Modesto Orozco Lpez

List of Publications by Year in Descending Order

395 papers	23,822 citations	78 h-index	138 g-index
412 ext. papers	26,470 ext. citations	9 avg, IF	6.78 L-index

#	Paper	IF	Citations
395	Molecular basis of Arginine and Lysine DNA sequence-dependent thermo-stability modulation.. *PLoS Computational Biology*, **2022**, 18, e1009749	5	0
394	The Impact of the HydroxyMethylCytosine epigenetic signature on DNA structure and function. *PLoS Computational Biology*, **2021**, 17, e1009547	5	1
393	Sequence-dependent structural properties of B-DNA: what have we learned in 40´years?. *Biophysical Reviews*, **2021**, 13, 995-1005	3.7	1
392	Mutation in KARS: A´novel mechanism for severe anaphylaxis. *Journal of Allergy and Clinical Immunology*, **2021**, 147, 1855-1864.e9	11.5	8
391	Impact of DNA methylation on 3D genome structure. *Nature Communications*, **2021**, 12, 3243	17.4	8
390	3dRS, a Web-Based Tool to Share Interactive Representations of 3D Biomolecular Structures and Molecular Dynamics Trajectories. *Frontiers in Molecular Biosciences*, **2021**, 8, 726232	5.6	1
389	Probing allosteric regulations with coevolution-driven molecular simulations. *Science Advances*, **2021**, 7, eabj0786	14.3	0
388	Protein disorder-to-order transition enhances the nucleosome-binding affinity of H1. *Nucleic Acids Research*, **2020**, 48, 5318-5331	20.1	11
387	Colibactin DNA-damage signature indicates mutational impact in colorectal cancer. *Nature Medicine* , **2020**, 26, 1063-1069	50.5	76
386	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	11.5	21
385	4D Genome Rewiring during Oncogene-Induced and Replicative Senescence. *Molecular Cell*, **2020**, 78, 522-538.e9	17.6	48
384	A multi-modal coarse grained model of DNA flexibility mappable to the atomistic level. *Nucleic Acids Research*, **2020**, 48, e29	20.1	10
383	Determination of a Structural Ensemble Representing the Dynamics of a G-Quadruplex DNA. *Biochemistry*, **2020**, 59, 379-388	3.2	2
382	Surviving the deluge of biosimulation data. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2020**, 10, e1449	7.9	5
381	Bioactive Conformational Ensemble Server and Database. A Public Framework to Speed Up Drug Discovery. *Journal of Chemical Theory and Computation*, **2020**, 16, 6586-6597	6.4	6
380	Exploring the Conformational Landscape of Bioactive Small Molecules. *Journal of Chemical Theory and Computation*, **2020**, 16, 6575-6585	6.4	10
379	DFFR: A New Method for High-Throughput Recalibration of Automatic Force-Fields for Drugs. *Journal of Chemical Theory and Computation*, **2020**, 16, 6598-6608	6.4	2

378	BioExcel Building Blocks, a software library for interoperable biomolecular simulation workflows. *Scientific Data*, **2019**, 6, 169	8.2	19
377	Nucleosome Dynamics: a new tool for the dynamic analysis of nucleosome positioning. *Nucleic Acids Research*, **2019**, 47, 9511-9523	20.1	3
376	Predicting the Limit of Intramolecular Hydrogen Bonding with Classical Molecular Dynamics. *Angewandte Chemie - International Edition*, **2019**, 58, 3759-3763	16.4	10
375	Predicting the Limit of Intramolecular Hydrogen Bonding with Classical Molecular Dynamics. *Angewandte Chemie*, **2019**, 131, 3799-3803	3.6	4
374	A multifunctional toolkit for target-directed cancer therapy. *Chemical Communications*, **2019**, 55, 802-805	5.8	1
373	An artificial DNAzyme RNA ligase shows a reaction mechanism resembling that of cellular polymerases. *Nature Catalysis*, **2019**, 2, 544-552	36.5	9
372	DNA specificities modulate the binding of human transcription factor A to mitochondrial DNA control region. *Nucleic Acids Research*, **2019**, 47, 6519-6537	20.1	6
371	The Origins and the Biological Consequences of the Pur/Pyr DNA–RNA Asymmetry. *CheM*, **2019**, 5, 1619-1631	16.2	6
370	Modulation of the helical properties of DNA: next-to-nearest neighbour effects and beyond. *Nucleic Acids Research*, **2019**, 47, 4418-4430	20.1	12
369	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	11.5	23
368	Epigenetic loss of RNA-methyltransferase NSUN5 in glioma targets ribosomes to drive a stress adaptive translational program. *Acta Neuropathologica*, **2019**, 138, 1053-1074	14.3	55
367	How B-DNA Dynamics Decipher Sequence-Selective Protein Recognition. *Journal of Molecular Biology*, **2019**, 431, 3845-3859	6.5	15
366	VeriNA3d: an R package for nucleic acids data mining. *Bioinformatics*, **2019**, 35, 5334-5336	7.2	2
365	The static and dynamic structural heterogeneities of B-DNA: extending Calladine-Dickerson rules. *Nucleic Acids Research*, **2019**, 47, 11090-11102	20.1	18
364	An In-Depth Look at DNA Crystals through the Prism of Molecular Dynamics Simulations. *CheM*, **2019**, 5, 649-663	16.2	9
363	Modeling, Simulations, and Bioinformatics at the Service of RNA Structure. *CheM*, **2019**, 5, 51-73	16.2	20
362	Inhibition of Human Enhancer of Zeste Homolog 2 with Tambjamine Analogs. *Journal of Chemical Information and Modeling*, **2018**, 57, 2089-2098	6.1	4
361	Protein Flexibility and Synergy of HMG Domains Underlie U-Turn Bending of DNA by TFAM in Solution. *Biophysical Journal*, **2018**, 114, 2386-2396	2.9	11

360	Plasticity in oligomerization, operator architecture, and DNA binding in the mode of action of a bacterial B-based photoreceptor. *Journal of Biological Chemistry*, **2018**, 293, 17888-17905	5.4	11
359	Allosterism and signal transfer in DNA. *Nucleic Acids Research*, **2018**, 46, 7554-7565	20.1	15
358	Targeting RNA structure in SMN2 reverses spinal muscular atrophy molecular phenotypes. *Nature Communications*, **2018**, 9, 2032	17.4	34
357	The Multiple Roles of Waters in Protein Solvation. *Journal of Physical Chemistry B*, **2017**, 121, 3636-3643	3.4	13
356	How accurate are accurate force-fields for B-DNA?. *Nucleic Acids Research*, **2017**, 45, 4217-4230	20.1	79
355	Proton Dynamics in Protein Mass Spectrometry. *Journal of Physical Chemistry Letters*, **2017**, 8, 1105-1112	6.4	26
354	Discrete Molecular Dynamics Approach to the Study of Disordered and Aggregating Proteins. *Journal of Chemical Theory and Computation*, **2017**, 13, 1454-1461	6.4	14
353	Efficient siRNA-peptide conjugation for specific targeted delivery into tumor cells. *Chemical Communications*, **2017**, 53, 2870-2873	5.8	15
352	Compaction of Duplex Nucleic Acids upon Native Electrospray Mass Spectrometry. *ACS Central Science*, **2017**, 3, 454-461	16.8	65
351	Mechanism of Structural Tuning of the Hepatitis C Virus Human Cellular Receptor CD81 Large Extracellular Loop. *Structure*, **2017**, 25, 53-65	5.2	13
350	PMut: a web-based tool for the annotation of pathological variants on proteins, 2017 update. *Nucleic Acids Research*, **2017**, 45, W222-W228	20.1	100
349	The Role of Unconventional Hydrogen Bonds in Determining BII Propensities in B-DNA. *Journal of Physical Chemistry Letters*, **2017**, 8, 21-28	6.4	15
348	DNA structure directs positioning of the mitochondrial genome packaging protein Abf2p. *Nucleic Acids Research*, **2017**, 45, 951-967	20.1	17
347	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	16.4	40
346	Repair of UV-Induced DNA Damage Independent of Nucleotide Excision Repair Is Masked by MUTYH. *Molecular Cell*, **2017**, 68, 797-807.e7	17.6	22
345	Quantification of Pathway Cross-talk Reveals Novel Synergistic Drug Combinations for Breast Cancer. *Cancer Research*, **2017**, 77, 459-469	10.1	47
344	Changes in the free-energy landscape of p38 MAP kinase through its canonical activation and binding events as studied by enhanced molecular dynamics simulations. *ELife*, **2017**, 6,	8.9	36
343	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	11.5	17

342	Mutations in JMJD1C are involved in Rett syndrome and intellectual disability. *Genetics in Medicine*, **2016**, 18, 378-85	8.1	28
341	Small Details Matter: The 2'-Hydroxyl as a Conformational Switch in RNA. *Journal of the American Chemical Society*, **2016**, 138, 16355-16363	16.4	16
340	Prediction and validation of protein intermediate states from structurally rich ensembles and coarse-grained simulations. *Nature Communications*, **2016**, 7, 12575	17.4	38
339	pyPcazip: A PCA-based toolkit for compression and analysis of molecular simulation data. *SoftwareX*, **2016**, 5, 44-50	2.7	23
338	Parmbsc1: a refined force field for DNA simulations. *Nature Methods*, **2016**, 13, 55-8	21.6	483
337	Multiscale simulation of DNA. *Current Opinion in Structural Biology*, **2016**, 37, 29-45	8.1	85
336	Residues Coevolution Guides the Systematic Identification of Alternative Functional Conformations in Proteins. *Structure*, **2016**, 24, 116-126	5.2	40
335	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, 1233-46	5.6	7
334	Rational design of novel N-alkyl-N capped biostable RNA nanostructures for efficient long-term inhibition of gene expression. *Nucleic Acids Research*, **2016**, 44, 4354-67	20.1	6
333	BIGNASim: a NoSQL database structure and analysis portal for nucleic acids simulation data. *Nucleic Acids Research*, **2016**, 44, D272-8	20.1	35
332	Epigenomic analysis detects aberrant super-enhancer DNA methylation in human cancer. *Genome Biology*, **2016**, 17, 11	18.3	141
331	The Differential Response of Proteins to Macromolecular Crowding. *PLoS Computational Biology*, **2016**, 12, e1005040	5	35
330	Nucleosome architecture throughout the cell cycle. *Scientific Reports*, **2016**, 6, 19729	4.9	23
329	Conformational plasticity of RepB, the replication initiator protein of promiscuous streptococcal plasmid pMV158. *Scientific Reports*, **2016**, 6, 20915	4.9	9
328	Saturation of recognition elements blocks evolution of new tRNA identities. *Science Advances*, **2016** , 2, e1501860	14.3	34
327	Computational Prediction of HIV-1 Resistance to Protease Inhibitors. *Journal of Chemical Information and Modeling*, **2016**, 56, 915-23	6.1	15
326	Long-timescale dynamics of the Drew-Dickerson dodecamer. *Nucleic Acids Research*, **2016**, 44, 4052-66	20.1	68
325	Challenges of docking in large, flexible and promiscuous binding sites. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 4961-4969	3.4	15

324	Structure and Dynamics of Oligonucleotides in the Gas Phase. *Angewandte Chemie*, **2015**, 127, 477-481	3.6	6
323	Synthesis and properties of 2'-deoxy-2',4'-difluoroarabinose-modified nucleic acids. *Journal of Organic Chemistry*, **2015**, 80, 3083-91	4.2	25
322	Chromatin Unfolding by Epigenetic Modifications Explained by Dramatic Impairment of Internucleosome Interactions: A Multiscale Computational Study. *Journal of the American Chemical Society*, **2015**, 137, 10205-15	16.4	96
321	Non-coding recurrent mutations in chronic lymphocytic leukaemia. *Nature*, **2015**, 526, 519-24	50.4	565
320	The structural impact of DNA mismatches. *Nucleic Acids Research*, **2015**, 43, 4309-21	20.1	80
319	SEABED: Small molEcule activity scanner weB servicE baseD. *Bioinformatics*, **2015**, 31, 773-5	7.2	7
318	Seven-Membered Ring Nucleoside Analogues: Stereoselective Synthesis and Studies on Their Conformational Properties. *Organic Letters*, **2015**, 17, 5416-9	6.2	9
317	Inntags: small self-structured epitopes for innocuous protein tagging. *Nature Methods*, **2015**, 12, 955-8	21.6	18
316	Visualizing phosphodiester-bond hydrolysis by an endonuclease. *Nature Structural and Molecular Biology*, **2015**, 22, 65-72	17.6	26
315	SDS-PAGE analysis of A□bligomers is disserving research into Alzheimer·s disease: appealing for ESI-IM-MS. *Scientific Reports*, **2015**, 5, 14809	4.9	70
314	Can A Denaturant Stabilize DNA? Pyridine Reverses DNA Denaturation in Acidic pH. *Angewandte Chemie*, **2015**, 127, 10634-10637	3.6	
313	Can A Denaturant Stabilize DNA? Pyridine Reverses DNA Denaturation in Acidic pH. *Angewandte Chemie - International Edition*, **2015**, 54, 10488-91	16.4	6
312	Molecular dynamics simulations: advances and applications. *Advances and Applications in Bioinformatics and Chemistry*, **2015**, 8, 37-47	1.5	229
311	PACSAB: Coarse-Grained Force Field for the Study of Protein-Protein Interactions and Conformational Sampling in Multiprotein Systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 5929-38	6.4	10
310	Assessing the suitability of the multilevel strategy for the conformational analysis of small ligands. *Journal of Physical Chemistry B*, **2015**, 119, 1164-72	3.4	16
309	Structure and dynamics of oligonucleotides in the gas phase. *Angewandte Chemie - International Edition*, **2015**, 54, 467-71	16.4	18
308	Molecular dynamics study of naturally existing cavity couplings in proteins. *PLoS ONE*, **2015**, 10, e0119978	3.7	7
307	Specific loop modifications of the thrombin-binding aptamer trigger the formation of parallel structures. *FEBS Journal*, **2014**, 281, 1085-99	5.7	21

306	The DNA-forming properties of 6-selenoguanine. *Physical Chemistry Chemical Physics*, **2014**, 16, 1101-10	3.6	9
305	Comprehensive characterization of complex structural variations in cancer by directly comparing genome sequence reads. *Nature Biotechnology*, **2014**, 32, 1106-12	44.5	62
304	Structure and properties of DNA in apolar solvents. *Journal of Physical Chemistry B*, **2014**, 118, 8540-8	3.4	14
303	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	11.5	119
302	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, 3075-86	16.4	39
301	A theoretical view of protein dynamics. *Chemical Society Reviews*, **2014**, 43, 5051-66	58.5	83
300	Correlated motions are a fundamental property of β-sheets. *Nature Communications*, **2014**, 5, 4070	17.4	52
299	ABC: a systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. *Nucleic Acids Research*, **2014**, 42, 12272-83	20.1	138
298	A comprehensive DNA methylation profile of epithelial-to-mesenchymal transition. *Cancer Research* , **2014**, 74, 5608-19	10.1	54
297	Unraveling the sequence-dependent polymorphic behavior of d(CpG) steps in B-DNA. *Nucleic Acids Research*, **2014**, 42, 11304-20	20.1	63
296	Fuzziness and noise in nucleosomal architecture. *Nucleic Acids Research*, **2014**, 42, 4934-46	20.1	19
295	Structure of Nucleic Acids in the Gas Phase. *Physical Chemistry in Action*, **2014**, 55-75		3
294	On the nature of DNA hyperchromic effect. *Journal of Physical Chemistry B*, **2013**, 117, 8697-704	3.4	31
293	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, 119-25	6.4	63
292	The conformational landscape of an intrinsically disordered DNA-binding domain of a transcription regulator. *Journal of Physical Chemistry B*, **2013**, 117, 13842-50	3.4	19
291	BioSuper: a web tool for the superimposition of biomolecules and assemblies with rotational symmetry. *BMC Structural Biology*, **2013**, 13, 32	2.7	5
290	Backbone FC-H···O hydrogen bonds in 2'F-substituted nucleic acids. *Angewandte Chemie - International Edition*, **2013**, 52, 12065-8	16.4	41
289	Backbone FC?H???O Hydrogen Bonds in 2?F-Substituted Nucleic Acids. *Angewandte Chemie*, **2013**, 125, 12287-12290	3.6	6

288	Efficient Relaxation of Protein-Protein Interfaces by Discrete Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2013**, 9, 1222-9	6.4	10
287	The dynamic view of proteins: comment on "Comparing proteins to their internal dynamics: exploring structure-function relationships beyond static structural alignments". *Physics of Life Reviews*, **2013**, 10, 29-30; discussion 39-40	2.1	2
286	The catalytic site structural gate of adenosine deaminase allosterically modulates ligand binding to adenosine receptors. *FASEB Journal*, **2013**, 27, 1048-61	0.9	30
285	Functionalization of the 3'-ends of DNA and RNA strands with N-ethyl-N-coupled nucleosides: a promising approach to avoid 3'-exonuclease-catalyzed hydrolysis of therapeutic oligonucleotides. *ChemBioChem*, **2013**, 14, 510-20	3.8	9
284	Structure, Stiffness and Substates of the Dickerson-Drew Dodecamer. *Journal of Chemical Theory and Computation*, **2013**, 9, 707-721	6.4	72
283	Dramatic effect of furanose C2' 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, 5344-7	16.4	55
282	Proteins in the gas phase. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 408-425	7.9	40
281	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, 5933-8	11.5	42
280	Understanding the connection between epigenetic DNA methylation and nucleosome positioning from computer simulations. *PLoS Computational Biology*, **2013**, 9, e1003354	5	40
279	Exploring early stages of the chemical unfolding of proteins at the proteome scale. *PLoS Computational Biology*, **2013**, 9, e1003393	5	11
278	NAFlex: a web server for the study of nucleic acid flexibility. *Nucleic Acids Research*, **2013**, 41, W47-55	20.1	30
277	Unravelling the hidden DNA structural/physical code provides novel insights on promoter location. *Nucleic Acids Research*, **2013**, 41, 7220-30	20.1	11
276	Improved nucleic acid descriptors for siRNA efficacy prediction. *Nucleic Acids Research*, **2013**, 41, 1383-94	20.1	15
275	Exploration of conformational transition pathways from coarse-grained simulations. *Bioinformatics*, **2013**, 29, 1980-6	7.2	21
274	Light on the structural communication in Ras GTPases. *Journal of Biomolecular Structure and Dynamics*, **2013**, 31, 142-57	3.6	17
273	Conformational dynamics of the human propeller telomeric DNA quadruplex on a microsecond time scale. *Nucleic Acids Research*, **2013**, 41, 2723-35	20.1	60
272	Geometry, Dynamics, and Electronic Structure of DNA–Carbon Nanotube Hybrids. *Journal of Physical Chemistry C*, **2012**, 116, 11278-11282	3.8	4
271	Hog1 bypasses stress-mediated down-regulation of transcription by RNA polymerase II redistribution and chromatin remodeling. *Genome Biology*, **2012**, 13, R106	18.3	43

270	Structure of triplex DNA in the gas phase. *Journal of the American Chemical Society*, **2012**, 134, 6596-606	16.4	49
269	Finding Conformational Transition Pathways from Discrete Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2012**, 8, 4707-18	6.4	25
268	Frontiers in molecular dynamics simulations of DNA. *Accounts of Chemical Research*, **2012**, 45, 196-205	24.3	171
267	Fast Atomistic Molecular Dynamics Simulations from Essential Dynamics Samplings. *Journal of Chemical Theory and Computation*, **2012**, 8, 792-9	6.4	9
266	Exploring polymorphisms in B-DNA helical conformations. *Nucleic Acids Research*, **2012**, 40, 10668-78	20.1	68
265	Epigenomic analysis detects widespread gene-body DNA hypomethylation in chronic lymphocytic leukemia. *Nature Genetics*, **2012**, 44, 1236-42	36.3	422
264	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, 2204-14	6.4	10
263	Impact of methylation on the physical properties of DNA. *Biophysical Journal*, **2012**, 102, 2140-8	2.9	89
262	A Multilevel Strategy for the Exploration of the Conformational Flexibility of Small Molecules. *Journal of Chemical Theory and Computation*, **2012**, 8, 1808-19	6.4	32
261	Defining the nature of thermal intermediate in 3 state folding proteins: apoflavodoxin, a study case. *PLoS Computational Biology*, **2012**, 8, e1002647	5	9
260	Evidence for transcript networks composed of chimeric RNAs in human cells. *PLoS ONE*, **2012**, 7, e28213	3.7	51
259	Characterization of the impact of alternative splicing on protein dynamics: the cases of glutathione S-transferase and ectodysplasin-A isoforms. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 2235-49	4.2	4
258	MDWeb and MDMoby: an integrated web-based platform for molecular dynamics simulations. *Bioinformatics*, **2012**, 28, 1278-9	7.2	120
257	Small Molecule Docking from Theoretical Structural Models **2012**, 75-95		1
256	Exome sequencing identifies recurrent mutations of the splicing factor SF3B1 gene in chronic lymphocytic leukemia. *Nature Genetics*, **2011**, 44, 47-52	36.3	752
255	Structural, dynamical, and electronic transport properties of modified DNA duplexes containing size-expanded nucleobases. *Journal of Physical Chemistry A*, **2011**, 115, 11344-54	2.8	15
254	Coarse-grained representation of protein flexibility. Foundations, successes, and shortcomings. *Advances in Protein Chemistry and Structural Biology*, **2011**, 85, 183-215	5.3	27
253	The native ensemble and folding of a protein molten-globule: functional consequence of downhill folding. *Journal of the American Chemical Society*, **2011**, 133, 12154-61	16.4	48

252	Structural analysis of an equilibrium folding intermediate in the apoflavodoxin native ensemble by small-angle X-ray scattering. *Journal of Molecular Biology*, **2011**, 406, 604-19	6.5	23
251	A systematic study of the energetics involved in structural changes upon association and connectivity in protein interaction networks. *Structure*, **2011**, 19, 881-9	5.2	38
250	Polarization effects in molecular interactions. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 844-854	7.9	26
249	Physical properties of naked DNA influence nucleosome positioning and correlate with transcription start and termination sites in yeast. *BMC Genomics*, **2011**, 12, 489	4.5	25
248	Effects of local electric fields on the redox free energy of single stranded DNA. *Chemical Communications*, **2011**, 47, 2646-8	5.8	6
247	The protein folding transition-state ensemble from a Gō-like model. *Physical Chemistry Chemical Physics*, **2011**, 13, 15166-74	3.6	12
246	Whole-genome sequencing identifies recurrent mutations in chronic lymphocytic leukaemia. *Nature* , **2011**, 475, 101-5	50.4	1206
245	nucleR: a package for non-parametric nucleosome positioning. *Bioinformatics*, **2011**, 27, 2149-50	7.2	54
244	Scoring by intermolecular pairwise propensities of exposed residues (SIPPER): a new efficient potential for protein-protein docking. *Journal of Chemical Information and Modeling*, **2011**, 51, 370-7	6.1	51
243	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, 3935-40	11.5	111
242	Nucleotide binding switches the information flow in ras GTPases. *PLoS Computational Biology*, **2011** , 7, e1001098	5	27
241	Structural properties of g,t-parallel duplexes. *Journal of Nucleic Acids*, **2010**, 2010,	2.3	3
240	Differential stability of 2'F-ANA*RNA and ANA*RNA hybrid duplexes: roles of structure, pseudohydrogen bonding, hydration, ion uptake and flexibility. *Nucleic Acids Research*, **2010**, 38, 2498-511	20.1	58
239	Toward a consensus view of duplex RNA flexibility. *Biophysical Journal*, **2010**, 99, 1876-85	2.9	46
238	Approaching Elastic Network Models to Molecular Dynamics Flexibility. *Journal of Chemical Theory and Computation*, **2010**, 6, 2910-23	6.4	52
237	Ensemble Docking from Homology Models. *Journal of Chemical Theory and Computation*, **2010**, 6, 2547-57	6.4	55
236	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	20.1	299
235	Structural characterization of protein-protein complexes by integrating computational docking with small-angle scattering data. *Journal of Molecular Biology*, **2010**, 403, 217-30	6.5	59

234	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	6.4	261
233	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, 281-91	4.2	22
232	Deciphering the deformation modes associated with function retention and specialization in members of the Ras superfamily. *Structure*, **2010**, 18, 402-14	5.2	40
231	MoDEL (Molecular Dynamics Extended Library): a database of atomistic molecular dynamics trajectories. *Structure*, **2010**, 18, 1399-409	5.2	100
230	A genomics method to identify pathogenicity-related proteins. Application to aminoacyl-tRNA synthetase-like proteins. *FEBS Letters*, **2010**, 584, 460-6	3.8	5
229	Real-Time Atomistic Description of DNA Unfolding. *Angewandte Chemie*, **2010**, 122, 4915-4918	3.6	2
228	Multiple Routes to Characterize the Folding of a Small DNA Hairpin. *Angewandte Chemie*, **2010**, 122, 7839-7842	3.6	4
227	Real-time atomistic description of DNA unfolding. *Angewandte Chemie - International Edition*, **2010**, 49, 4805-8	16.4	26
226	Multiple routes to characterize the folding of a small DNA hairpin. *Angewandte Chemie - International Edition*, **2010**, 49, 7673-6	16.4	40
225	Protein flexibility from discrete molecular dynamics simulations using quasi-physical potentials. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 83-94	4.2	20
224	Conformationally rigid nucleoside probes help understand the role of sugar pucker and nucleobase orientation in the thrombin-binding aptamer. *Nucleic Acids Research*, **2009**, 37, 5589-601	20.1	33
223	Alternative splicing of transcription factors' genes: beyond the increase of proteome diversity. *Comparative and Functional Genomics*, **2009**, 905894		13
222	FlexServ: an integrated tool for the analysis of protein flexibility. *Bioinformatics*, **2009**, 25, 1709-10	7.2	67
221	An atomistic view to the gas phase proteome. *Structure*, **2009**, 17, 88-95	5.2	37
220	Solvation enthalpies of neutral solutes in water and octanol. *Theoretical Chemistry Accounts*, **2009**, 123, 11-20	1.9	7
219	COCO: a simple tool to enrich the representation of conformational variability in NMR structures. *Proteins: Structure, Function and Bioinformatics*, **2009**, 75, 206-16	4.2	17
218	Comparison of molecular dynamics and superfamily spaces of protein domain deformation. *BMC Structural Biology*, **2009**, 9, 6	2.7	29
217	On the performance of continuum solvation methods. A comment on "Universal approaches to solvation modeling". *Accounts of Chemical Research*, **2009**, 42, 489-92; discussion 493-7	24.3	152

216	Theoretical characterization of the dynamical behavior and transport properties of alpha,gamma-peptide nanotubes in solution. *Journal of the American Chemical Society*, **2009**, 131, 15678-86	16.4	40
215	Performance of the IEF-MST solvation continuum model in a blind test prediction of hydration free energies. *Journal of Physical Chemistry B*, **2009**, 113, 9330-4	3.4	17
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