# 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 |

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

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | 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 |
| 2 | Whole-genome sequencing identifies recurrent mutations in chronic lymphocytic leukaemia. Nature, 2011, 475, 101-105. | 13.7 | 1,364 |
| 3 | Exome sequencing identifies recurrent mutations of the splicing factor SF3B1 gene in chronic lymphocytic leukemia. Nature Genetics, 2012, 44, 47-52. | 9.4 | 893 |
| 4 | Parmbsc1: a refined force field for DNA simulations. Nature Methods, 2016, 13, 55-58. | 9.0 | 790 |
| 5 | Non-coding recurrent mutations in chronic lymphocytic leukaemia. Nature, 2015, 526, 519-524. | 13.7 | 749 |
| 6 | 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 |
| 7 | Theoretical Methods for the Description of the Solvent Effect in Biomolecular Systems. Chemical Reviews, 2000, 100, 4187-4226. | 23.0 | 571 |
| 8 | Epigenomic analysis detects widespread gene-body DNA hypomethylation in chronic lymphocytic leukemia. Nature Genetics, 2012, 44, 1236-1242. | 9.4 | 525 |
| 9 | PMUT: a web-based tool for the annotation of pathological mutations on proteins. Bioinformatics, 2005, 21, 3176-3178. | 1.8 | 441 |
| 10 | Molecular dynamics simulations: advances and applications. Advances and Applications in Bioinformatics and Chemistry, 2015, 8, 37. | 1.6 | 409 |
| 11 | 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 |
| 12 | 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 |
| 13 | 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 |
| 14 | Target Flexibility: An Emerging Consideration in Drug Discovery and Design. Journal of Medicinal Chemistry, 2008, 51, 6237-6255. | 2.9 | 280 |
| 15 | 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 |
| 16 | Dynamics of B-DNA on the Microsecond Time Scale. Journal of the American Chemical Society, 2007, 129, 14739-14745. | 6.6 | 250 |
| 17 | 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 |
| 18 | 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 |

| # | Article | IF | Citations |
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| 19 | 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 |
| 20 | 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 |
| 21 | Frontiers in Molecular Dynamics Simulations of DNA. Accounts of Chemical Research, 2012, 45, 196-205. | 7.6 | 194 |
| 22 | 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 |
| 23 | Î¼ABC: a systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. Nucleic Acids Research, 2014, 42, 12272-12283. | 6.5 | 186 |
| 24 | 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 |
| 25 | Epigenomic analysis detects aberrant super-enhancer DNA methylation in human cancer. Genome Biology, 2016, 17, 11. | 3.8 | 184 |
| 26 | 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 |
| 27 | Molecular Dynamics Simulations of the Unfolding of Barnase in Water and 8 M Aqueous Urea. Biochemistry, 1997, 36, 7313-7329. | 1.2 | 173 |
| 28 | 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 |
| 29 | Molecular Dynamics Simulations of the d(TÂ·AÂ·T) Triple Helix. Journal of the American Chemical Society, 1997, 119, 7463-7469. | 6.6 | 160 |
| 30 | 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 |
| 31 | 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 |
| 32 | MDWeb and MDMoby: an integrated web-based platform for molecular dynamics simulations. Bioinformatics, 2012, 28, 1278-1279. | 1.8 | 153 |
| 33 | Cooperativity in Drugâ¯DNA Recognition:â€‰ A Molecular Dynamics Study. Journal of the American Chemical Society, 2001, 123, 12658-12663. | 6.6 | 150 |
| 34 | Theoretical methods for the simulation of nucleic acids. Chemical Society Reviews, 2003, 32, 350-364. | 18.7 | 150 |
| 35 | Triplex-forming oligonucleotide target sequences in the human genome. Nucleic Acids Research, 2004, 32, 354-360. | 6.5 | 149 |
| 36 | Colibactin DNA-damage signature indicates mutational impact in colorectal cancer. Nature Medicine, 2020, 26, 1063-1069. | 15.2 | 149 |

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| 37 | Towards a molecular dynamics consensus view of B-DNA flexibility. Nucleic Acids Research, 2008, 36, 2379-2394. | 6.5 | 147 |
| 38 | Thorough Validation of Protein Normal Mode Analysis: A Comparative Study with Essential Dynamics. Structure, 2007, 15, 565-575. | 1.6 | 144 |
| 39 | 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 |
| 40 | 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 |
| 41 | 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 |
| 42 | 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 |
| 43 | Functional and structural conservation of CBS domains from CLC chloride channels. Journal of Physiology, 2004, 557, 363-378. | 1.3 | 131 |
| 44 | 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 |
| 45 | 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 |
| 46 | Multiscale simulation of DNA. Current Opinion in Structural Biology, 2016, 37, 29-45. | 2.6 | 124 |
| 47 | MoDEL (Molecular Dynamics Extended Library): AÂDatabase of Atomistic Molecular Dynamics Trajectories. Structure, 2010, 18, 1399-1409. | 1.6 | 123 |
| 48 | The Structure and Dynamics of DNA in the Gas Phase. Journal of the American Chemical Society, 2003, 125, 8007-8014. | 6.6 | 121 |
| 49 | Determining promoter location based on DNA structure first-principles calculations. Genome Biology, 2007, 8, R263. | 13.9 | 121 |
| 50 | 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 |
| 51 | 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 |
| 52 | Solvation in octanol: parametrization of the continuum MST model. Journal of Computational Chemistry, 2001, 22, 1180-1193. | 1.5 | 120 |
| 53 | Theoretical Study of Alkyl-Ï€ and Aryl-Ï€ Interactions. Reconciling Theory and Experiment. Journal of Organic Chemistry, 2002, 67, 7057-7065. | 1.7 | 119 |
| 54 | The relative flexibility of B-DNA and A-RNA duplexes: database analysis. Nucleic Acids Research, 2004, 32, 6144-6151. | 6.5 | 119 |

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| 55 | 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 |
| 56 | Impact of Methylation on the Physical Properties of DNA. Biophysical Journal, 2012, 102, 2140-2148. | 0.2 | 118 |
| 57 | Recent advances in the study of nucleic acid flexibility by molecular dynamics. Current Opinion in Structural Biology, 2008, 18, 185-193. | 2.6 | 113 |
| 58 | The structural impact of DNA mismatches. Nucleic Acids Research, 2015, 43, 4309-4321. | 6.5 | 113 |
| 59 | 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 |
| 60 | 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 |
| 61 | A theoretical view of protein dynamics. Chemical Society Reviews, 2014, 43, 5051-5066. | 18.7 | 111 |
| 62 | 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 |
| 63 | How accurate are accurate force-fields for B-DNA?. Nucleic Acids Research, 2017, 45, gkw1355. | 6.5 | 107 |
| 64 | 4D Genome Rewiring during Oncogene-Induced and Replicative Senescence. Molecular Cell, 2020, 78, 522-538.e9. | 4.5 | 107 |
| 65 | 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 |
| 66 | 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 |
| 67 | Molecular Dynamics Studies of DNA A-Tract Structure and Flexibility. Journal of the American Chemical Society, 1999, 121, 5981-5991. | 6.6 | 101 |
| 68 | 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 |
| 69 | 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 |
| 70 | Essential Dynamics:â€‰ A Tool for Efficient Trajectory Compression and Management. Journal of Chemical Theory and Computation, 2006, 2, 251-258. | 2.3 | 98 |
| 71 | Exploring the Counterion Atmosphere around DNA: What Can Be Learned from Molecular Dynamics Simulations?. Biophysical Journal, 2004, 87, 800-811. | 0.2 | 96 |
| 72 | 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 |

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| 73 | 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 |
| 74 | 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 |
| 75 | Relative Flexibility of DNA and RNA: a Molecular Dynamics Study. Journal of Molecular Biology, 2004, 343, 627-638. | 2.0 | 94 |
| 76 | Interoperability with Moby 1.0--It's better than sharing your toothbrush!. Briefings in Bioinformatics, 2008, 9, 220-231. | 3.2 | 91 |
| 77 | Continuum solvation models: Dissecting the free energy of solvation. Physical Chemistry Chemical Physics, 2003, 5, 3827-3836. | 1.3 | 89 |
| 78 | Exploring polymorphisms in B-DNA helical conformations. Nucleic Acids Research, 2012, 40, 10668-10678. | 6.5 | 89 |
| 79 | 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 |
| 80 | 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 |
| 81 | 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 |
| 82 | Electrostatic component of solvation: Comparison of SCRF continuum models. Journal of Computational Chemistry, 2003, 24, 284-297. | 1.5 | 86 |
| 83 | Long-timescale dynamics of the Drewâ€“Dickerson dodecamer. Nucleic Acids Research, 2016, 44, 4052-4066. | 6.5 | 86 |
| 84 | G-Quadruplexes Can Maintain Their Structure in the Gas Phase. Journal of the American Chemical Society, 2006, 128, 3608-3619. | 6.6 | 85 |
| 85 | 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 |
| 86 | 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 |
| 87 | Ab InitioStudy of Stacking Interactions in A- and B-DNA. Journal of Physical Chemistry B, 1997, 101, 3846-3853. | 1.2 | 82 |
| 88 | Correlated motions are a fundamental property of Î²-sheets. Nature Communications, 2014, 5, 4070. | 5.8 | 82 |
| 89 | nucleR: a package for non-parametric nucleosome positioning. Bioinformatics, 2011, 27, 2149-2150. | 1.8 | 81 |
| 90 | Unraveling the sequence-dependent polymorphic behavior of d(CpG) steps in B-DNA. Nucleic Acids Research, 2014, 42, 11304-11320. | 6.5 | 81 |

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| 91 | Compaction of Duplex Nucleic Acids upon Native Electrospray Mass Spectrometry. ACS Central Science, 2017, 3, 454-461. | 5.3 | 81 |
| 92 | 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 |
| 93 | 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 |
| 94 | Extension of the MST model to the IEF formalism: HF and B3LYP parametrizations. Computational and Theoretical Chemistry, 2005, 727, 29-40. | 1.5 | 79 |
| 95 | Induction effects in metal cationâ€“benzene complexes. Physical Chemistry Chemical Physics, 2008, 10, 2616. | 1.3 | 78 |
| 96 | Structure, Stiffness and Substates of the Dickerson-Drew Dodecamer. Journal of Chemical Theory and Computation, 2013, 9, 707-721. | 2.3 | 78 |
| 97 | Quantification of Pathway Cross-talk Reveals Novel Synergistic Drug Combinations for Breast Cancer. Cancer Research, 2017, 77, 459-469. | 0.4 | 75 |
| 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 | An optimized AM1/MST method for the MST-SCRF representation of solvated systems. Journal of Computational Chemistry, 1994, 15, 847-857. | 1.5 | 73 |
| 100 | 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 |
| 101 | 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 |
| 102 | FlexServ: an integrated tool for the analysis of protein flexibility. Bioinformatics, 2009, 25, 1709-1710. | 1.8 | 72 |
| 103 | Tautomerism of Xanthine Oxidase Substrates Hypoxanthine and Allopurinol. Journal of Organic Chemistry, 1996, 61, 5964-5971. | 1.7 | 71 |
| 104 | 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 |
| 105 | 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 |
| 106 | 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 |
| 107 | Conformational dynamics of the human propeller telomeric DNA quadruplex on a microsecond time scale. Nucleic Acids Research, 2013, 41, 2723-2735. | 6.5 | 70 |
| 108 | A Comprehensive DNA Methylation Profile of Epithelial-to-Mesenchymal Transition. Cancer Research, 2014, 74, 5608-5619. | 0.4 | 69 |

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| 109 | 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 |
| 110 | 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 |
| 111 | The (In)dependence of Alternative Splicing and Gene Duplication. PLoS Computational Biology, 2007, 3, e33. | 1.5 | 66 |
| 112 | Optimization of the cavity size for ab initio MST-SCRF calculations of monovalent ions. Chemical Physics, 1994, 182, 237-248. | 0.9 | 65 |
| 113 | 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 |
| 114 | Ensemble Docking from Homology Models. Journal of Chemical Theory and Computation, 2010, 6, 2547-2557. | 2.3 | 65 |
| 115 | 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 |
| 116 | Structure, Recognition Properties, and Flexibility of the DNAÂ·RNA Hybrid. Journal of the American Chemical Society, 2005, 127, 4910-4920. | 6.6 | 64 |
| 117 | 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 |
| 118 | The impact of monovalent ion force field model in nucleic acids simulations. Physical Chemistry Chemical Physics, 2009, 11, 10596. | 1.3 | 62 |
| 119 | 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 |
| 120 | Prediction and validation of protein intermediate states from structurally rich ensembles and coarse-grained simulations. Nature Communications, 2016, 7, 12575. | 5.8 | 62 |
| 121 | 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 |
| 122 | Theoretical Methods for the Representation of Solvent. Journal of Molecular Modeling, 1996, 2, 1-15. | 0.8 | 61 |
| 123 | Exploring the Essential Dynamics of B-DNA. Journal of Chemical Theory and Computation, 2005, 1, 790-800. | 2.3 | 61 |
| 124 | Evidence for Transcript Networks Composed of Chimeric RNAs in Human Cells. PLoS ONE, 2012, 7, e28213. | 1.1 | 61 |
| 125 | Impact of DNA methylation on 3D genome structure. Nature Communications, 2021, 12, 3243. | 5.8 | 61 |
| 126 | Approaching Elastic Network Models to Molecular Dynamics Flexibility. Journal of Chemical Theory and Computation, 2010, 6, 2910-2923. | 2.3 | 60 |

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| 127 | Targeting RNA structure in SMN2 reverses spinal muscular atrophy molecular phenotypes. Nature Communications, 2018, 9, 2032. | 5.8 | 60 |
| 128 | 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 |
| 129 | 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 |
| 130 | Nucleic Acid Triple Helices: Stability Effects of Nucleobase Modifications. Current Organic Chemistry, 2002, 6, 1333-1368. | 0.9 | 59 |
| 131 | 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 |
| 132 | BIGNASim: a NoSQL database structure and analysis portal for nucleic acids simulation data. Nucleic Acids Research, 2016, 44, D272-D278. | 6.5 | 57 |
| 133 | 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 |
| 134 | Structure of Triplex DNA in the Gas Phase. Journal of the American Chemical Society, 2012, 134, 6596-6606. | 6.6 | 56 |
| 135 | Residues Coevolution Guides the Systematic Identification of Alternative Functional Conformations in Proteins. Structure, 2016, 24, 116-126. | 1.6 | 56 |
| 136 | Role of Intramolecular Hydrogen Bonds in the Intermolecular Hydrogen Bonding of Carbohydrates. Journal of Physical Chemistry A, 1998, 102, 6690-6696. | 1.1 | 54 |
| 137 | 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 |
| 138 | Toward a Consensus View of Duplex RNA Flexibility. Biophysical Journal, 2010, 99, 1876-1885. | 0.2 | 54 |
| 139 | Unique Tautomeric Properties of Isoguanine. Journal of the American Chemical Society, 2004, 126, 154-164. | 6.6 | 53 |
| 140 | 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 |
| 141 | Local Aromaticity in Natural Nucleobases and Their Size-Expanded Benzo-Fused Derivatives. Journal of Physical Chemistry A, 2006, 110, 12249-12258. | 1.1 | 52 |
| 142 | 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 |
| 143 | Molecular interaction potential: A new tool for the theoretical study of molecular reactivity. Journal of Computational Chemistry, 1993, 14, 587-602. | 1.5 | 50 |
| 144 | Theoretical Study of the Mechanisms of Substrate Recognition by Catalase. Journal of the American Chemical Society, 2001, 123, 9665-9672. | 6.6 | 50 |

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| 145 | Hog1 bypasses stress-mediated down-regulation of transcription by RNA polymerase II redistribution and chromatin remodeling. Genome Biology, 2012, 13, R106. | 13.9 | 50 |
| 146 | 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 |
| 147 | Understanding the Connection between Epigenetic DNA Methylation and Nucleosome Positioning from Computer Simulations. PLoS Computational Biology, 2013, 9, e1003354. | 1.5 | 50 |
| 148 | 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 |
| 149 | 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 |
| 150 | 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 |
| 151 | Proteins in the gas phase. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 408-425. | 6.2 | 49 |
| 152 | Generalization of the Molecular Electrostatic Potential for the Study of Noncovalent interactions. Theoretical and Computational Chemistry, 1996, 3, 181-218. | 0.2 | 47 |
| 153 | Ligand-induced changes in the binding sites of proteins. Bioinformatics, 2002, 18, 939-948. | 1.8 | 46 |
| 154 | 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 |
| 155 | Deciphering the Deformation Modes Associated with Function Retention and Specialization in Members of the Ras Superfamily. Structure, 2010, 18, 402-414. | 1.6 | 46 |
| 156 | Saturation of recognition elements blocks evolution of new tRNA identities. Science Advances, 2016, 2, e1501860. | 4.7 | 46 |
| 157 | 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 |
| 158 | Synthesis, in Vitro Pharmacology, and Molecular Modeling ofsyn-Huprines as Acetylcholinesterase Inhibitors. Journal of Medicinal Chemistry, 2001, 44, 4733-4736. | 2.9 | 45 |
| 159 | Multiple Routes to Characterize the Folding of a Small DNA Hairpin. Angewandte Chemie - International Edition, 2010, 49, 7673-7676. | 7.2 | 45 |
| 160 | NAFlex: a web server for the study of nucleic acid flexibility. Nucleic Acids Research, 2013, 41, W47-W55. | 6.5 | 45 |
| 161 | The static and dynamic structural heterogeneities of B-DNA: extending Calladineâ€“Dickerson rules. Nucleic Acids Research, 2019, 47, 11090-11102. | 6.5 | 45 |
| 162 | Mechanism for the rotamase activity of FK506 binding protein from molecular dynamics simulations. Biochemistry, 1993, 32, 12864-12874. | 1.2 | 44 |

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