology, 2009, 5, e1000461.	3.2	67
39	Fatty Acids Derived from Royal Jelly Are Modulators of Estrogen Receptor Functions. PLoS ONE, 2010, 5, e15594.	2.5	66
40	Potential of mean force calculations of the stacking-unstacking process in single-stranded deoxyribodinucleoside monophosphates. Biophysical Journal, 1995, 69, 2277-2285.	0.5	64
41	Toward a Full Characterization of Nucleic Acid Components in Aqueous Solution:Â Simulations of Nucleosides. Journal of Physical Chemistry B, 2005, 109, 9119-9131.	2.6	63
42	Additive <scp>CHARMM</scp> force field for naturally occurring modified ribonucleotides. Journal of Computational Chemistry, 2016, 37, 896-912.	3.3	63
43	Structural fluctuations of a helical polypeptide traversing a lipid bilayer.. Proceedings of the National Academy of Sciences of the United States of America, 1988, 85, 5067-5071.	7.1	58
44	A comparison of15N NMR relaxation measurements with a molecular dynamics simulation: Backbone dynamics of the glucocorticoid receptor DNA-binding domain. Proteins: Structure, Function and Bioinformatics, 1993, 17, 375-390.	2.6	57
45	Promotion of helix formation in peptides dissolved in alcohol and water-alcohol mixtures. Journal of the American Chemical Society, 1993, 115, 11034-11035.	13.7	57
46	Structureâ€“Function Defects of the TWINKLE Linker Region in Progressive External Ophthalmoplegia. Journal of Molecular Biology, 2008, 377, 691-705.	4.2	57
47	Three-dimensional model for the membrane domain of Escherichia coli leader peptidase based on disulfide mapping. Biochemistry, 1993, 32, 8534-8539.	2.5	54
48	Molecular dynamics simulations of the glucocorticoid receptor DNA-binding domain in complex with DNA and free in solution. Biophysical Journal, 1995, 68, 402-426.	0.5	54
49	Insights into structure, dynamics and hydration of locked nucleic acid (LNA) strand-based duplexes from molecular dynamics simulations. Nucleic Acids Research, 2008, 36, 1508-1516.	14.5	54
50	Molecular Dynamics Simulations of the Complex between Human U1A Protein and Hairpin II of U1 Small Nuclear RNA and of Free RNA in Solution. Biophysical Journal, 1999, 77, 1284-1305.	0.5	53
51	Revisiting sulfur H-bonds in proteins: The example of peroxiredoxin AhpE. Scientific Reports, 2016, 6, 30369.	3.3	52
52	Glass transition in DNA from molecular dynamics simulations.. Proceedings of the National Academy of Sciences of the United States of America, 1996, 93, 10173-10176.	7.1	51
53	Mitochondrial targeting sequences why â€˜non-amphiphilicâ€™ peptides may still be amphiphilic. FEBS Letters, 1988, 235, 173-177.	2.8	50
54	Molecular dynamics simulations of ribonuclease T1: analysis of the effect of solvent on the structure, fluctuations, and active site of the free enzyme. Biochemistry, 1988, 27, 4547-4556.	2.5	49

#	Article	IF	Citations
55	Nuclear Receptorâ"DNA Binding Specificity:Â A COMBINE and Freeâ"Wilson QSAR Analysisâ€–. Journal of Medicinal Chemistry, 2000, 43, 1780-1792.	6.4	49
56	Structural fluctuations between two conformational states of a transmembrane helical peptide are related to its channel-forming properties in planar lipid membranes. FEBS Journal, 1993, 212, 305-313.	0.2	47
57	Structural Basis of SH2 Domain Mutations in X-Linked Agammaglobulinemia. Biochemical and Biophysical Research Communications, 1994, 205, 1270-1277.	2.1	47
58	On the pH dependence of amide proton exchange rates in proteins. Biophysical Journal, 1995, 69, 329-339.	0.5	46
59	Protein dynamics. Biophysical Chemistry, 1987, 26, 247-261.	2.8	45
60	Structure, Thermodynamics and Cooperativity of the Glucocorticoid Receptor DNA-binding Domain in Complex with Different Response Elements. Molecular Dynamics Simulation and Free Energy Perturbation Studies. Journal of Molecular Biology, 1995, 253, 453-472.	4.2	45
61	Molecular dynamics simulations and free energy calculations of base flipping in dsRNA. Rna, 2005, 11, 609-618.	3.5	45
62	Nucleotide modifications and tRNA anticodonâ€"mRNA codon interactions on the ribosome. Rna, 2011, 17, 2177-2188.	3.5	45
63	Constant pressure molecular dynamics simulations of the dodecamers: d(GCGCGCGCGCGC)2 and r(GCGCGCGCGCGC)2. Journal of Chemical Physics, 1996, 104, 6052-6057.	3.0	44
64	DNA and Estrogen Receptor Interaction Revealed by Fragment Molecular Orbital Calculations. Journal of Physical Chemistry B, 2007, 111, 9621-9627.	2.6	43
65	Loopâ€"loop interaction in an adenine-sensing riboswitch: A molecular dynamics study. Rna, 2013, 19, 916-926.	3.5	43
66	Structural insights into the DNA-binding specificity of E2F family transcription factors. Nature Communications, 2015, 6, 10050.	12.8	43
67	Structure, Interaction, Dynamics and Solvent Effects on the DNA-EcoRI complex in Aqueous Solution from Molecular Dynamics Simulation. Biophysical Journal, 1999, 77, 1782-1800.	0.5	40
68	Structural and functional analysis of mutations at the human hypoxanthine phosphoribosyl transferase (HPRT1) locus. Human Mutation, 2004, 23, 599-611.	2.5	39
69	Efficient table lookup without inverse square roots for calculation of pair wise atomic interactions in classical simulations. Journal of Computational Chemistry, 2009, 30, 1490-1498.	3.3	39
70	Effects of Base Substitutions in an RNA Hairpin from Molecular Dynamics and Free Energy Simulations. Biophysical Journal, 2003, 85, 3445-3459.	0.5	37
71	Conformational Free Energy Landscape of ApApA from Molecular Dynamics Simulations. The Journal of Physical Chemistry, 1996, 100, 2550-2554.	2.9	36
72	Molecular dynamics simulations of ribonuclease T1: Comparison of the free enzyme and 2â€² GMP-enzyme complex. Proteins: Structure, Function and Bioinformatics, 1989, 6, 20-31.	2.6	34

#	Article	IF	Citations
73	The Glutaredoxin -C-P-Y-C- Motif: Influence of Peripheral Residues. Structure, 2004, 12, 289-300.	3.3	34
74	Temperature dependence of the stacking propensity of adenylyl-3',5'-adenosine. The Journal of Physical Chemistry, 1995, 99, 13056-13058.	2.9	32
75	Structureâ€"function defects of the twinkle amino-terminal region in progressive external ophthalmoplegia. Biochimica Et Biophysica Acta - Molecular Basis of Disease, 2009, 1792, 132-139.	3.8	32
76	Two distinct DNA sequences recognized by transcription factors represent enthalpy and entropy optima. ELife, 2018, 7, .	6.0	32
77	Conformational Dynamics of a 5S rRNA Hairpin Domain Containing Loop D and a Single Nucleotide Bulge. Biophysical Journal, 2000, 79, 1213-1227.	0.5	31
78	A Molecular Dynamics Study of Tryptophan in Water. Journal of Physical Chemistry B, 2002, 106, 9440-9445.	2.6	31
79	Cytosine ribose flexibility in DNA: a combined NMR 13C spin relaxation and molecular dynamics simulation study. Nucleic Acids Research, 2008, 36, 4211-4219.	14.5	29
80	Ligand unbinding from the estrogen receptor: A computational study of pathways and ligand specificity. Proteins: Structure, Function and Bioinformatics, 2009, 77, 842-856.	2.6	29
81	LNA effects on DNA binding and conformation: from single strand to duplex and triplex structures. Scientific Reports, 2017, 7, 11043.	3.3	28
82	Models for mRNA Translation: Theory versus Experiment. FEBS Journal, 1978, 92, 397-402.	0.2	27
83	Structural variability of tRNA: small-angle x-ray scattering of the yeast tRNAphe-Escherichia coli tRNAGlu2 complex.. Proceedings of the National Academy of Sciences of the United States of America, 1982, 79, 5891-5895.	7.1	27
84	Stacking-unstacking of the dinucleoside monophosphate guanylyl-3',5'-uridine studied with molecular dynamics. Biophysical Journal, 1994, 67, 812-824.	0.5	26
85	Stabilization of the Catalytic Thiolate in a Mammalian Glutaredoxin: Structure, Dynamics and Electrostatics of Reduced Pig Glutaredoxin and its Mutants. Journal of Molecular Biology, 2007, 372, 798-816.	4.2	26
86	Structural Determination of Functional Domains in Early B-cell Factor (EBF) Family of Transcription Factors Reveals Similarities to Rel DNA-binding Proteins and a Novel Dimerization Motif. Journal of Biological Chemistry, 2010, 285, 25875-25879.	3.4	26
87	Unfolding of the Amyloid Î²-Peptide Central Helix: Mechanistic Insights from Molecular Dynamics Simulations. PLoS ONE, 2011, 6, e17587.	2.5	26
88	Molecular Dynamics of the Anticodon Domain of Yeast tRNAPhe:Codon-Anticodon Interaction. Biophysical Journal, 2000, 79, 2276-2289.	0.5	25
89	Dynamic Arrangement of Ion Pairs and Individual Contributions to the Thermal Stability of the Cofactor-Binding Domain of Glutamate Dehydrogenase from Thermotoga maritima. Biochemistry, 2007, 46, 8537-8549.	2.5	25
90	Functional Fluorescence Microscopy Imaging: Quantitative Scanning-Free Confocal Fluorescence Microscopy for the Characterization of Fast Dynamic Processes in Live Cells. Analytical Chemistry, 2019, 91, 11129-11137.	6.5	25

#	Article	IF	Citations
91	Modeling zinc sulfhydryl bonds in zinc fingers. International Journal of Quantum Chemistry, 2001, 83, 230-244.	2.0	24
92	Intrinsic Relative Stabilities of the Neutral Tautomers of Arginine Side-Chain Models. Journal of Chemical Theory and Computation, 2005, 1, 986-993.	5.3	24
93	Urea parametrization for molecular dynamics simulations. Computational and Theoretical Chemistry, 2006, 758, 139-148.	1.5	24
94	Interaction of human SRY protein with DNA: A molecular dynamics study. , 1998, 31, 417-433.		23
95	Virtual screening, selection and development of a benzindolone structural scaffold for inhibition of lumazine synthase. Bioorganic and Medicinal Chemistry, 2010, 18, 3518-3534.	3.0	23
96	Molecular Dynamics Simulations of the Ala-Pro Dipeptide in Water:Â Conformational Dynamics of Trans and Cis Isomers Using Different Water Models. Journal of Physical Chemistry B, 2001, 105, 8028-8035.	2.6	22
97	Motion of aromatic side chains, picosecond fluorescence, and internal energy transfer in Escherichia coli thioredoxin studied by site-directed mutagenesis, time-resolved fluorescence spectroscopy, and molecular dynamics simulations. Biochemistry, 1991, 30, 9648-9656.	2.5	21
98	The role of residue 50 and hydration water molecules in homeodomain DNA recognition. European Biophysics Journal, 2002, 31, 306-316.	2.2	21
99	Analysis of the Stability and Flexibility of RNA Complexes Containing Bulge Loops of Different Sizes. Journal of Biomolecular Structure and Dynamics, 2008, 26, 163-173.	3.5	21
100	Thermodynamics of interaction of a fluorescent DNA oligomer with the anti-tumour drug netropsin. FEBS Journal, 1992, 203, 361-366.	0.2	20
101	Structural analysis of an anti-estradiol antibody. Molecular Immunology, 1997, 34, 1215-1226.	2.2	20
102	Free Energy Calculations and Molecular Dynamics Simulations of Wild-Type and Variants of the DNA-EcoRI Complex. Biophysical Journal, 1999, 77, 1801-1810.	0.5	20
103	Triple helical DNA in a duplex context and base pair opening. Nucleic Acids Research, 2014, 42, 11329-11338.	14.5	20
104	Computational studies of LXR molecular interactions reveal an allosteric communication pathway. Proteins: Structure, Function and Bioinformatics, 2012, 80, 294-306.	2.6	19
105	Conformational Preferences of Modified Uridines: Comparison of AMBER Derived Force Fields. Journal of Chemical Information and Modeling, 2014, 54, 1129-1142.	5.4	19
106	Glucocorticoid Receptor Point Mutation V571M Facilitates Coactivator and Ligand Binding by Structural Rearrangement and Stabilization. Molecular Endocrinology, 2005, 19, 1960-1977.	3.7	17
107	Effects of Ligands on Unfolding of the Amyloid Î²-Peptide Central Helix: Mechanistic Insights from Molecular Dynamics Simulations. PLoS ONE, 2012, 7, e30510.	2.5	17
108	Implicit Solvent Models and Stabilizing Effects of Mutations and Ligands on the Unfolding of the Amyloid Î²-Peptide Central Helix. Journal of Chemical Theory and Computation, 2013, 9, 834-846.	5.3	17

#	Article	IF	Citations
109	High-pressure molecular dynamics of a nucleic acid fragment. Chemical Physics Letters, 1994, 224, 219-224.	2.6	16
110	The Reducing Activity of Glutaredoxin 3 toward Cytoplasmic Substrate Proteins Is Restricted by Methionine 43â€. Biochemistry, 2007, 46, 3366-3377.	2.5	16
111	Influence of adjacent bases on the stacking-unstacking process of single-stranded oligonucleotides. Biopolymers, 1996, 39, 765-768.	2.4	15
112	Conformational states of the glucocorticoid receptor DNA-binding domain from molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2002, 49, 24-36.	2.6	15
113	Collective Dynamics ofEcoRI-DNA Complex by Elastic Network Model and Molecular Dynamics Simulations. Journal of Biomolecular Structure and Dynamics, 2006, 24, 1-15.	3.5	15
114	NMR Relaxation Times, Dynamics, and Hydration of a Nucleic Acid Fragment from Molecular Dynamics Simulations. The Journal of Physical Chemistry, 1995, 99, 14876-14884.	2.9	14
115	Thermal unfolding simulations of a multimeric protein-Transition state and unfolding pathways. Proteins: Structure, Function and Bioinformatics, 2005, 59, 170-182.	2.6	14
116	The influence of spermine on the structural dynamics of yeast tRNAPhe. Biochimica Et Biophysica Acta Gene Regulatory Mechanisms, 1983, 740, 460-465.	2.4	12
117	Modulation of DNA-binding specificity within the nuclear receptor family by substitutions at a single amino acid position. Proteins: Structure, Function and Bioinformatics, 1995, 21, 57-67.	2.6	12
118	Internal mobility of the ologonucleotide duplexes d(TCGCG)2 and d(CGCGCG)2 in aqueous solution from molecular dynamics simulations. Journal of Biomolecular NMR, 1996, 7, 305-14.	2.8	12
119	Molecular Dynamics Simulations of Human LRH-1: The Impact of Ligand Binding in a Constitutively Active Nuclear Receptor. Biochemistry, 2008, 47, 5205-5215.	2.5	12
120	Three-dimensional model and molecular dynamics simulation of the active site of the self-splicing intervening sequence of the bacteriophage T4 nrdB messenger RNA. Biochemistry, 1990, 29, 10317-10322.	2.5	11
121	Structural and dynamic differences of the estrogen receptor DNA-binding domain, binding as a dimer and as a monomer to DNA: molecular dynamics simulation studies. European Biophysics Journal, 1999, 28, 102-111.	2.2	11
122	A single residue exchange between two HLA-B27 alleles triggers increased peptide flexibility. European Biophysics Journal, 2004, 33, 651-655.	2.2	11
123	Site specific point mutation changes specificity: A molecular modeling study by free energy simulations and enzyme kinetics of the thermodynamics in ribonuclease T1 substrate interactions. Proteins: Structure, Function and Bioinformatics, 1993, 17, 161-175.	2.6	10
124	The elastic network model reveals a consistent picture on intrinsic functional dynamics of type II restriction endonucleases. Physical Biology, 2011, 8, 056001.	1.8	10
125	Multiple pH Regime Molecular Dynamics Simulation for pK Calculations. PLoS ONE, 2011, 6, e20116.	2.5	10
126	Exploring the idea of self-guided dynamics. Journal of Chemical Physics, 2001, 114, 5993-5999.	3.0	9

#	Article	IF	Citations
127	Human hereditary glutathione synthetase deficiency: kinetic properties of mutant enzymes. Biochemical Journal, 2004, 381, 489-494.	3.7	9
128	Molecular dynamics simulation of the preferred conformations of 2-thiouridine in aqueous solution. Theoretical Chemistry Accounts, 2007, 117, 267-273.	1.4	9
129	Investigation of transcription factor Ndt80 affinity differences for wild type and mutant DNA: A molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2008, 73, 325-337.	2.6	9
130	Elucidating the Relation between Internal Motions and Dihedral Angles in an RNA Hairpin Using Molecular Dynamics. Journal of Chemical Theory and Computation, 2014, 10, 3532-3540.	5.3	9
131	Motions and Entropies in Proteins as Seen in NMR Relaxation Experiments and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2015, 119, 1114-1128.	2.6	9
132	Structural effects of modified ribonucleotides and magnesium in transfer RNAs. Bioorganic and Medicinal Chemistry, 2016, 24, 4826-4834.	3.0	9
133	Role of Pseudoisocytidine Tautomerization in Triplex-Forming Oligonucleotides: In Silico and in Vitro Studies. ACS Omega, 2017, 2, 2165-2177.	3.5	9
134	Influence of adjacent bases on the stackingâ€unstacking process of singleâ€stranded oligonucleotides. Biopolymers, 1996, 39, 765-768.	2.4	9
135	Conformational states of yeast tRNAPhein the complex with congnate and non cognate synthetases. Nucleic Acids Research, 1981, 9, 1031-1044.	14.5	8
136	Free Energy Perturbations in Ribonuclease T₁Substrate Binding. A Study of the Influence of Simulation Length, Internal Degrees of Freedom and Structure in Free Energy Perturbations. Molecular Simulation, 1993, 10, 255-276.	2.0	8
137	Molecular Dynamics Study of Intrinsic Stability in Six RNA Terminal Loop Motifs. Journal of Biomolecular Structure and Dynamics, 2007, 24, 525-535.	3.5	8
138	Merging Implicit with Explicit Solvent Simulations: Polyethylene Glycol. Journal of Chemical Theory and Computation, 2010, 6, 1871-1883.	5.3	8
139	The free energy of locking a ring: Changing a deoxyribonucleoside to a locked nucleic acid. Journal of Computational Chemistry, 2017, 38, 1147-1157.	3.3	8
140	A subset of functional adaptation mutations alter propensity for Î±-helical conformation in the intrinsically disordered glucocorticoid receptor tau1core activation domain. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 1452-1461.	2.4	8
141	Computational Study of Uracil Tautomeric Forms in the Ribosome: The Case of Uracil and 5-Oxyacetic Acid Uracil in the First Anticodon Position of tRNA. Journal of Physical Chemistry B, 2018, 122, 1152-1160.	2.6	8
142	Biomolecular dynamics: A report from a workshop in Gysinge, Sweden, October 4â€“7, 1982. Quarterly Reviews of Biophysics, 1984, 17, 125-151.	5.7	7
143	A 1.2 ns Molecular Dynamics Simulation of the Ribonuclease T1â^'3â€˜-Guanosine Monophosphate Complex. The Journal of Physical Chemistry, 1996, 100, 2480-2488.	2.9	7
144	Examining the characteristics of chaos in biomolecular dynamics: a random matrix approximation. Chemical Physics Letters, 1999, 311, 459-466.	2.6	7

#	Article	IF	Citations
145	Molecular Dynamics Simulations of the E1/E2 Transmembrane Domain of the Semliki Forest Virus. Biophysical Journal, 2003, 85, 3646-3658.	0.5	7
146	A molecular dynamics study of Cyclophilin A free and in complex with the Ala-Pro dipeptide. European Biophysics Journal, 2007, 36, 213-224.	2.2	7
147	Crystal Structure of the HIV-2 Neutralizing Fab Fragment 7C8 with High Specificity to the V3 Region of gp125. PLoS ONE, 2011, 6, e18767.	2.5	7
148	Understanding the â^'Câ€“X1â€“X2â€“Câ€“ Motif in the Active Site of the Thioredoxin Superfamily: E. coli DsbA and Its Mutants as a Model System. Biochemistry, 2013, 52, 5730-5745.	2.5	7
149	Amyloid-Î² Peptide Targeting Peptidomimetics for Prevention of Neurotoxicity. ACS Chemical Neuroscience, 2019, 10, 1462-1477.	3.5	7
150	The ability of locked nucleic acid oligonucleotides to pre-structure the double helix: A molecular simulation and binding study. PLoS ONE, 2019, 14, e0211651.	2.5	7
151	Free Energy Calculations Predict Sequence Specificity in DNA-Drug Complexes. Nucleosides & Nucleotides, 1992, 11, 167-173.	0.5	6
152	Some practical aspects of free energy calculations from molecular dynamics simulation. Journal of Computational Chemistry, 1999, 20, 877-885.	3.3	6
153	Effect of G40R mutation on the binding of human SRY protein to DNA: A molecular dynamics view. , 1999, 35, 101-113.		6
154	Synthesis and evaluation of antineurotoxicity properties of an amyloid-Î² peptide targeting ligand containing a triamino acid. Organic and Biomolecular Chemistry, 2014, 12, 6684-6693.	2.8	6
155	The -Cys-X1-X2-Cys- Motif of Reduced Glutaredoxins Adopts a Consensus Structure That Explains the Low pK_a of Its Catalytic Cysteine. Biochemistry, 2012, 51, 8189-8207.	2.5	5
156	A â€œspindle and threadâ€•mechanism unblocks p53 translation by modulating N-terminal disorder. Structure, 2022, 30, 733-742.e7.	3.3	5
157	Theoretical Studies of Nucleic Acids and Nucleic Acid-Protein Complexes using Charmm. , 2006, , 73-94.		4
158	Rapid communication capturing the destabilizing effect of dihydrouridine through molecular simulations. Biopolymers, 2014, 101, 985-991.	2.4	4
159	Modeling pK Shift in DNA Triplexes Containing Locked Nucleic Acids. Journal of Chemical Information and Modeling, 2018, 58, 773-783.	5.4	4
160	Effect of mutations on internal dynamics of an RNA hairpin from hepatitis B virus. Biophysical Chemistry, 2016, 218, 7-13.	2.8	3
161	Quantitative confocal fluorescence microscopy of dynamic processes by multifocal fluorescence correlation spectroscopy. , 2015, , .		3
162	Comment on `Free energy calculations for DNA base stacking by replica-exchange umbrella sampling' by Katsumi Murata, Yuji Sugita, Yuko Okamoto. Chemical Physics Letters, 2004, 393, 282-283.	2.6	2

#	Article	IF	Citations
163	An Additive Charmm Force Field for Modified Nucleic Acids. Biophysical Journal, 2015, 108, 235a-236a.	0.5	2
164	Molecular Dynamics and NMR Shed Light on Motions Underpinning Dynamical Transitions in Biomolecules. Biophysical Journal, 2015, 108, 2755-2756.	0.5	2
165	Structural basis of biotinâ€"RNA aptamer binding: a theoretical study. Chemical Physics Letters, 2002, 363, 39-44.	2.6	1
166	Editorial preface. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 859-860.	2.4	1
167	Structural Stability of the Anticodon Stem Loop Domains of the Unmodified Yeast and Escherichia coli tRNA^{Phe}: Differing Views from Different Force Fields. ACS Omega, 2019, 4, 3029-3044.	3.5	1
168	Nucleic Acid Simulations. , 2001, , .		1
169	Molecular Dynamics Simulation of the Anticodon Arm of Phenylalanine Transfer RNA. , 1986, , 151-159.		1
170	Structural Fluctuations of Polypeptides in Lipid Membranes. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1988, 92, 1004-1006.	0.9	0
171	Computer Graphics Modelling and Molecular Dynamics Simulation of the Core of the Self Splicing Intervening Sequence of the T4 nrDB mRNA in the Presence of the Guanosine Cofactor. Nucleosides & Nucleotides, 1991, 10, 207-213.	0.5	0
172	Improved precision and efficiency of free energy calculations for small systems using ?-scaled atomic masses and separating conformational and transformational sampling. Journal of Computational Chemistry, 2003, 24, 1383-1389.	3.3	0
173	Studies on somatostatin with timeâ€resolved spectroscopy and molecular dynamics simulations. International Journal of Peptide and Protein Research, 1990, 36, 297-301.	0.1	0
174	Sophisticated Modeling Uncovers Atomic DNA Structure in Bacteriophage Î¦29ÂCavity. Biophysical Journal, 2013, 104, 1840-1841.	0.5	0
175	Combine and Free-Wilson QSAR Analysis of Nuclear Receptor-DNA Binding. , 2000, , 269-270.		0
176	Solvent effects on biomolecular dynamics simulations: A comparison between TIP3P, SPC and SPC/E water models acting on the Glucocorticoid receptor DNA-binding domain. , 2006, , 123-135.		0
177	The Structure of the tRNA Anticodon Arm as Determined by Restrained Molecular Dynamics in Combination with NMR Interproton Distance Data. Springer Series in Biophysics, 1987, , 113-117.	0.4	0
178	Dynamics of Nucleic Acids and Nucleic Acid:Protein Complexes. Springer Series in Synergetics, 1995, , 156-164.	0.4	0
179	Computer Simulations of Protein-DNA Interactions. , 1997, , 279-286.		0
180	Modeling and Simulation of Oligonucleotide Hybrids: Outlining a Strategy. Methods in Molecular Biology, 2019, 2036, 113-126.	0.9	0

#	Article	IF	Citations
181	A Highly Efficient Ab Initio Tight-Binding-Like Approximate Density-Functional Quantum Mechanical Method. , 2007, , 100-108.		0