Modesto Orozco LÃ³pez

List of Publications by Year
in descending order

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		5558	8138
392	28,596	82	148
papers	citations	h-index	g-index

412	412	412	28681
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	<scp>Preâ€exascale HPC</scp> approaches for molecular dynamics simulations. Covidâ€19 research: A use case. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	6.2	6
2	Molecular basis of Arginine and Lysine DNA sequence-dependent thermo-stability modulation. PLoS Computational Biology, 2022, 18, e1009749.	1.5	1
3	Mechanism of reaction of RNA-dependent RNA polymerase from SARS-CoV-2. Chem Catalysis, 2022, 2, 1084-1099.	2.9	20
4	BioExcel Building Blocks Workflows (BioBB-Wfs), an integrated web-based platform for biomolecular simulations. Nucleic Acids Research, 2022, 50, W99-W107.	6.5	7
5	Mutation in KARS: AÂnovel mechanism for severe anaphylaxis. Journal of Allergy and Clinical Immunology, 2021, 147, 1855-1864.e9.	1.5	14
6	Impact of DNA methylation on 3D genome structure. Nature Communications, 2021, 12, 3243.	5.8	61
7	3dRS, a Web-Based Tool to Share Interactive Representations of 3D Biomolecular Structures and Molecular Dynamics Trajectories. Frontiers in Molecular Biosciences, 2021, 8, 726232.	1.6	6
8	Probing allosteric regulations with coevolution-driven molecular simulations. Science Advances, 2021, 7, eabj0786.	4.7	8
9	The Impact of the HydroxyMethylCytosine epigenetic signature on DNA structure and function. PLoS Computational Biology, 2021, 17, e1009547.	1.5	6
10	Sequence-dependent structural properties of B-DNA: what have we learned in 40Âyears?. Biophysical Reviews, 2021, 13, 995-1005.	1.5	13
11	Determination of a Structural Ensemble Representing the Dynamics of a G-Quadruplex DNA. Biochemistry, 2020, 59, 379-388.	1.2	3
12	Surviving the deluge of biosimulation data. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1449.	6.2	16
13	Bioactive Conformational Ensemble Server and Database. A Public Framework to Speed Up In Silico Drug Discovery. Journal of Chemical Theory and Computation, 2020, 16, 6586-6597.	2.3	10
14	Exploring the Conformational Landscape of Bioactive Small Molecules. Journal of Chemical Theory and Computation, 2020, 16, 6575-6585.	2.3	17
15	DFFR: A New Method for High-Throughput Recalibration of Automatic Force-Fields for Drugs. Journal of Chemical Theory and Computation, 2020, 16, 6598-6608.	2.3	5
16	Protein disorder-to-order transition enhances the nucleosome-binding affinity of H1. Nucleic Acids Research, 2020, 48, 5318-5331.	6.5	19
17	Colibactin DNA-damage signature indicates mutational impact in colorectal cancer. Nature Medicine, 2020, 26, 1063-1069.	15.2	149
18	Emergence of chromatin hierarchical loops from protein disorder and nucleosome asymmetry. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 7216-7224.	3.3	32

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19	4D Genome Rewiring during Oncogene-Induced and Replicative Senescence. Molecular Cell, 2020, 78, 522-538.e9.	4.5	107
20	A multi-modal coarse grained model of DNA flexibility mappable to the atomistic level. Nucleic Acids Research, 2020, 48, e29-e29.	6.5	27
21	Epigenetic loss of RNA-methyltransferase NSUN5 in glioma targets ribosomes to drive a stress adaptive translational program. Acta Neuropathologica, 2019, 138, 1053-1074.	3.9	106
22	How B-DNA Dynamics Decipher Sequence-Selective Protein Recognition. Journal of Molecular Biology, 2019, 431, 3845-3859.	2.0	34
23	VeriNA3d: an R package for nucleic acids data mining. Bioinformatics, 2019, 35, 5334-5336.	1.8	4
24	The static and dynamic structural heterogeneities of B-DNA: extending Calladineâ€“Dickerson rules. Nucleic Acids Research, 2019, 47, 11090-11102.	6.5	45
25	BioExcel Building Blocks, a software library for interoperable biomolecular simulation workflows. Scientific Data, 2019, 6, 169.	2.4	35
26	Nucleosome Dynamics: a new tool for the dynamic analysis of nucleosome positioning. Nucleic Acids Research, 2019, 47, 9511-9523.	6.5	12
27	Predicting the Limit of Intramolecular Hydrogen Bonding with Classical Molecular Dynamics. Angewandte Chemie - International Edition, 2019, 58, 3759-3763.	7.2	15
28	Predicting the Limit of Intramolecular Hydrogen Bonding with Classical Molecular Dynamics. Angewandte Chemie, 2019, 131, 3799-3803.	1.6	4
29	A multifunctional toolkit for target-directed cancer therapy. Chemical Communications, 2019, 55, 802-805.	2.2	1
30	An artificial DNAzyme RNA ligase shows a reaction mechanism resembling that of cellular polymerases. Nature Catalysis, 2019, 2, 544-552.	16.1	18
31	DNA specificities modulate the binding of human transcription factor A to mitochondrial DNA control region. Nucleic Acids Research, 2019, 47, 6519-6537.	6.5	17
32	The Origins and the Biological Consequences of the Pur/Pyr DNAÂ·RNA Asymmetry. CheM, 2019, 5, 1619-1631.	5.8	13
33	Modulation of the helical properties of DNA: next-to-nearest neighbour effects and beyond. Nucleic Acids Research, 2019, 47, 4418-4430.	6.5	32
34	Oncogenic mutations at the EGFR ectodomain structurally converge to remove a steric hindrance on a kinase-coupled cryptic epitope. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 10009-10018.	3.3	46
35	An In-Depth Look at DNA Crystals through the Prism of Molecular Dynamics Simulations. CheM, 2019, 5, 649-663.	5.8	11
36	Modeling, Simulations, and Bioinformatics at the Service of RNA Structure. CheM, 2019, 5, 51-73.	5.8	25

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37	Protein Flexibility and Synergy of HMG Domains Underlie U-Turn Bending of DNA by TFAM in Solution. Biophysical Journal, 2018, 114, 2386-2396.	0.2	16
38	Plasticity in oligomerization, operator architecture, and DNA binding in the mode of action of a bacterial B12-based photoreceptor. Journal of Biological Chemistry, 2018, 293, 17888-17905.	1.6	12
39	Allosterism and signal transfer in DNA. Nucleic Acids Research, 2018, 46, 7554-7565.	6.5	30
40	Targeting RNA structure in SMN2 reverses spinal muscular atrophy molecular phenotypes. Nature Communications, 2018, 9, 2032.	5.8	60
41	The Multiple Roles of Waters in Protein Solvation. Journal of Physical Chemistry B, 2017, 121, 3636-3643.	1.2	17
42	How accurate are accurate force-fields for B-DNA?. Nucleic Acids Research, 2017, 45, gkw1355.	6.5	107
43	Proton Dynamics in Protein Mass Spectrometry. Journal of Physical Chemistry Letters, 2017, 8, 1105-1112.	2.1	34
44	Discrete Molecular Dynamics Approach to the Study of Disordered and Aggregating Proteins. Journal of Chemical Theory and Computation, 2017, 13, 1454-1461.	2.3	24
45	Efficient siRNAâ€“peptide conjugation for specific targeted delivery into tumor cells. Chemical Communications, 2017, 53, 2870-2873.	2.2	16
46	Compaction of Duplex Nucleic Acids upon Native Electrospray Mass Spectrometry. ACS Central Science, 2017, 3, 454-461.	5.3	81
47	Mechanism of Structural Tuning of the Hepatitis C Virus Human Cellular Receptor CD81 Large Extracellular Loop. Structure, 2017, 25, 53-65.	1.6	25
48	PMut: a web-based tool for the annotation of pathological variants on proteins, 2017 update. Nucleic Acids Research, 2017, 45, W222-W228.	6.5	184
49	The Role of Unconventional Hydrogen Bonds in Determining BII Propensities in B-DNA. Journal of Physical Chemistry Letters, 2017, 8, 21-28.	2.1	18
50	Prevalent Sequences in the Human Genome Can Form Mini i-Motif Structures at Physiological pH. Journal of the American Chemical Society, 2017, 139, 13985-13988.	6.6	68
51	Inhibition of Human Enhancer of Zeste Homolog 2 with Tambjamine Analogs. Journal of Chemical Information and Modeling, 2017, 57, 2089-2098.	2.5	5
52	Repair of UV-Induced DNA Damage Independent of Nucleotide Excision Repair Is Masked by MUTYH. Molecular Cell, 2017, 68, 797-807.e7.	4.5	29
53	Quantification of Pathway Cross-talk Reveals Novel Synergistic Drug Combinations for Breast Cancer. Cancer Research, 2017, 77, 459-469.	0.4	75
54	DNA structure directs positioning of the mitochondrial genome packaging protein Abf2p. Nucleic Acids Research, 2017, 45, 951-967.	6.5	23

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55	Structural basis of a histidine-DNA nicking/joining mechanism for gene transfer and promiscuous spread of antibiotic resistance. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E6526-E6535.	3.3	27
56	Changes in the free-energy landscape of p38Î± MAP kinase through its canonical activation and binding events as studied by enhanced molecular dynamics simulations. ELife, 2017, 6, .	2.8	65
57	Nucleosome architecture throughout the cell cycle. Scientific Reports, 2016, 6, 19729.	1.6	29
58	Conformational plasticity of RepB, the replication initiator protein of promiscuous streptococcal plasmid pMV158. Scientific Reports, 2016, 6, 20915.	1.6	11
59	Saturation of recognition elements blocks evolution of new tRNA identities. Science Advances, 2016, 2, e1501860.	4.7	46
60	Editorial overview: Theory and simulation. Current Opinion in Structural Biology, 2016, 37, iv-v.	2.6	0
61	Computational Prediction of HIV-1 Resistance to Protease Inhibitors. Journal of Chemical Information and Modeling, 2016, 56, 915-923.	2.5	19
62	Long-timescale dynamics of the Drewâ€“Dickerson dodecamer. Nucleic Acids Research, 2016, 44, 4052-4066.	6.5	86
63	Challenges of docking in large, flexible and promiscuous binding sites. Bioorganic and Medicinal Chemistry, 2016, 24, 4961-4969.	1.4	19
64	Small Details Matter: The 2â€²-Hydroxyl as a Conformational Switch in RNA. Journal of the American Chemical Society, 2016, 138, 16355-16363.	6.6	23
65	Prediction and validation of protein intermediate states from structurally rich ensembles and coarse-grained simulations. Nature Communications, 2016, 7, 12575.	5.8	62
66	pyPcazip: A PCA-based toolkit for compression and analysis of molecular simulation data. SoftwareX, 2016, 5, 44-50.	1.2	37
67	Parmbsc1: a refined force field for DNA simulations. Nature Methods, 2016, 13, 55-58.	9.0	790
68	Multiscale simulation of DNA. Current Opinion in Structural Biology, 2016, 37, 29-45.	2.6	124
69	Residues Coevolution Guides the Systematic Identification of Alternative Functional Conformations in Proteins. Structure, 2016, 24, 116-126.	1.6	56
70	Exploring the complete mutational space of the LDL receptor LA5 domain using molecular dynamics: linking SNPs with disease phenotypes in familial hypercholesterolemia. Human Molecular Genetics, 2016, 25, 1233-1246.	1.4	9
71	Rational design of novel N-alkyl-N capped biostable RNA nanostructures for efficient long-term inhibition of gene expression. Nucleic Acids Research, 2016, 44, 4354-4367.	6.5	9
72	BIGNASim: a NoSQL database structure and analysis portal for nucleic acids simulation data. Nucleic Acids Research, 2016, 44, D272-D278.	6.5	57

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73	Epigenomic analysis detects aberrant super-enhancer DNA methylation in human cancer. Genome Biology, 2016, 17, 11.	3.8	184
74	Mutations in JMJD1C are involved in Rett syndrome and intellectual disability. Genetics in Medicine, 2016, 18, 378-385.	1.1	40
75	The Differential Response of Proteins to Macromolecular Crowding. PLoS Computational Biology, 2016, 12, e1005040.	1.5	44
76	Chapter 7. Methods to Trace Conformational Transitions. RSC Theoretical and Computational Chemistry Series, 2016, , 215-244.	0.7	0
77	Structure and Dynamics of Oligonucleotides in the Gas Phase. Angewandte Chemie - International Edition, 2015, 54, 467-471.	7.2	26
78	SDS-PAGE analysis of AÎ² oligomers is disserving research into AlzheimerÂ´s disease: appealing for ESI-IM-MS. Scientific Reports, 2015, 5, 14809.	1.6	88
79	Can A Denaturant Stabilize DNA? Pyridine Reverses DNA Denaturation in Acidic pH. Angewandte Chemie - International Edition, 2015, 54, 10488-10491.	7.2	7
80	Molecular dynamics simulations: advances and applications. Advances and Applications in Bioinformatics and Chemistry, 2015, 8, 37.	1.6	409
81	PACSAB: Coarse-Grained Force Field for the Study of Proteinâ€“Protein Interactions and Conformational Sampling in Multiprotein Systems. Journal of Chemical Theory and Computation, 2015, 11, 5929-5938.	2.3	14
82	Assessing the Suitability of the Multilevel Strategy for the Conformational Analysis of Small Ligands. Journal of Physical Chemistry B, 2015, 119, 1164-1172.	1.2	16
83	Synthesis and Properties of 2â€²-Deoxy-2â€²,4â€²-difluoroarabinose-Modified Nucleic Acids. Journal of Organic Chemistry, 2015, 80, 3083-3091.	1.7	32
84	Chromatin Unfolding by Epigenetic Modifications Explained by Dramatic Impairment of Internucleosome Interactions: A Multiscale Computational Study. Journal of the American Chemical Society, 2015, 137, 10205-10215.	6.6	135
85	Non-coding recurrent mutations in chronic lymphocytic leukaemia. Nature, 2015, 526, 519-524.	13.7	749
86	The structural impact of DNA mismatches. Nucleic Acids Research, 2015, 43, 4309-4321.	6.5	113
87	SEABED: Small molEcule activity scanner weB servicE baseD. Bioinformatics, 2015, 31, 773-775.	1.8	8
88	Seven-Membered Ring Nucleoside Analogues: Stereoselective Synthesis and Studies on Their Conformational Properties. Organic Letters, 2015, 17, 5416-5419.	2.4	12
89	Inntags: small self-structured epitopes for innocuous protein tagging. Nature Methods, 2015, 12, 955-958.	9.0	22
90	Visualizing phosphodiester-bond hydrolysis by an endonuclease. Nature Structural and Molecular Biology, 2015, 22, 65-72.	3.6	30

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91	Molecular Dynamics Study of Naturally Existing Cavity Couplings in Proteins. PLoS ONE, 2015, 10, e0119978.	1.1	10
92	Î¼ABC: a systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. Nucleic Acids Research, 2014, 42, 12272-12283.	6.5	186
93	A Comprehensive DNA Methylation Profile of Epithelial-to-Mesenchymal Transition. Cancer Research, 2014, 74, 5608-5619.	0.4	69
94	Unraveling the sequence-dependent polymorphic behavior of d(CpG) steps in B-DNA. Nucleic Acids Research, 2014, 42, 11304-11320.	6.5	81
95	Fuzziness and noise in nucleosomal architecture. Nucleic Acids Research, 2014, 42, 4934-4946.	6.5	28
96	Specific loop modifications of the thrombinâ€‘binding aptamer trigger the formation of parallel structures. FEBS Journal, 2014, 281, 1085-1099.	2.2	25
97	The DNA-forming properties of 6-selenoguanine. Physical Chemistry Chemical Physics, 2014, 16, 1101-1110.	1.3	13
98	Comprehensive characterization of complex structural variations in cancer by directly comparing genome sequence reads. Nature Biotechnology, 2014, 32, 1106-1112.	9.4	74
99	Structure and Properties of DNA in Apolar Solvents. Journal of Physical Chemistry B, 2014, 118, 8540-8548.	1.2	22
100	Direct measurement of the dielectric polarization properties of DNA. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E3624-30.	3.3	160
101	MD and NMR Analyses of Choline and TMA Binding to Duplex DNA: On the Origins of Aberrant Sequence-Dependent Stability by Alkyl Cations in Aqueous and Water-Free Solvents. Journal of the American Chemical Society, 2014, 136, 3075-3086.	6.6	44
102	A theoretical view of protein dynamics. Chemical Society Reviews, 2014, 43, 5051-5066.	18.7	111
103	Correlated motions are a fundamental property of Î²-sheets. Nature Communications, 2014, 5, 4070.	5.8	82
104	Structure of Nucleic Acids in the Gas Phase. Physical Chemistry in Action, 2014, , 55-75.	0.1	5
105	On the Nature of DNA Hyperchromic Effect. Journal of Physical Chemistry B, 2013, 117, 8697-8704.	1.2	44
106	Consistent View of Protein Fluctuations from All-Atom Molecular Dynamics and Coarse-Grained Dynamics with Knowledge-Based Force-Field. Journal of Chemical Theory and Computation, 2013, 9, 119-125.	2.3	85
107	The Conformational Landscape of an Intrinsically Disordered DNA-Binding Domain of a Transcription Regulator. Journal of Physical Chemistry B, 2013, 117, 13842-13850.	1.2	27
108	BioSuper: A web tool for the superimposition of biomolecules and assemblies with rotational symmetry. BMC Structural Biology, 2013, 13, 32.	2.3	8

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109	Backbone FCï£¿Hâ‹…â‹…â‹…O Hydrogen Bonds in 2â€²Fâ€Substituted Nucleic Acids. Angewandte Chemie - International Edition, 2013, 52, 12065-12068.	7.2	44
110	Backbone FCï£¿Hâ‹…â‹…â‹…O Hydrogen Bonds in 2â€²Fâ€Substituted Nucleic Acids. Angewandte Chemie, 2013, 125, 12287-12290.	1.6	7
111	Efficient Relaxation of Proteinâ€“Protein Interfaces by Discrete Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 1222-1229.	2.3	13
112	The dynamic view of proteins. Physics of Life Reviews, 2013, 10, 29-30.	1.5	2
113	The catalytic site structural gate of adenosine deaminase allosterically modulates ligand binding to adenosine receptors. FASEB Journal, 2013, 27, 1048-1061.	0.2	35
114	Functionalization of the 3â€²â€Ends of DNA and RNA Strands with Nâ€ethylâ€Nâ€coupled Nucleosides: A Promising Approach To Avoid 3â€²â€Exonucleaseâ€Catalyzed Hydrolysis of Therapeutic Oligonucleotides. ChemBioChem, 2013, 14, 510-520.	1.3	13
115	Structure, Stiffness and Substates of the Dickerson-Drew Dodecamer. Journal of Chemical Theory and Computation, 2013, 9, 707-721.	2.3	78
116	Dramatic Effect of Furanose C2â€² Substitution on Structure and Stability: Directing the Folding of the Human Telomeric Quadruplex with a Single Fluorine Atom. Journal of the American Chemical Society, 2013, 135, 5344-5347.	6.6	62
117	Proteins in the gas phase. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 408-425.	6.2	49
118	Toward an atomistic description of the urea-denatured state of proteins. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 5933-5938.	3.3	50
119	Understanding the Connection between Epigenetic DNA Methylation and Nucleosome Positioning from Computer Simulations. PLoS Computational Biology, 2013, 9, e1003354.	1.5	50
120	Exploring Early Stages of the Chemical Unfolding of Proteins at the Proteome Scale. PLoS Computational Biology, 2013, 9, e1003393.	1.5	14
121	NAFlex: a web server for the study of nucleic acid flexibility. Nucleic Acids Research, 2013, 41, W47-W55.	6.5	45
122	Unravelling the hidden DNA structural/physical code provides novel insights on promoter location. Nucleic Acids Research, 2013, 41, 7220-7230.	6.5	13
123	Improved nucleic acid descriptors for siRNA efficacy prediction. Nucleic Acids Research, 2013, 41, 1383-1394.	6.5	17
124	Exploration of conformational transition pathways from coarse-grained simulations. Bioinformatics, 2013, 29, 1980-1986.	1.8	26
125	Light on the structural communication in Ras GTPases. Journal of Biomolecular Structure and Dynamics, 2013, 31, 142-157.	2.0	19
126	Conformational dynamics of the human propeller telomeric DNA quadruplex on a microsecond time scale. Nucleic Acids Research, 2013, 41, 2723-2735.	6.5	70

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127	MDWeb and MDMoby: an integrated web-based platform for molecular dynamics simulations. Bioinformatics, 2012, 28, 1278-1279.	1.8	153
128	Geometry, Dynamics, and Electronic Structure of DNAâ€“Carbon Nanotube Hybrids. Journal of Physical Chemistry C, 2012, 116, 11278-11282.	1.5	5
129	Hog1 bypasses stress-mediated down-regulation of transcription by RNA polymerase II redistribution and chromatin remodeling. Genome Biology, 2012, 13, R106.	13.9	50
130	Structure of Triplex DNA in the Gas Phase. Journal of the American Chemical Society, 2012, 134, 6596-6606.	6.6	56
131	Finding Conformational Transition Pathways from Discrete Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 4707-4718.	2.3	29
132	Frontiers in Molecular Dynamics Simulations of DNA. Accounts of Chemical Research, 2012, 45, 196-205.	7.6	194
133	Fast Atomistic Molecular Dynamics Simulations from Essential Dynamics Samplings. Journal of Chemical Theory and Computation, 2012, 8, 792-799.	2.3	10
134	Exploring polymorphisms in B-DNA helical conformations. Nucleic Acids Research, 2012, 40, 10668-10678.	6.5	89
135	Epigenomic analysis detects widespread gene-body DNA hypomethylation in chronic lymphocytic leukemia. Nature Genetics, 2012, 44, 1236-1242.	9.4	525
136	Application of Drug-Perturbed Essential Dynamics/Molecular Dynamics (ED/MD) to Virtual Screening and Rational Drug Design. Journal of Chemical Theory and Computation, 2012, 8, 2204-2214.	2.3	11
137	Impact of Methylation on the Physical Properties of DNA. Biophysical Journal, 2012, 102, 2140-2148.	0.2	118
138	A Multilevel Strategy for the Exploration of the Conformational Flexibility of Small Molecules. Journal of Chemical Theory and Computation, 2012, 8, 1808-1819.	2.3	35
139	Defining the Nature of Thermal Intermediate in 3 State Folding Proteins: Apoflavodoxin, a Study Case. PLoS Computational Biology, 2012, 8, e1002647.	1.5	14
140	Evidence for Transcript Networks Composed of Chimeric RNAs in Human Cells. PLoS ONE, 2012, 7, e28213.	1.1	61
141	Characterization of the impact of alternative splicing on protein dynamics: The cases of glutathione Sâ€transferase and ectodysplasinâ€A isoforms. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2235-2249.	1.5	5
142	Exome sequencing identifies recurrent mutations of the splicing factor SF3B1 gene in chronic lymphocytic leukemia. Nature Genetics, 2012, 44, 47-52.	9.4	893
143	Small Molecule Docking from Theoretical Structural Models. Biological and Medical Physics Series, 2012, , 75-95.	0.3	1
144	Effects of local electric fields on the redox free energy of single stranded DNA. Chemical Communications, 2011, 47, 2646-2648.	2.2	8

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145	The protein folding transition-state ensemble from a GÅ•like model. Physical Chemistry Chemical Physics, 2011, 13, 15166.	1.3	14
146	Whole-genome sequencing identifies recurrent mutations in chronic lymphocytic leukaemia. Nature, 2011, 475, 101-105.	13.7	1,364
147	nucleR: a package for non-parametric nucleosome positioning. Bioinformatics, 2011, 27, 2149-2150.	1.8	81
148	Scoring by Intermolecular Pairwise Propensities of Exposed Residues (SIPPER): A New Efficient Potential for Proteinâ^'Protein Docking. Journal of Chemical Information and Modeling, 2011, 51, 370-377.	2.5	70
149	Structural, Dynamical, and Electronic Transport Properties of Modified DNA Duplexes Containing Size-Expanded Nucleobases. Journal of Physical Chemistry A, 2011, 115, 11344-11354.	1.1	16
150	Coarse-grained Representation of Protein Flexibility. Foundations, Successes, and Shortcomings. Advances in Protein Chemistry and Structural Biology, 2011, 85, 183-215.	1.0	33
151	The Native Ensemble and Folding of a Protein Molten-Globule: Functional Consequence of Downhill Folding. Journal of the American Chemical Society, 2011, 133, 12154-12161.	6.6	57
152	Structural Analysis of an Equilibrium Folding Intermediate in the Apoflavodoxin Native Ensemble by Small-Angle X-ray Scattering. Journal of Molecular Biology, 2011, 406, 604-619.	2.0	27
153	A Systematic Study of the Energetics Involved in Structural Changes upon Association and Connectivity in Protein Interaction Networks. Structure, 2011, 19, 881-889.	1.6	42
154	Polarization effects in molecular interactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 844-854.	6.2	28
155	Physical properties of naked DNA influence nucleosome positioning and correlate with transcription start and termination sites in yeast. BMC Genomics, 2011, 12, 489.	1.2	31
156	Molecular basis of substrate-induced permeation by an amino acid antiporter. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 3935-3940.	3.3	139
157	Nucleotide Binding Switches the Information Flow in Ras GTPases. PLoS Computational Biology, 2011, 7, e1001098.	1.5	39
158	Performance of the IEF-MST solvation continuum model in the SAMPL2 blind test prediction of hydration and tautomerization free energies. Journal of Computer-Aided Molecular Design, 2010, 24, 281-291.	1.3	24
159	Deciphering the Deformation Modes Associated with Function Retention and Specialization in Members of the Ras Superfamily. Structure, 2010, 18, 402-414.	1.6	46
160	MoDEL (Molecular Dynamics Extended Library): AÂDatabase of Atomistic Molecular Dynamics Trajectories. Structure, 2010, 18, 1399-1409.	1.6	123
161	A genomics method to identify pathogenicityâ€related proteins. Application to aminoacylâ€tRNA synthetaseâ€like proteins. FEBS Letters, 2010, 584, 460-466.	1.3	5
162	Realâ€Time Atomistic Description of DNA Unfolding. Angewandte Chemie - International Edition, 2010, 49, 4805-4808.	7.2	30

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163	Multiple Routes to Characterize the Folding of a Small DNA Hairpin. Angewandte Chemie - International Edition, 2010, 49, 7673-7676.	7.2	45
164	Protein flexibility from discrete molecular dynamics simulations using quasiâ€physical potentials. Proteins: Structure, Function and Bioinformatics, 2010, 78, 83-94.	1.5	24
165	Structural Properties of G,T-Parallel Duplexes. Journal of Nucleic Acids, 2010, 2010, 1-11.	0.8	4
166	Differential stability of 2â€²F-ANAâ€¢RNA and ANAâ€¢RNA hybrid duplexes: roles of structure, pseudohydrogen bonding, hydration, ion uptake and flexibility. Nucleic Acids Research, 2010, 38, 2498-2511.	6.5	65
167	Toward a Consensus View of Duplex RNA Flexibility. Biophysical Journal, 2010, 99, 1876-1885.	0.2	54
168	Approaching Elastic Network Models to Molecular Dynamics Flexibility. Journal of Chemical Theory and Computation, 2010, 6, 2910-2923.	2.3	60
169	Ensemble Docking from Homology Models. Journal of Chemical Theory and Computation, 2010, 6, 2547-2557.	2.3	65
170	A systematic molecular dynamics study of nearest-neighbor effects on base pair and base pair step conformations and fluctuations in B-DNA. Nucleic Acids Research, 2010, 38, 299-313.	6.5	349
171	Structural Characterization of Proteinâ€“Protein Complexes by Integrating Computational Docking with Small-angle Scattering Data. Journal of Molecular Biology, 2010, 403, 217-230.	2.0	64
172	Performance of Molecular Mechanics Force Fields for RNA Simulations: Stability of UUCG and GNRA Hairpins. Journal of Chemical Theory and Computation, 2010, 6, 3836-3849.	2.3	339
173	Conformationally rigid nucleoside probes help understand the role of sugar pucker and nucleobase orientation in the thrombin-binding aptamer. Nucleic Acids Research, 2009, 37, 5589-5601.	6.5	35
174	Alternative Splicing of Transcription Factors' Genes: Beyond the Increase of Proteome Diversity. Comparative and Functional Genomics, 2009, 2009, 1-6.	2.0	14
175	FlexServ: an integrated tool for the analysis of protein flexibility. Bioinformatics, 2009, 25, 1709-1710.	1.8	72
176	An Atomistic View to the Gas Phase Proteome. Structure, 2009, 17, 88-95.	1.6	44
177	Solvation enthalpies of neutral solutes in water and octanol. Theoretical Chemistry Accounts, 2009, 123, 11-20.	0.5	7
178	COCO: A simple tool to enrich the representation of conformational variability in NMR structures. Proteins: Structure, Function and Bioinformatics, 2009, 75, 206-216.	1.5	17
179	Comparison of molecular dynamics and superfamily spaces of protein domain deformation. BMC Structural Biology, 2009, 9, 6.	2.3	35
180	On the Performance of Continuum Solvation Methods. A Comment on â€œUniversal Approaches to Solvation Modelingâ€• Accounts of Chemical Research, 2009, 42, 489-492.	7.6	171

#	Article	IF	Citations
181	Theoretical Characterization of the Dynamical Behavior and Transport Properties of Î±,Î³-Peptide Nanotubes in Solution. Journal of the American Chemical Society, 2009, 131, 15678-15686.	6.6	41
182	Performance of the IEF-MST Solvation Continuum Model in a Blind Test Prediction of Hydration Free Energies. Journal of Physical Chemistry B, 2009, 113, 9330-9334.	1.2	17
183	Ab initio Study of the Structural, Tautomeric, Pairing, and Electronic Properties of Seleno-Derivatives of Thymine. Journal of Physical Chemistry B, 2009, 113, 14465-14472.	1.2	15
184	Nucleic acid simulations themed issue. Physical Chemistry Chemical Physics, 2009, 11, 10541.	1.3	5
185	X-Pol Potential: An Electronic Structure-Based Force Field for Molecular Dynamics Simulation of a Solvated Protein in Water. Journal of Chemical Theory and Computation, 2009, 5, 459-467.	2.3	121
186	On the Use of low-resolution Data to Improve Structure Prediction of Proteins and Protein Complexes. Journal of Chemical Theory and Computation, 2009, 5, 3129-3137.	2.3	7
187	Unique Tautomeric and Recognition Properties of Thioketothymines?. Journal of the American Chemical Society, 2009, 131, 12845-12853.	6.6	4
188	Single Stranded Loops of Quadruplex DNA As Key Benchmark for Testing Nucleic Acids Force Fields. Journal of Chemical Theory and Computation, 2009, 5, 2514-2530.	2.3	121
189	The impact of monovalent ion force field model in nucleic acids simulations. Physical Chemistry Chemical Physics, 2009, 11, 10596.	1.3	62
190	GRIDâ€¥MDâ€”A tool for massive simulation of protein channels. Proteins: Structure, Function and Bioinformatics, 2008, 70, 892-899.	1.5	13
191	Extension of the MST continuum solvation model to the RM1 semiempirical hamiltonian. Journal of Computational Chemistry, 2008, 29, 578-587.	1.5	17
192	Towards a molecular dynamics consensus view of B-DNA flexibility. Nucleic Acids Research, 2008, 36, 2379-2394.	6.5	147
193	Recent advances in the study of nucleic acid flexibility by molecular dynamics. Current Opinion in Structural Biology, 2008, 18, 185-193.	2.6	113
194	Ab Initio Study of Naphtho-Homologated DNA Bases. Journal of Physical Chemistry B, 2008, 112, 2179-2186.	1.2	23
195	Exploring the Suitability of Coarse-Grained Techniques for the Representation of Protein Dynamics. Biophysical Journal, 2008, 95, 2127-2138.	0.2	42
196	Geometrical and Electronic Structure Variability of the Sugarâ”phosphate Backbone in Nucleic Acids. Journal of Physical Chemistry B, 2008, 112, 8188-8197.	1.2	52
197	Target Flexibility: An Emerging Consideration in Drug Discovery and Design. Journal of Medicinal Chemistry, 2008, 51, 6237-6255.	2.9	280
198	Induction effects in metal cationâ€“benzene complexes. Physical Chemistry Chemical Physics, 2008, 10, 2616.	1.3	78

#	Article	IF	Citations
199	8-Amino guanine accelerates tetramolecular G-quadruplex formation. Chemical Communications, 2008, , 2926.	2.2	32
200	Structure-Directed Reversion in the Ï€-Facial Stereoselective Alkylation of Chiral Bicyclic Lactams. Journal of Organic Chemistry, 2008, 73, 7756-7763.	1.7	13
201	United-Atom Discrete Molecular Dynamics of Proteins Using Physics-Based Potentials. Journal of Chemical Theory and Computation, 2008, 4, 2001-2010.	2.3	17
202	Theoretical Analysis of Antisense Duplexes:â€‰ Determinants of the RNase H Susceptibility. Journal of the American Chemical Society, 2008, 130, 3486-3496.	6.6	30
203	DNAlive: a tool for the physical analysis of DNA at the genomic scale. Bioinformatics, 2008, 24, 1731-1732.	1.8	28
204	Interoperability with Moby 1.0--It's better than sharing your toothbrush!. Briefings in Bioinformatics, 2008, 9, 220-231.	3.2	91
205	Thermochemical Analysis of the Hydration of Neutral Solutes. Challenges and Advances in Computational Chemistry and Physics, 2008, , 103-113.	0.6	0
206	The (In)dependence of Alternative Splicing and Gene Duplication. PLoS Computational Biology, 2007, 3, e33.	1.5	66
207	The Structure of Human 4F2hc Ectodomain Provides a Model for Homodimerization and Electrostatic Interaction with Plasma Membrane. Journal of Biological Chemistry, 2007, 282, 31444-31452.	1.6	101
208	A consensus view of protein dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 796-801.	3.3	223
209	Refinement of the AMBER Force Field for Nucleic Acids: Improving the Description of Î±/Î³ Conformers. Biophysical Journal, 2007, 92, 3817-3829.	0.2	2,036
210	Theoretical study of large conformational transitions in DNA: the Bâ†”A conformational change in water and ethanol/water. Nucleic Acids Research, 2007, 35, 3330-3338.	6.5	71
211	Dynamics of B-DNA on the Microsecond Time Scale. Journal of the American Chemical Society, 2007, 129, 14739-14745.	6.6	250
212	Determining promoter location based on DNA structure first-principles calculations. Genome Biology, 2007, 8, R263.	13.9	121
213	Characterization of Compensated Mutations in Terms of Structural and Physico-Chemical Properties. Journal of Molecular Biology, 2007, 365, 249-256.	2.0	43
214	Binding Affinities of Oligonucleotides and PNAs Containing Phenoxazine and G-Clamp Cytosine Analogues Are Unusually Sequence-Dependent. Organic Letters, 2007, 9, 4503-4506.	2.4	54
215	Derivation of Distributed Models of Atomic Polarizability for Molecular Simulations. Journal of Chemical Theory and Computation, 2007, 3, 1901-1913.	2.3	41
216	Triplex Formation Using Oligonucleotide Clamps Carrying 8-Aminopurines. Nucleosides, Nucleotides and Nucleic Acids, 2007, 26, 979-983.	0.4	2

#	Article	IF	Citations
217	Dissection of the Recognition Properties of p38 MAP Kinase. Determination of the Binding Mode of a New Pyridinylâ"Heterocycle Inhibitor Family. Journal of Medicinal Chemistry, 2007, 50, 283-293.	2.9	24
218	Exploring the Dynamics of Calix[4]pyrrole: Effect of Solvent and Fluorine Substitution. Chemistry - A European Journal, 2007, 13, 1108-1116.	1.7	37
219	A procedure for identifying homologous alternative splicing events. BMC Bioinformatics, 2007, 8, 260.	1.2	5
220	Thorough Validation of Protein Normal Mode Analysis: A Comparative Study with Essential Dynamics. Structure, 2007, 15, 565-575.	1.6	144
221	A hydrophobic similarity analysis of solvation effects on nucleic acid bases. Journal of Molecular Modeling, 2007, 13, 357-365.	0.8	8
222	Essential Dynamics:â€‰ A Tool for Efficient Trajectory Compression and Management. Journal of Chemical Theory and Computation, 2006, 2, 251-258.	2.3	98
223	Local Aromaticity in Natural Nucleobases and Their Size-Expanded Benzo-Fused Derivatives. Journal of Physical Chemistry A, 2006, 110, 12249-12258.	1.1	52
224	Theoretical Study of the Hoogsteenâ€"Watson-Crick Junctions in DNA. Biophysical Journal, 2006, 90, 1000-1008.	0.2	17
225	Data Mining of Molecular Dynamics Trajectories of Nucleic Acids. Journal of Biomolecular Structure and Dynamics, 2006, 23, 447-455.	2.0	12
226	G-Quadruplexes Can Maintain Their Structure in the Gas Phase. Journal of the American Chemical Society, 2006, 128, 3608-3619.	6.6	85
227	Benzoderivatives of Nucleic Acid Bases as Modified DNA Building Blocksâ€. Journal of Physical Chemistry A, 2006, 110, 510-518.	1.1	21
228	On the Origin of the Stereoselectivity in the Alkylation of Oxazolopiperidone Enolates. Journal of the American Chemical Society, 2006, 128, 6581-6588.	6.6	17
229	Aromaticity-induced changes in electronic properties of size-expanded DNA bases: Case of xC. International Journal of Quantum Chemistry, 2006, 106, 2339-2346.	1.0	17
230	Ligand-induced dynamical regulation of NO conversion in Mycobacterium tuberculosis truncated hemoglobin-N. Proteins: Structure, Function and Bioinformatics, 2006, 64, 457-464.	1.5	95
231	A fast method for the determination of fractional contributions to solvation in proteins. Protein Science, 2006, 15, 2525-2533.	3.1	3
232	Exploring the reasons for the large density of triplex-forming oligonucleotide target sequences in the human regulatory regions. BMC Genomics, 2006, 7, 63.	1.2	46
233	Nature of Base Stacking: Reference Quantum-Chemical Stacking Energies in Ten Unique B-DNA Base-Pair Steps. Chemistry - A European Journal, 2006, 12, 2854-2865.	1.7	211
234	Destabilization of Quadruplex DNA by 8-Aminoguanine. ChemBioChem, 2006, 7, 46-48.	1.3	20

#	Article	IF	Citations
235	Dispersion and repulsion contributions to the solvation free energy: Comparison of quantum mechanical and classical approaches in the polarizable continuum model. Journal of Computational Chemistry, 2006, 27, 1769-1780.	1.5	49
236	Extension of the MST model to the IEF formalism: HF and B3LYP parametrizations. Computational and Theoretical Chemistry, 2005, 727, 29-40.	1.5	79
237	Are the Hydrogen Bonds of RNA (Aâ‹…U) Stronger Than those of DNA (Aâ‹…T)? A Quantum Mechanics Study. Chemistry - A European Journal, 2005, 11, 5062-5066.	1.7	42
238	Hydrophobic Molecular Similarity from MST Fractional Contributions to the Octanol/water Partition Coefficient. Journal of Computer-Aided Molecular Design, 2005, 19, 401-419.	1.3	9
239	Use of bioinformatics tools for the annotation of disease-associated mutations in animal models. Proteins: Structure, Function and Bioinformatics, 2005, 61, 878-887.	1.5	19
240	PMUT: a web-based tool for the annotation of pathological mutations on proteins. Bioinformatics, 2005, 21, 3176-3178.	1.8	441
241	PupasView: a visual tool for selecting suitable SNPs, with putative pathological effect in genes, for genotyping purposes. Nucleic Acids Research, 2005, 33, W501-W505.	6.5	253
242	Structure, Recognition Properties, and Flexibility of the DNAÂ·RNA Hybrid. Journal of the American Chemical Society, 2005, 127, 4910-4920.	6.6	64
243	Nature of Minor-Groove Bindersâ”DNA Complexes in the Gas Phase. Journal of the American Chemical Society, 2005, 127, 11690-11698.	6.6	35
244	Theoretical Study of the Truncated Hemoglobin HbN:Â Exploring the Molecular Basis of the NO Detoxification Mechanism. Journal of the American Chemical Society, 2005, 127, 4433-4444.	6.6	111
245	Exploring the Essential Dynamics of B-DNA. Journal of Chemical Theory and Computation, 2005, 1, 790-800.	2.3	61
246	Design, Synthesis, and Biological Evaluation of Dual Binding Site Acetylcholinesterase Inhibitors:â€‰ New Disease-Modifying Agents for Alzheimer's Disease. Journal of Medicinal Chemistry, 2005, 48, 7223-7233.	2.9	203
247	MST Continuum Study of the Hydration Free Energies of Monovalent Ionic Species. Journal of Physical Chemistry B, 2005, 109, 3565-3574.	1.2	44
248	Group contributions to the solvation free energy from MST continuum calculations. Brazilian Journal of Physics, 2004, 34, 48-57.	0.7	7
249	The relative flexibility of B-DNA and A-RNA duplexes: database analysis. Nucleic Acids Research, 2004, 32, 6144-6151.	6.5	119
250	Triplex-forming oligonucleotide target sequences in the human genome. Nucleic Acids Research, 2004, 32, 354-360.	6.5	149
251	Effect of Bulky Lesions on DNA. Journal of Biological Chemistry, 2004, 279, 24552-24560.	1.6	18
252	Functional and structural conservation of CBS domains from CLC chloride channels. Journal of Physiology, 2004, 557, 363-378.	1.3	131

#	Article	IF	Citations
253	Linear response theory: An alternative to PB and GB methods for the analysis of molecular dynamics trajectories?. Proteins: Structure, Function and Bioinformatics, 2004, 57, 458-467.	1.5	8
254	Unconventional interactions between water and heterocyclic nitrogens in protein structures. Proteins: Structure, Function and Bioinformatics, 2004, 57, 1-8.	1.5	38
255	Partition of protein solvation into group contributions from molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2004, 58, 101-109.	1.5	8
256	MST study of group contributions for alkane derivatives: effect of the charge normalization. Chemical Physics Letters, 2004, 384, 299-305.	1.2	6
257	Exploring the Binding Mode of Semicarbazide-Sensitive Amine Oxidase/VAP-1:Â Identification of Novel Substrates with Insulin-like Activity. Journal of Medicinal Chemistry, 2004, 47, 4865-4874.	2.9	27
258	Exploring the Counterion Atmosphere around DNA: What Can Be Learned from Molecular Dynamics Simulations?. Biophysical Journal, 2004, 87, 800-811.	0.2	96
259	Alternative Splicing Mechanisms for the Modulation of Protein Function: Conservation Between Human and Other Species. Journal of Molecular Biology, 2004, 335, 495-502.	2.0	21
260	Relative Flexibility of DNA and RNA: a Molecular Dynamics Study. Journal of Molecular Biology, 2004, 343, 627-638.	2.0	94
261	Theoretical Study of the Guanine â†' 6-Thioguanine Substitution in Duplexes, Triplexes, and Tetraplexes. Journal of the American Chemical Society, 2004, 126, 14642-14650.	6.6	52
262	Unique Tautomeric Properties of Isoguanine. Journal of the American Chemical Society, 2004, 126, 154-164.	6.6	53
263	Solute-Solvent Interactions from QM SCRF Methods. , 2004, , 475-495.		2
264	Molecular Modelling Approaches to the Design of Acetylcholinesterase Inhibitors: New Challenges for the Treatment of Alzheimers Disease. Current Pharmaceutical Design, 2004, 10, 3131-3140.	0.9	29
265	Electrostatic component of solvation: Comparison of SCRF continuum models. Journal of Computational Chemistry, 2003, 24, 284-297.	1.5	86
266	Transferability of fragmental contributions to the octanol/water partition coefficient: An NDDO-based MST study. Journal of Computational Chemistry, 2003, 24, 32-45.	1.5	11
267	Energy decomposition in molecular complexes: Implications for the treatment of polarization in molecular simulations. Journal of Computational Chemistry, 2003, 24, 1263-1275.	1.5	14
268	Continuum and discrete calculation of fractional contributions to solvation free energy. Journal of Computational Chemistry, 2003, 24, 1610-1623.	1.5	8
269	Molecular Dynamics Study of [2]Rotaxanes: Influence of Solvation and Cation on Co-conformation.. ChemInform, 2003, 34, no.	0.1	0
270	Theoretical Studies on the Inhibition Mechanism of Cyclooxygenase-2. Is There a Unique Recognition Site?. Journal of Medicinal Chemistry, 2003, 46, 1372-1382.	2.9	49

#	Article	IF	Citations
271	Continuum solvation models: Dissecting the free energy of solvation. Physical Chemistry Chemical Physics, 2003, 5, 3827-3836.	1.3	89
272	Perturbation Approach to Combined QM/MM Simulation of Soluteâ˜'Solvent Interactions in Solution. Journal of Physical Chemistry B, 2003, 107, 1664-1671.	1.2	30
273	Four-Stranded DNA Structure Stabilized by a Novel G:C:A:T Tetrad. Journal of the American Chemical Society, 2003, 125, 5654-5662.	6.6	29
274	Molecular Dynamics Study of [2]Rotaxanes:Â Influence of Solvation and Cation on Co-conformation. Journal of Organic Chemistry, 2003, 68, 4663-4673.	1.7	24
275	Theoretical Study of a New DNA Structure:â€‰ The Antiparallel Hoogsteen Duplex. Journal of the American Chemical Society, 2003, 125, 14603-14612.	6.6	41
276	The Structure and Dynamics of DNA in the Gas Phase. Journal of the American Chemical Society, 2003, 125, 8007-8014.	6.6	121
277	Theoretical methods for the simulation of nucleic acids. Chemical Society Reviews, 2003, 32, 350-364.	18.7	150
278	Antiparallel Triple Helices. Structural Characteristics and Stabilization by 8-Amino Derivatives. Journal of the American Chemical Society, 2003, 125, 16127-16138.	6.6	38
279	Properties of triple helices formed by parallel-stranded hairpins containing 8-aminopurines. Nucleic Acids Research, 2002, 30, 2609-2619.	6.5	39
280	Can Divalent Metal Cations Stabilize the Triplex Motif? Theoretical Study of the Interaction of the Hydrated Mg2+ Cation with the Gâ˜'GÂ·C Triplet. Journal of Physical Chemistry B, 2002, 106, 8849-8857.	1.2	20
281	Rational Design of Reversible Acetylcholinesterase Inhibitors. Mini-Reviews in Medicinal Chemistry, 2002, 2, 27-36.	1.1	22
282	Ligand-induced changes in the binding sites of proteins. Bioinformatics, 2002, 18, 939-948.	1.8	46
283	Hoogsteen-Based Parallel-Stranded Duplexes of DNA. Effect of 8-Amino-purine Derivatives. Journal of the American Chemical Society, 2002, 124, 3133-3142.	6.6	38
284	Characterization of disease-associated single amino acid polymorphisms in terms of sequence and structure properties 1 1Edited by J. Thornton. Journal of Molecular Biology, 2002, 315, 771-786.	2.0	194
285	Theoretical Study of Anion Binding to Calix[4]pyrrole:Â the Effects of Solvent, Fluorine Substitution, Cosolute, and Water Traces. Journal of the American Chemical Society, 2002, 124, 12796-12805.	6.6	71
286	Correlated ab initio study of nucleic acid bases and their tautomers in the gas phase, in a microhydrated environment and in aqueous solution : Part 1. Cytosine. Physical Chemistry Chemical Physics, 2002, 4, 4192-4203.	1.3	187
287	Theoretical Study of Alkyl-Ï€ and Aryl-Ï€ Interactions. Reconciling Theory and Experiment. Journal of Organic Chemistry, 2002, 67, 7057-7065.	1.7	119
288	Hydrophobic similarity between molecules: A MST-based hydrophobic similarity index. Journal of Computational Chemistry, 2002, 23, 554-563.	1.5	18

#	Article	IF	Citations
289	Fast estimation of hydrogen-bonding donor and acceptor propensities: a GMIPp study. Journal of Computer-Aided Molecular Design, 2002, 16, 569-583.	1.3	3
290	Nucleic Acid Triple Helices: Stability Effects of Nucleobase Modifications. Current Organic Chemistry, 2002, 6, 1333-1368.	0.9	59
291	Synthesis, in Vitro Pharmacology, and Molecular Modeling ofsyn-Huprines as Acetylcholinesterase Inhibitors. Journal of Medicinal Chemistry, 2001, 44, 4733-4736.	2.9	45
292	Cooperativity in Drugâ˜DNA Recognition:â€‰ A Molecular Dynamics Study. Journal of the American Chemical Society, 2001, 123, 12658-12663.	6.6	150
293	Theoretical Study of the Mechanisms of Substrate Recognition by Catalase. Journal of the American Chemical Society, 2001, 123, 9665-9672.	6.6	50
294	Aminoâ˜Imino Tautomerism in Derivatives of Cytosine:Â Effect on Hydrogen-Bonding and Stacking Properties. Journal of Physical Chemistry A, 2001, 105, 6575-6580.	1.1	34
295	Interactions of Hydrated Mg2+ Cation with Bases, Base Pairs, and Nucleotides. Electron Topology, Natural Bond Orbital, Electrostatic, and Vibrational Study. Journal of Physical Chemistry B, 2001, 105, 6051-6060.	1.2	95
296	Theoretical Studies of d(A:T)-Based Parallel-Stranded DNA Duplexes. Journal of the American Chemical Society, 2001, 123, 12018-12025.	6.6	33
297	Parallel-stranded hairpins containing 8-aminopurines. novel efficient probes for triple-helix formation. Bioorganic and Medicinal Chemistry Letters, 2001, 11, 1761-1763.	1.0	15
298	Classical molecular interaction potentials: Improved setup procedure in molecular dynamics simulations of proteins. Proteins: Structure, Function and Bioinformatics, 2001, 45, 428-437.	1.5	87
299	Solvation in octanol: parametrization of the continuum MST model. Journal of Computational Chemistry, 2001, 22, 1180-1193.	1.5	120
300	General Access to Tacamine and Vinca-Eburna Alkaloids through Tandem Non-Biomimetic Oxidation of Dihydropyridines/Zn-Mediated Radical Addition Processes â˜ Unexpected Facial Selectivity of Flattened Cyclohexyl-Type Radicals. European Journal of Organic Chemistry, 2001, 2001, 3719.	1.2	31
301	Mixed QM/MM molecular electrostatic potentials. Journal of Computer-Aided Molecular Design, 2000, 14, 329-339.	1.3	9
302	Synthesis of Enantiopuretrans-3,4-Disubstituted Piperidines. An Enantiodivergent Synthesis of (+)- and (â˜)-Paroxetine. Journal of Organic Chemistry, 2000, 65, 3074-3084.	1.7	135
303	Perspective on "Electrostatic interactions of a solute with a continuum. A direct utilization of ab initio molecular potentials for the prevision of solvent effects". Theoretical Chemistry Accounts, 2000, 103, 343-345.	0.5	712
304	Glutaryl-CoA Dehydrogenase Deficiency in Spain: Evidence of Two Groups of Patients, Genetically, and Biochemically Distinct. Pediatric Research, 2000, 48, 315-322.	1.1	127
305	New Tacrineâ˜Huperzine A Hybrids (Huprines):â€‰ Highly Potent Tight-Binding Acetylcholinesterase Inhibitors of Interest for the Treatment of Alzheimer's Disease. Journal of Medicinal Chemistry, 2000, 43, 4657-4666.	2.9	185
306	Theoretical Methods for the Description of the Solvent Effect in Biomolecular Systems. Chemical Reviews, 2000, 100, 4187-4226.	23.0	571

#	Article	IF	Citations
307	Simplified descriptions of the topological distribution of hydrophilic/hydrophobic characteristics of molecules. Physical Chemistry Chemical Physics, 2000, 2, 4897-4905.	1.3	13
308	Molecular Dynamics Simulations of PNAÂ·DNA and PNAÂ·RNA Duplexes in Aqueous Solution. Journal of the American Chemical Society, 2000, 122, 5997-6008.	6.6	67
309	Molecular Dynamics Study of Oligonucleotides Containing Difluorotoluene. Journal of the American Chemical Society, 2000, 122, 6891-6899.	6.6	29
310	Câ^'HÂ·Â·Â·O Contacts in the AdenineÂ·Â·Â·Uracil Watsonâ^'Crick and UracilÂ·Â·Â·Uracil Nucleic Acid Base Pairs:â€‰ Nonempirical ab Initio Study with Inclusion of Electron Correlation Effects. Journal of Physical Chemistry B, 2000, 104, 6286-6292.	1.2	125
311	On the Use of SCRF Methods in Drug Design Studies. , 2000, , 129-134.		1
312	Nucleic Acid Bases in Solution. Theoretical and Computational Chemistry, 1999, 8, 119-166.	0.2	7
313	Modified Oligonucleotides with Triple-Helix Stabilization Properties. Nucleosides & Nucleotides, 1999, 18, 1619-1621.	0.5	3
314	Cavitation contribution to the free energy of solvation.. Chemical Physics, 1999, 240, 253-264.	0.9	38
315	Fractional description of free energies of solvation. Journal of Computer-Aided Molecular Design, 1999, 13, 139-152.	1.3	33
316	Monte Carlo-MST: New strategy for representation of solvent configurational space in solution. Journal of Computational Chemistry, 1999, 20, 665-678.	1.5	15
317	Parametrization of the GMIPp for the study of stacking interactions. Journal of Computational Chemistry, 1999, 20, 937-946.	1.5	11
318	Role of Sugar Re-Puckering in the Transition of A and B Forms of DNA in Solution. A Molecular Dynamics Study. Journal of Biomolecular Structure and Dynamics, 1999, 17, 89-99.	2.0	28
319	Predicting Relative Binding Free Energies of Tacrineâ^'Huperzine A Hybrids as Inhibitors of AcetylcholinesteraseÂ§. Journal of Medicinal Chemistry, 1999, 42, 5110-5119.	2.9	36
320	Theoretical Evaluation of Solvent Effects on the Conformational and Tautomeric Equilibria of 2-(2â€˜-Hydroxyphenyl)benzimidazole and on Its Absorption and Fluorescence Spectra. Journal of Physical Chemistry A, 1999, 103, 4525-4532.	1.1	79
321	Observation of Spontaneous Base Pair Breathing Events in the Molecular Dynamics Simulation of a Difluorotoluene-Containing DNA Oligonucleotide. Journal of the American Chemical Society, 1999, 121, 8653-8654.	6.6	59
322	Dimerization of Formamide in Gas Phase and Solution. An Ab Initio MCâ^'MST Study. Journal of Physical Chemistry A, 1999, 103, 6200-6208.	1.1	30
323	Synthesis, in Vitro Pharmacology, and Molecular Modeling of Very Potent Tacrineâ^'Huperzine A Hybrids as Acetylcholinesterase Inhibitors of Potential Interest for the Treatment of Alzheimer's Disease. Journal of Medicinal Chemistry, 1999, 42, 3227-3242.	2.9	101
324	Molecular Dynamics Studies of DNA A-Tract Structure and Flexibility. Journal of the American Chemical Society, 1999, 121, 5981-5991.	6.6	101

#	Article	IF	Citations
325	Interactions of Nucleic Acid Bases: The Role of Solvent. Computational Chemistry - Reviews of Current Trends, 1999, , 191-225.	0.4	2
326	Polarization effects in generalized molecular interaction potential: New Hamiltonian for reactivity studies and mixed QM/MM calculations. Journal of Computational Chemistry, 1998, 19, 866-881.	1.5	83
327	Triple helix stabilization properties of oligonucleotides containing 8-amino-2â€²-deoxyguanosine. Bioorganic and Medicinal Chemistry Letters, 1998, 8, 3011-3016.	1.0	11
328	Tautomerism of 1-Methyl Derivatives of Uracil, Thymine, and 5-Bromouracil. Is Tautomerism the Basis for the Mutagenicity of 5-Bromouridine?. Journal of Physical Chemistry B, 1998, 102, 5228-5233.	1.2	73
329	Azidoazomethineâ^'Tetrazole Isomerism in Solution:Â A Thermochemical Study. Journal of Organic Chemistry, 1998, 63, 2354-2356.	1.7	25
330	Molecular Dynamics Simulations in Aqueous Solution of Triple Helices Containing d(GÂ·CÂ·C) Trios. Journal of the American Chemical Society, 1998, 120, 11226-11233.	6.6	59
331	A Priori Prediction of Substituent and Solvent Effects in the Basicity of Nitriles. Journal of Organic Chemistry, 1998, 63, 4947-4953.	1.7	27
332	Dimerization of Carboxylic Acids:â€‰ Reliability of Theoretical Calculations and the Effect of Solvent. Journal of Physical Chemistry B, 1998, 102, 2269-2276.	1.2	80
333	On the potential role of the amino nitrogen atom as a hydrogen bond acceptor in macromolecules. Journal of Molecular Biology, 1998, 279, 1123-1136.	2.0	110
334	Theoretical Study of Azidoâ^'Tetrazole Isomerism:Â Effect of Solvent and Substituents and Mechanism of Isomerization. Journal of the American Chemical Society, 1998, 120, 4723-4731.	6.6	73
335	Molecular Dynamics Simulation of a PNAÂ·DNAÂ·PNA Triple Helix in Aqueous Solution. Journal of the American Chemical Society, 1998, 120, 5895-5904.	6.6	99
336	Role of Intramolecular Hydrogen Bonds in the Intermolecular Hydrogen Bonding of Carbohydrates. Journal of Physical Chemistry A, 1998, 102, 6690-6696.	1.1	54
337	The GAGA Factor of Drosophila Binds Triple-stranded DNA. Journal of Biological Chemistry, 1998, 273, 24640-24648.	1.6	41
338	Molecular Dynamics Simulations of the Unfolding of Barnase in Water and 8 M Aqueous Urea. Biochemistry, 1997, 36, 7313-7329.	1.2	173
339	Molecular Dynamics Simulations of the d(TÂ·AÂ·T) Triple Helix. Journal of the American Chemical Society, 1997, 119, 7463-7469.	6.6	160
340	Ab InitioStudy of Stacking Interactions in A- and B-DNA. Journal of Physical Chemistry B, 1997, 101, 3846-3853.	1.2	82
341	Role of tautomerism of 2-azaadenine and 2-azahypoxanthine in substrate recognition by xanthine oxidase. Journal of Computer-Aided Molecular Design, 1997, 11, 153-162.	1.3	43
342	Reliability of MEP and MEP-derived properties computed from DFT methods for molecules containing P, S and CL. Theoretical Chemistry Accounts, 1997, 98, 42-49.	0.5	25

#	Article	IF	Citations
343	Suitability of density functional methods for calculation of electrostatic properties. Journal of Computational Chemistry, 1997, 18, 980-991.	1.5	37
344	Helical preferences of alanine, glycine, and aminoisobutyric homopeptides. , 1997, 28, 83-93.		39
345	On the reaction mechanism of class Pi glutathione S-transferase. , 1997, 28, 530-542.		11
346	Tautomerism of Xanthine Oxidase Substrates Hypoxanthine and Allopurinol. Journal of Organic Chemistry, 1996, 61, 5964-5971.	1.7	71
347	Tautomerism and Protonation of Guanine and Cytosine. Implications in the Formation of Hydrogen-Bonded Complexes. Journal of the American Chemical Society, 1996, 118, 6811-6821.	6.6	318
348	Theoretical Methods for the Representation of Solvent. Journal of Molecular Modeling, 1996, 2, 1-15.	0.8	61
349	Extension of MST/SCRF method to organic solvents:Ab initio and semiempirical parametrization for neutral solutes in CCl4. Journal of Computational Chemistry, 1996, 17, 806-820.	1.5	111
350	Theoretical representation of solvation in biochemical systems: From discrete solute-solvent interactions to bulk solvation. International Journal of Quantum Chemistry, 1996, 60, 1179-1187.	1.0	3
351	Synthesis, chemical trapping and dimerization of tricyclo[3.3.0.03,7]oct-1(5)-ene, the consummate member of a series of pyramidalized alkenes. Tetrahedron Letters, 1996, 37, 8605-8608.	0.7	29
352	Theoretical determination of the solvation free energy in water and chloroform of the nucleic acid bases. Chemical Physics, 1996, 209, 19-29.	0.9	27
353	Tautomerism of xanthine and alloxanthine: A model for substrate recognition by xanthine oxidase. Journal of Computer-Aided Molecular Design, 1996, 10, 535-544.	1.3	29
354	Effect of Solvation on the Charge Distribution of a Series of Anionic, Neutral, and Cationic Species. A Quantum Molecular Similarity Study. The Journal of Physical Chemistry, 1996, 100, 606-610.	2.9	27
355	Generalization of the Molecular Electrostatic Potential for the Study of Noncovalent interactions. Theoretical and Computational Chemistry, 1996, 3, 181-218.	0.2	47
356	Molecular Dynamics Study of the Binding of Elsamicin A to DNA. FEBS Journal, 1995, 230, 555-566.	0.2	9
357	The effect of hydration on the molecular charge distribution of cations. An ab initio SCRF study. Chemical Physics Letters, 1995, 232, 509-517.	1.2	19
358	Development of optimized MST/SCRF methods for semiempirical calculations: The MNDO and PM3 Hamiltonians. Journal of Computational Chemistry, 1995, 16, 563-575.	1.5	94
359	Synthetic studies on indole alkaloids VIII. 1 Synthesis and reactivity of asymmetric 2-indolyi-4-methylenepiperidines. Tetrahedron, 1995, 51, 7527-7546.	1.0	5
360	The polarization contribution to the free energy of hydration. Journal of Chemical Physics, 1995, 102, 6145-6152.	1.2	41

#	Article	IF	Citations
361	New strategies to incorporate the solvent polarization in selfâ€consistent reaction field and freeâ€energy perturbation simulations. Journal of Chemical Physics, 1995, 103, 10183-10191.	1.2	49
362	Molecular Solvation Potential. A New Tool for the Quantum Mechanical Description of Hydration in Organic and Bioorganic Molecules. The Journal of Physical Chemistry, 1995, 99, 3084-3092.	2.9	39
363	Theoretical Study of the Tautomerism and Protonation of 7-Aminopyrazolopyrimidine in the Gas Phase and in Aqueous Solution. Journal of the American Chemical Society, 1995, 117, 1378-1386.	6.6	43
364	Tautomerism of Neutral and Protonated 6-Thioguanine in the Gas Phase and in Aqueous Solution. An ab Initio Study. Journal of Organic Chemistry, 1995, 60, 969-976.	1.7	41
365	Effect of Solvent Polarization on Bimolecular Interactions. The Journal of Physical Chemistry, 1995, 99, 11344-11349.	2.9	8
366	Effect of solvation on the shapes, sizes, and anisotropies of polyatomic anions via molecular electrostatic potential topography: Anab initioselfâ€consistent reaction field approach. Journal of Chemical Physics, 1994, 100, 6718-6726.	1.2	33
367	Comparison of NDDO and quasi-ab initio approaches to compute semiempirical molecular electrostatic potentials. Journal of Computational Chemistry, 1994, 15, 12-22.	1.5	43
368	Optimization of solute cavities and van der Waals parameters inab initio MST-SCRF calculations of neutral molecules. Journal of Computational Chemistry, 1994, 15, 446-454.	1.5	135
369	An optimized AM1/MST method for the MST-SCRF representation of solvated systems. Journal of Computational Chemistry, 1994, 15, 847-857.	1.5	73
370	PAPQMD/AM1 Parametrization of the bonded term of aromatic biomolecules. Biopolymers, 1994, 34, 941-955.	1.2	9
371	Optimization of the cavity size for ab initio MST-SCRF calculations of monovalent ions. Chemical Physics, 1994, 182, 237-248.	0.9	65
372	Multicentric charges for the accurate representation of electrostatic interactions in force-field calculations for small molecules. Chemical Physics, 1994, 189, 573-584.	0.9	15
373	DNA Sequence-Specific Reading by Echinomycin: Role of Hydrogen Bonding and Stacking Interactions. Journal of Medicinal Chemistry, 1994, 37, 1602-1609.	2.9	33
374	Self-consistent reaction field computation of the reactive characteristics of DNA bases in water. Biopolymers, 1993, 33, 1851-1869.	1.2	35
375	Molecular interaction potential: A new tool for the theoretical study of molecular reactivity. Journal of Computational Chemistry, 1993, 14, 587-602.	1.5	50
376	Ab initio study of bond stretching: Implications in force-field parametrization for molecular mechanics and dynamics. Journal of Computational Chemistry, 1993, 14, 881-894.	1.5	13
377	Accuracy of free energies of hydration for organic molecules from 6-31g*-derived partial charges. Journal of Computational Chemistry, 1993, 14, 1240-1249.	1.5	154
378	Comparison of 6-31G*-based MST/SCRF and FEP evaluations of the free energies of hydration for small neutral molecules. Journal of Computational Chemistry, 1993, 14, 1498-1503.	1.5	61

#	Article	IF	Citations
379	A new scaling procedure to correct semiempirical MEP and MEP-derived properties. Journal of Computer-Aided Molecular Design, 1993, 7, 721-742.	1.3	25
380	Reactivity of planar and twisted amides in vacuum and aqueous environments: an ab initio MEP study. Journal of the Chemical Society Perkin Transactions II, 1993, , 683.	0.9	24
381	Mechanism for the rotamase activity of FK506 binding protein from molecular dynamics simulations. Biochemistry, 1993, 32, 12864-12874.	1.2	44
382	Theoretical study of N-methylacetamide in vacuum and aqueous solution: implications for the peptide bond isomerization. Journal of Organic Chemistry, 1993, 58, 6397-6405.	1.7	56
383	An AM1-SCRF approach to the study of changes in molecular properties induced by solvent. The Journal of Physical Chemistry, 1993, 97, 4386-4391.	2.9	88
384	Induced dipole moment and atomic charges based on average electrostatic potentials in aqueous solution. Journal of Chemical Physics, 1993, 98, 2975-2982.	1.2	118
385	Experimental and modelling studies on the DNA cleavage by elsamicin A. FEBS Journal, 1992, 208, 227-233.	0.2	13
386	Conformational Analysis of 2-Aryl-4-piperidones. Effect of the Indole Protective Phenylsulfonyl Group. Heterocycles, 1992, 34, 449.	0.4	3
387	A new strategy for the evaluation of force parameters from quantum mechanical computations. Journal of Computational Chemistry, 1991, 12, 664-674.	1.5	39
388	A quantum chemical study of the enzymatic deamination of benzoadenine derivatives. A theoretical model of the interactions occurring between nucleosides and the active site of adenosine deaminase. FEBS Journal, 1990, 188, 155-163.	0.2	19
389	Theoretical study of the hydroxyl nucleophilic attack on the 6-aminopyrimidine molecule: functional implications in the reaction mechanism of nucleoside deaminative enzymes. Journal of Organic Chemistry, 1990, 55, 2630-2637.	1.7	15
390	Ab initio study of the protonation and the tautomerism of the 7-aminopyrazolopyrimidine molecule. Journal of Organic Chemistry, 1990, 55, 753-756.	1.7	9
391	Theoretical Approximation to the Reaction Mechanism of Adenosine Deaminase. QSAR and Combinatorial Science, 1989, 8, 109-114.	1.4	9
392	Beyond the Continuum Approach. , 0, , 499-605.		6