Modesto Orozco Lpez

List of Publications by Citations

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	Refinement of the AMBER force field for nucleic acids: improving the description of alpha/gamma conformers. *Biophysical Journal*, **2007**, 92, 3817-29	2.9	1705
394	Whole-genome sequencing identifies recurrent mutations in chronic lymphocytic leukaemia. *Nature* , **2011**, 475, 101-5	50.4	1206
393	Exome sequencing identifies recurrent mutations of the splicing factor SF3B1 gene in chronic lymphocytic leukemia. *Nature Genetics*, **2011**, 44, 47-52	36.3	752
392	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	1.9	592
391	Non-coding recurrent mutations in chronic lymphocytic leukaemia. *Nature*, **2015**, 526, 519-24	50.4	565
390	Theoretical Methods for the Description of the Solvent Effect in Biomolecular Systems. *Chemical Reviews*, **2000**, 100, 4187-4226	68.1	538
389	Parmbsc1: a refined force field for DNA simulations. *Nature Methods*, **2016**, 13, 55-8	21.6	483
388	Epigenomic analysis detects widespread gene-body DNA hypomethylation in chronic lymphocytic leukemia. *Nature Genetics*, **2012**, 44, 1236-42	36.3	422
387	PMUT: a web-based tool for the annotation of pathological mutations on proteins. *Bioinformatics*, **2005**, 21, 3176-8	7.2	404
386	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
385	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	16.4	292
384	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
383	Target flexibility: an emerging consideration in drug discovery and design. *Journal of Medicinal Chemistry*, **2008**, 51, 6237-55	8.3	244
382	Molecular dynamics simulations: advances and applications. *Advances and Applications in Bioinformatics and Chemistry*, **2015**, 8, 37-47	1.5	229
381	Dynamics of B-DNA on the microsecond time scale. *Journal of the American Chemical Society*, **2007**, 129, 14739-45	16.4	224
380	Nature of base stacking: reference quantum-chemical stacking energies in ten unique B-DNA base-pair steps. *Chemistry - A European Journal*, **2006**, 12, 2854-65	4.8	204
379	A consensus view of protein dynamics. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 796-801	11.5	194

378	PupasView: a visual tool for selecting suitable SNPs, with putative pathological effect in genes, for genotyping purposes. *Nucleic Acids Research*, **2005**, 33, W501-5	20.1	192
377	Design, synthesis, and biological evaluation of dual binding site acetylcholinesterase inhibitors: new disease-modifying agents for Alzheimer's disease. *Journal of Medicinal Chemistry*, **2005**, 48, 7223-33	8.3	179
376	Correlated ab initio study of nucleic acid bases and their tautomers in the gas phase, in a microhydrated environment and in aqueous solution. *Physical Chemistry Chemical Physics*, **2002**, 4, 4192-4203	3.6	175
375	Frontiers in molecular dynamics simulations of DNA. *Accounts of Chemical Research*, **2012**, 45, 196-205	24.3	171
374	Characterization of disease-associated single amino acid polymorphisms in terms of sequence and structure properties. *Journal of Molecular Biology*, **2002**, 315, 771-86	6.5	171
373	Molecular dynamics simulations of the unfolding of barnase in water and 8 M aqueous urea. *Biochemistry*, **1997**, 36, 7313-29	3.2	162
372	New tacrine-huperzine A hybrids (huprines): highly potent tight-binding acetylcholinesterase inhibitors of interest for the treatment of Alzheimer's disease. *Journal of Medicinal Chemistry*, **2000**, 43, 4657-66	8.3	160
371	Molecular Dynamics Simulations of the d(T•A•T) Triple Helix. *Journal of the American Chemical Society*, **1997**, 119, 7463-7469	16.4	156
370	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
369	Accuracy of free energies of hydration for organic molecules from 6-31g*-derived partial charges. *Journal of Computational Chemistry*, **1993**, 14, 1240-1249	3.5	142
368	Epigenomic analysis detects aberrant super-enhancer DNA methylation in human cancer. *Genome Biology*, **2016**, 17, 11	18.3	141
367	Theoretical methods for the simulation of nucleic acids. *Chemical Society Reviews*, **2003**, 32, 350-64	58.5	141
366	ABC: a systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. *Nucleic Acids Research*, **2014**, 42, 12272-83	20.1	138
365	Cooperativity in drug-DNA recognition: a molecular dynamics study. *Journal of the American Chemical Society*, **2001**, 123, 12658-63	16.4	133
364	Optimization of solute cavities and van der Waals parameters in ab initio MST-SCRF calculations of neutral molecules. *Journal of Computational Chemistry*, **1994**, 15, 446-454	3.5	131
363	Thorough validation of protein normal mode analysis: a comparative study with essential dynamics. *Structure*, **2007**, 15, 565-75	5.2	130
362	Towards a molecular dynamics consensus view of B-DNA flexibility. *Nucleic Acids Research*, **2008**, 36, 2379-94	20.1	128
361	Triplex-forming oligonucleotide target sequences in the human genome. *Nucleic Acids Research*, **2004**, 32, 354-60	20.1	127

360	Synthesis of enantiopure trans-3,4-disubstituted piperidines. An enantiodivergent synthesis of (+)- and (-)-paroxetine. *Journal of Organic Chemistry*, **2000**, 65, 3074-84	4.2	122
359	MDWeb and MDMoby: an integrated web-based platform for molecular dynamics simulations. *Bioinformatics*, **2012**, 28, 1278-9	7.2	120
358	Functional and structural conservation of CBS domains from CLC chloride channels. *Journal of Physiology*, **2004**, 557, 363-78	3.9	120
357	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
356	CH···O Contacts in the Adenine···Uracil Watson–Crick and Uracil···Uracil Nucleic Acid Base Pairs: Nonempirical ab Initio Study with Inclusion of Electron Correlation Effects. *Journal of Physical Chemistry B*, **2000**, 104, 6286-6292	3.4	118
355	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	6.4	114
354	Induced dipole moment and atomic charges based on average electrostatic potentials in aqueous solution. *Journal of Chemical Physics*, **1993**, 98, 2975-2982	3.9	113
353	Single Stranded Loops of Quadruplex DNA As Key Benchmark for Testing Nucleic Acids Force Fields. *Journal of Chemical Theory and Computation*, **2009**, 5, 2514-30	6.4	112
352	Solvation in octanol: parametrization of the continuum MST model. *Journal of Computational Chemistry*, **2001**, 22, 1180-1193	3.5	112
351	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
350	The structure and dynamics of DNA in the gas phase. *Journal of the American Chemical Society*, **2003**, 125, 8007-14	16.4	111
349	Glutaryl-CoA dehydrogenase deficiency in Spain: evidence of two groups of patients, genetically, and biochemically distinct. *Pediatric Research*, **2000**, 48, 315-22	3.2	111
348	Recent advances in the study of nucleic acid flexibility by molecular dynamics. *Current Opinion in Structural Biology*, **2008**, 18, 185-93	8.1	105
347	The relative flexibility of B-DNA and A-RNA duplexes: database analysis. *Nucleic Acids Research*, **2004**, 32, 6144-51	20.1	105
346	On the potential role of the amino nitrogen atom as a hydrogen bond acceptor in macromolecules. *Journal of Molecular Biology*, **1998**, 279, 1123-36	6.5	105
345	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	3.5	104
344	Theoretical study of the truncated hemoglobin HbN: exploring the molecular basis of the NO detoxification mechanism. *Journal of the American Chemical Society*, **2005**, 127, 4433-44	16.4	102
343	Theoretical study of alkyl-pi and aryl-pi interactions. Reconciling theory and experiment. *Journal of Organic Chemistry*, **2002**, 67, 7057-65	4.2	101

342	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
341	MoDEL (Molecular Dynamics Extended Library): a database of atomistic molecular dynamics trajectories. *Structure*, **2010**, 18, 1399-409	5.2	100
340	Determining promoter location based on DNA structure first-principles calculations. *Genome Biology*, **2007**, 8, R263	18.3	98
339	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
338	Molecular Dynamics Studies of DNA A-Tract Structure and Flexibility. *Journal of the American Chemical Society*, **1999**, 121, 5981-5991	16.4	96
337	Molecular Dynamics Simulation of a PNA□DNA□PNA Triple Helix in Aqueous Solution. *Journal of the American Chemical Society*, **1998**, 120, 5895-5904	16.4	94
336	Essential Dynamics: A Tool for Efficient Trajectory Compression and Management. *Journal of Chemical Theory and Computation*, **2006**, 2, 251-8	6.4	90
335	Synthesis, in vitro pharmacology, and molecular modeling of very potent tacrine-huperzine A hybrids as acetylcholinesterase inhibitors of potential interest for the treatment of Alzheimer's disease. *Journal of Medicinal Chemistry*, **1999**, 42, 3227-42	8.3	90
334	Impact of methylation on the physical properties of DNA. *Biophysical Journal*, **2012**, 102, 2140-8	2.9	89
333	Ligand-induced dynamical regulation of NO conversion in Mycobacterium tuberculosis truncated hemoglobin-N. *Proteins: Structure, Function and Bioinformatics*, **2006**, 64, 457-64	4.2	89
332	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	3.4	89
331	An AM1-SCRF approach to the study of changes in molecular properties induced by solvent. *The Journal of Physical Chemistry*, **1993**, 97, 4386-4391		88
330	Exploring the counterion atmosphere around DNA: what can be learned from molecular dynamics simulations?. *Biophysical Journal*, **2004**, 87, 800-11	2.9	86
329	Development of optimized MST/SCRF methods for semiempirical calculations: The MNDO and PM3 Hamiltonians. *Journal of Computational Chemistry*, **1995**, 16, 563-575	3.5	86
328	Multiscale simulation of DNA. *Current Opinion in Structural Biology*, **2016**, 37, 29-45	8.1	85
327	A theoretical view of protein dynamics. *Chemical Society Reviews*, **2014**, 43, 5051-66	58.5	83
326	G-quadruplexes can maintain their structure in the gas phase. *Journal of the American Chemical Society*, **2006**, 128, 3608-19	16.4	82
325	Electrostatic component of solvation: comparison of SCRF continuum models. *Journal of Computational Chemistry*, **2003**, 24, 284-97	3.5	82

324	The structure of human 4F2hc ectodomain provides a model for homodimerization and electrostatic interaction with plasma membrane. *Journal of Biological Chemistry*, **2007**, 282, 31444-52	5.4	81
323	Continuum solvation models: Dissecting the free energy of solvation. *Physical Chemistry Chemical Physics*, **2003**, 5, 3827-3836	3.6	81
322	The structural impact of DNA mismatches. *Nucleic Acids Research*, **2015**, 43, 4309-21	20.1	80
321	How accurate are accurate force-fields for B-DNA?. *Nucleic Acids Research*, **2017**, 45, 4217-4230	20.1	79
320	Ab Initio Study of Stacking Interactions in A- and B-DNA. *Journal of Physical Chemistry B*, **1997**, 101, 3846-3853	3.4	79
319	Relative flexibility of DNA and RNA: a molecular dynamics study. *Journal of Molecular Biology*, **2004**, 343, 627-38	6.5	79
318	Classical molecular interaction potentials: improved setup procedure in molecular dynamics simulations of proteins. *Proteins: Structure, Function and Bioinformatics*, **2001**, 45, 428-37	4.2	79
317	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	3.5	78
316	Dimerization of Carboxylic Acids: Reliability of Theoretical Calculations and the Effect of Solvent. *Journal of Physical Chemistry B*, **1998**, 102, 2269-2276	3.4	77
315	Colibactin DNA-damage signature indicates mutational impact in colorectal cancer. *Nature Medicine* , **2020**, 26, 1063-1069	50.5	76
314	Extension of the MST model to the IEF formalism: HF and B3LYP parametrizations. *Computational and Theoretical Chemistry*, **2005**, 727, 29-40		74
313	. *Journal of Physical Chemistry A*, **1999**, 103, 4525-4532	2.8	74
312	Induction effects in metal cation-benzene complexes. *Physical Chemistry Chemical Physics*, **2008**, 10, 2616-24	3.6	73
311	Interoperability with Moby 1.0--it's better than sharing your toothbrush!. *Briefings in Bioinformatics*, **2008**, 9, 220-31	13.4	73
310	Structure, Stiffness and Substates of the Dickerson-Drew Dodecamer. *Journal of Chemical Theory and Computation*, **2013**, 9, 707-721	6.4	72
309	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	3.4	71
308	SDS-PAGE analysis of Aβ oligomers is disserving research into Alzheimer's disease: appealing for ESI-IM-MS. *Scientific Reports*, **2015**, 5, 14809	4.9	70
307	Exploring polymorphisms in B-DNA helical conformations. *Nucleic Acids Research*, **2012**, 40, 10668-78	20.1	68

306	Theoretical study of large conformational transitions in DNA: the BA conformational change in water and ethanol/water. *Nucleic Acids Research*, **2007**, 35, 3330-8	20.1	68
305	An optimized AM1/MST method for the MST-SCRF representation of solvated systems. *Journal of Computational Chemistry*, **1994**, 15, 847-857	3.5	68
304	Long-timescale dynamics of the Drew-Dickerson dodecamer. *Nucleic Acids Research*, **2016**, 44, 4052-66	20.1	68
303	FlexServ: an integrated tool for the analysis of protein flexibility. *Bioinformatics*, **2009**, 25, 1709-10	7.2	67
302	Compaction of Duplex Nucleic Acids upon Native Electrospray Mass Spectrometry. *ACS Central Science*, **2017**, 3, 454-461	16.8	65
301	Theoretical Study of Azido‐Tetrazole Isomerism: Effect of Solvent and Substituents and Mechanism of Isomerization. *Journal of the American Chemical Society*, **1998**, 120, 4723-4731	16.4	65
300	Tautomerism of Xanthine Oxidase Substrates Hypoxanthine and Allopurinol. *Journal of Organic Chemistry*, **1996**, 61, 5964-5971	4.2	64
299	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
298	Unraveling the sequence-dependent polymorphic behavior of d(CpG) steps in B-DNA. *Nucleic Acids Research*, **2014**, 42, 11304-20	20.1	63
297	Theoretical study of anion binding to calix[4]pyrrole: the effects of solvent, fluorine substitution, cosolute, and water traces. *Journal of the American Chemical Society*, **2002**, 124, 12796-805	16.4	63
296	Molecular Dynamics Simulations of PNA‐DNA and PNA‐RNA Duplexes in Aqueous Solution. *Journal of the American Chemical Society*, **2000**, 122, 5997-6008	16.4	63
295	Optimization of the cavity size for ab initio MST-SCRF calculations of monovalent ions. *Chemical Physics*, **1994**, 182, 237-248	2.3	63
294	Comprehensive characterization of complex structural variations in cancer by directly comparing genome sequence reads. *Nature Biotechnology*, **2014**, 32, 1106-12	44.5	62
293	Conformational dynamics of the human propeller telomeric DNA quadruplex on a microsecond time scale. *Nucleic Acids Research*, **2013**, 41, 2723-35	20.1	60
292	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
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289	Nucleic Acid Triple Helices: Stability Effects of Nucleobase Modifications. *Current Organic Chemistry* , **2002**, 6, 1333-1368	1.7	59

288	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
287	The (in)dependence of alternative splicing and gene duplication. *PLoS Computational Biology*, **2007**, 3, e33	5	57
286	Molecular Dynamics Simulations in Aqueous Solution of Triple Helices Containing d(GCC) Trios. *Journal of the American Chemical Society*, **1998**, 120, 11226-11233	16.4	57
285	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	16.4	57
284	Theoretical Methods for the Representation of Solvent. *Journal of Molecular Modeling*, **1996**, 2, 1-15	2	57
283	Exploring the Essential Dynamics of B-DNA. *Journal of Chemical Theory and Computation*, **2005**, 1, 790-800	6.4	56
282	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
281	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
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276	Theoretical study of N-methylacetamide in vacuum and aqueous solution: implications for the peptide bond isomerization. *Journal of Organic Chemistry*, **1993**, 58, 6397-6405	4.2	53
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272	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
271	Local aromaticity in natural nucleobases and their size-expanded benzo-fused derivatives. *Journal of Physical Chemistry A*, **2006**, 110, 12249-58	2.8	51

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269	Geometrical and electronic structure variability of the sugar-phosphate backbone in nucleic acids. *Journal of Physical Chemistry B*, **2008**, 112, 8188-97	3.4	50
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267	4D Genome Rewiring during Oncogene-Induced and Replicative Senescence. *Molecular Cell*, **2020**, 78, 522-538.e9	17.6	48
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264	Quantification of Pathway Cross-talk Reveals Novel Synergistic Drug Combinations for Breast Cancer. *Cancer Research*, **2017**, 77, 459-469	10.1	47
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262	New strategies to incorporate the solvent polarization in self-consistent reaction field and free-energy perturbation simulations. *Journal of Chemical Physics*, **1995**, 103, 10183-10191	3.9	46
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237	Binding affinities of oligonucleotides and PNAs containing phenoxazine and G-clamp cytosine analogues are unusually sequence-dependent. *Organic Letters*, **2007**, 9, 4503-6	6.2	39
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226	Generalization of the Molecular Electrostatic Potential for the Study of Noncovalent interactions. *Theoretical and Computational Chemistry*, **1996**, 3, 181-218		37
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