Lalith Perera

List of Publications by Year
in descending order

125 papers	24,371 citations	70961 41 h-index	19136 118 g-index
131 all docs	131 docs citations	131 times ranked	25582 citing authors

#	Article	IF	Citations
1	A smooth particle mesh Ewald method. Journal of Chemical Physics, 1995, 103, 8577-8593.	1.2	18,266
2	New tricks for modelers from the crystallography toolkit: the particle mesh Ewald algorithm and its use in nucleic acid simulations. Structure, 1999, 7, R55-R60.	1.6	571
3	Molecular Dynamics Simulation of Sodium Dodecyl Sulfate Micelle in Water:Â Micellar Structural Characteristics and Counterion Distribution. Journal of Physical Chemistry B, 2002, 106, 3788-3793.	1.2	334
4	Manyâ€body effects in molecular dynamics simulations of Na+(H2O)n and Clâ^'(H2O)n clusters. Journal of Chemical Physics, 1991, 95, 1954-1963.	1.2	322
5	Molecular Dynamics Simulations of Sodium Dodecyl Sulfate Micelle in Water:â€‰ The Behavior of Water. Journal of Physical Chemistry B, 2002, 106, 10902-10907.	1.2	173
6	Towards accurate solvation dynamics of divalent cations in water using the polarizable amoeba force field: From energetics to structure. Journal of Chemical Physics, 2006, 125, 054511.	1.2	169
7	Phenobarbital Indirectly Activates the Constitutive Active Androstane Receptor (CAR) by Inhibition of Epidermal Growth Factor Receptor Signaling. Science Signaling, 2013, 6, ra31.	1.6	163
8	Structures of Clâ^'(H2O)n and Fâ^'(H2O)n (n=2,3,...,15) clusters. Molecular dynamics computer simulations. Journal of Chemical Physics, 1994, 100, 3085-3093.	1.2	154
9	Effect of the treatment of longâ€range forces on the dynamics of ions in aqueous solutions. Journal of Chemical Physics, 1995, 102, 450-456.	1.2	148
10	Plasminogen Alleles Influence Susceptibility to Invasive Aspergillosis. PLoS Genetics, 2008, 4, e1000101.	1.5	145
11	Uncovering the polymerase-induced cytotoxicity of an oxidized nucleotide. Nature, 2015, 517, 635-639.	13.7	133
12	Potential SARS-CoV-2 main protease inhibitors. Drug Discovery Today, 2021, 26, 804-816.	3.2	128
13	GATA3-dependent cellular reprogramming requires activation-domain dependent recruitment of a chromatin remodeler. Genome Biology, 2016, 17, 36.	3.8	121
14	Structure and dynamics of Clâ^'(H2O)20 clusters: The effect of the polarizability and the charge of the ion. Journal of Chemical Physics, 1992, 96, 8288-8294.	1.2	118
15	The Origin of the Hydration Interaction of Lipid Bilayers from MD Simulation of Dipalmitoylphosphatidylcholine Membranes in Gel and Liquid Crystalline Phases. Langmuir, 1995, 11, 4519-4531.	1.6	117
16	Dephosphorylation of Threonine 38 Is Required for Nuclear Translocation and Activation of Human Xenobiotic Receptor CAR (NR1I3). Journal of Biological Chemistry, 2009, 284, 34785-34792.	1.6	117
17	Dynamics of ion solvation in a Stockmayer fluid. Journal of Chemical Physics, 1992, 96, 3092-3101.	1.2	104
18	The solvation of Clâ^', Brâ^', and Iâ^' in acetonitrile clusters: Photoelectron spectroscopy and molecular dynamics simulations. Journal of Chemical Physics, 1996, 105, 2675-2685.	1.2	103

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19	Stabilization energies of Clâ¯, Brâ¯, and Iâ¯ ions in water clusters. Journal of Chemical Physics, 1993, 99, 4222-4224.	1.2	100
20	Spectral shifts and structural classes in microsolutions of rare gas clusters containing a molecular chromophore. Journal of Chemical Physics, 1990, 93, 4884-4897.	1.2	95
21	Cryo-EM structures of the SARS-CoV-2 endoribonuclease Nsp15 reveal insight into nuclease specificity and dynamics. Nature Communications, 2021, 12, 636.	5.8	80
22	Charge localization in negative ion dynamics: Effect on caging of Brâ¯2 in Arn and (CO2)n clusters. Journal of Chemical Physics, 1989, 90, 7354-7368.	1.2	79
23	Surface solvation for an ion in a water cluster. Journal of Chemical Physics, 2005, 122, 024513.	1.2	78
24	Characterization of Estrogenic and Androgenic Activities for Bisphenol A-like Chemicals (BPs): In Vitro Estrogen and Androgen Receptors Transcriptional Activation, Gene Regulation, and Binding Profiles. Toxicological Sciences, 2019, 172, 23-37.	1.4	76
25	Differential in Vitro Biological Action, Coregulator Interactions, and Molecular Dynamic Analysis of Bisphenol A (BPA), BPAF, and BPS Ligandâ€“ERÎ± Complexes. Environmental Health Perspectives, 2018, 126, 017012.	2.8	74
26	Structure and Dynamics of Zymogen Human Blood Coagulation Factor X. Biophysical Journal, 2002, 82, 1190-1206.	0.2	73
27	GATA3 zinc finger 2 mutations reprogram the breast cancer transcriptional network. Nature Communications, 2018, 9, 1059.	5.8	72
28	Role of Water in the Hydration Force Acting between Lipid Bilayers. Langmuir, 1996, 12, 2625-2629.	1.6	71
29	Serological, genomic and structural analyses of the major mite allergen Der p 23. Clinical and Experimental Allergy, 2016, 46, 365-376.	1.4	69
30	Enthalpies of formation and stabilization energies of Brâ¯ (H2O)n (n=1,2, â€¦, 15) clusters. Comparisons between molecular dynamics computer simulations and experiment. Chemical Physics Letters, 1994, 218, 377-382.	1.2	65
31	Reaction Mechanism of the Îµ Subunit of E. coli DNA Polymerase III: Insights into Active Site Metal Coordination and Catalytically Significant Residues. Journal of the American Chemical Society, 2009, 131, 1550-1556.	6.6	64
32	Cube to cage transitions in (H2O)n (n=12, 16, and 20). Journal of Chemical Physics, 1996, 105, 3715-3721.	1.2	63
33	Solution Structure of the Dickerson DNA Dodecamer Containing a Single Ribonucleotide. Biochemistry, 2012, 51, 2407-2416.	1.2	56
34	An Ancient Family of RNA-Binding Proteins: Still Important!. Trends in Biochemical Sciences, 2017, 42, 285-296.	3.7	55
35	The structure of water at platinum/water interfaces Molecular dynamics computer simulations. Surface Science, 1995, 335, 401-415.	0.8	54
36	Simple formulas for improved pointâ€charge electrostatics in classical force fields and hybrid quantum mechanical/molecular mechanical embedding. International Journal of Quantum Chemistry, 2008, 108, 1905-1912.	1.0	53

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37	Catalytic mechanism of human DNA polymerase Î» with Mg2+ and Mn2+ from ab initio quantum mechanical/molecular mechanical studies. DNA Repair, 2008, 7, 1824-1834.	1.3	52
38	Template strand scrunching during DNA gap repair synthesis by human polymerase Î». Nature Structural and Molecular Biology, 2009, 16, 967-972.	3.6	49
39	Requirement for transient metal ions revealed through computational analysis for DNA polymerase going in reverse. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E5228-36.	3.3	49
40	Molecular Insights into DNA Polymerase Deterrents for Ribonucleotide Insertion. Journal of Biological Chemistry, 2011, 286, 31650-31660.	1.6	45
41	Binding of 5-phospho-D-arabinonohydroxamate and 5-phospho-D-arabinonate inhibitors to zinc phosphomannose isomerase fromCandida albicans studied by polarizable molecular mechanics and quantum mechanics. Journal of Computational Chemistry, 2007, 28, 938-957.	1.5	44
42	Binding of bisphenol A, bisphenol AF, and bisphenol S on the androgen receptor: Coregulator recruitment and stimulation of potential interaction sites. Toxicology in Vitro, 2017, 44, 287-302.	1.1	44
43	Characterization of SARS2 Nsp15 nuclease activity reveals it's mad about U. Nucleic Acids Research, 2021, 49, 10136-10149.	6.5	44
44	Amino Acid Substitution in the Active Site of DNA Polymerase Î² Explains the Energy Barrier of the Nucleotidyl Transfer Reaction. Journal of the American Chemical Society, 2013, 135, 8078-8088.	6.6	40
45	Thermally Induced Structural Changes in F-(H2O)11and Cl-(H2O)11Clusters:Â Molecular Dynamics Computer Simulations. The Journal of Physical Chemistry, 1996, 100, 1350-1356.	2.9	39
46	Molecular Mechanism of Substrate Specificity for Heparan Sulfate 2-O-Sulfotransferase. Journal of Biological Chemistry, 2014, 289, 13407-13418.	1.6	39
47	Phylogenetic Distribution and Evolution of the Linked RNA-Binding and NOT1-Binding Domains in the Tristetraprolin Family of Tandem CCCH Zinc Finger Proteins. Journal of Interferon and Cytokine Research, 2014, 34, 297-306.	0.5	38
48	Energetics and structure in I 2 ? (CO2) n clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1991, 20, 173-175.	1.0	37
49	Ultrafast solvation dynamics in a Stockmayer fluid. Journal of Chemical Physics, 1992, 97, 5253-5254.	1.2	35
50	Conformational dependence of 13C shielding and coupling constants for methionine methyl groups. Journal of Biomolecular NMR, 2010, 48, 31-47.	1.6	35
51	Free energy profiles for lithium(1+) and iodide ions approaching the platinum(100) surface: a molecular dynamics study. The Journal of Physical Chemistry, 1993, 97, 13803-13806.	2.9	33
52	Mitochondrial single-stranded DNA binding protein novel de novo SSBP1 mutation in a child with single large-scale mtDNA deletion (SLSMD) clinically manifesting as Pearson, Kearns-Sayre, and Leigh syndromes. PLoS ONE, 2019, 14, e0221829.	1.1	32
53	Modeling Zymogen Protein C. Biophysical Journal, 2000, 79, 2925-2943.	0.2	31
54	Phosphorylated Nuclear Receptor CAR Forms a Homodimer To Repress Its Constitutive Activity for Ligand Activation. Molecular and Cellular Biology, 2017, 37, .	1.1	31

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55	Cooperative damage recognition by UvrA and UvrB: Identification of UvrA residues that mediate DNA binding. DNA Repair, 2008, 7, 392-404.	1.3	29
56	Molecular mechanisms for the regulation of histone mRNA stem-loopâ€“binding protein by phosphorylation. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E2937-46.	3.3	29
57	Largazole Analogues Embodying Radical Changes in the Depsipeptide Ring: Development of a More Selective and Highly Potent Analogue. Journal of Medicinal Chemistry, 2016, 59, 10642-10660.	2.9	29
58	Engineering of betabellinâ€15d: A 64 residue beta sheet protein that forms long narrow multimeric fibrils. Protein Science, 1998, 7, 1545-1554.	3.1	28
59	An all-atom solution-equilibrated model for human extrinsic blood coagulation complex (sTF-VIIa-Xa): a protein-protein docking and molecular dynamics refinement study. Journal of Thrombosis and Haemostasis, 2003, 1, 2577-2588.	1.9	27
60	Proposed structural models of human factor Va and prothrombinase. Journal of Thrombosis and Haemostasis, 2008, 6, 83-89.	1.9	27
61	Revealing the role of the product metal in DNA polymerase Î² catalysis. Nucleic Acids Research, 2017, 45, gkw1363.	6.5	27
62	Mobility of stretched water. Journal of Chemical Physics, 1993, 98, 9859-9862.	1.2	25
63	A finite field method for calculating molecular polarizability tensors for arbitrary multipole rank. Journal of Computational Chemistry, 2011, 32, 3283-3295.	1.5	24
64	Reversal of DNA damage induced Topoisomerase 2 DNAâ€“protein crosslinks by Tdp2. Nucleic Acids Research, 2016, 44, 3829-3844.	6.5	23
65	Identification of the effector domain of biglycan that facilitates BMP-2 osteogenic function. Scientific Reports, 2018, 8, 7022.	1.6	23
66	Ion solvation in water clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 166-168.	1.0	22
67	Modeling Human Zymogen Factor IX. Thrombosis and Haemostasis, 2001, 85, 596-603.	1.8	22
68	Determining the endocrine disruption potential of industrial chemicals using an integrative approach: Public databases, in vitro exposure, and modeling receptor interactions. Environment International, 2019, 131, 104969.	4.8	22
69	Heparan Sulfate Biosynthesis: A Theoretical Study of the Initial Sulfation Step by N-Deacetylase/N-Sulfotransferase. Biophysical Journal, 2000, 79, 2909-2917.	0.2	21
70	Four loops of the catalytic domain of factor VIIa mediate the effect of the first EGF-like domain substitution on factor VIIa catalytic activity11Edited by R. Huber. Journal of Molecular Biology, 2001, 307, 1503-1517.	2.0	20
71	The discovery of new coding alleles of human CYP26A1 that are potentially defective in the metabolism of all-trans retinoic acid and their assessment in a recombinant cDNA expression system. Pharmacogenetics and Genomics, 2007, 17, 169-180.	0.7	20
72	Transâ^'CisIsomerization of Proline 22 in Bovine Prothrombin Fragment 1:Â A Surprising Result of Structural Characterizationâ€. Biochemistry, 1998, 37, 10920-10927.	1.2	19

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73	Reversal of drug resistance by JS-K and nitric oxide in ABCB1- and ABCG2-expressing multi-drug resistant human tumor cells. Biomedicine and Pharmacotherapy, 2019, 120, 109468.	2.5	19
74	Asymmetric conformational maturation of HIV-1 reverse transcriptase. ELife, 2015, 4, .	2.8	19
75	Atomic forces for geometryâ€dependent point multipole and Gaussian multipole models. Journal of Computational Chemistry, 2010, 31, 2702-2713.	1.5	18
76	Genomic, RNAseq, and Molecular Modeling Evidence Suggests That the Major Allergen Domain in Insects Evolved from a Homodimeric Origin. Genome Biology and Evolution, 2013, 5, 2344-2358.	1.1	18
77	Mutational and Structural Analysis of the Tandem Zinc Finger Domain of Tristetraprolin. Journal of Biological Chemistry, 2014, 289, 565-580.	1.6	18
78	The tandem zinc finger RNA binding domain of members of the tristetraprolin protein family. Wiley Interdisciplinary Reviews RNA, 2019, 10, e1531.	3.2	17
79	Unusual Fragmentation Pathways in Collagen Glycopeptides. Journal of the American Society for Mass Spectrometry, 2013, 24, 1072-1081.	1.2	16
80	The Drosophila Tis11 Protein and Its Effects on mRNA Expression in Flies. Journal of Biological Chemistry, 2014, 289, 35042-35060.	1.6	16
81	Synthesis and biological evaluation of largazole analogues with modified surface recognition cap groups. European Journal of Medicinal Chemistry, 2014, 86, 528-541.	2.6	16
82	Predicted solution structure of zymogen human coagulation FVII. Journal of Computational Chemistry, 2002, 23, 35-47.	1.5	15
83	HPAM: Hirshfeld partitioned atomic multipoles. Computer Physics Communications, 2012, 183, 390-397.	3.0	15
84	Functional Equivalence of an Evolutionarily Conserved RNA Binding Module. Journal of Biological Chemistry, 2015, 290, 24413-24423.	1.6	15
85	Explicit Water Near the Catalytic I Helix Thr in the Predicted Solution Structure of CYP2A4. Biophysical Journal, 2003, 84, 57-68.	0.2	14
86	Binuclear manganese(II) complexes in biological systems. Molecular Physics, 2007, 105, 2893-2898.	0.8	14
87	Hydrophobic ligands influence the structure, stability, and processing of the major cockroach allergen Bla g 1. Scientific Reports, 2019, 9, 18294.	1.6	14
88	Probing the Structural Changes in the Light Chain of Human Coagulation Factor VIIa Due to Tissue Factor Association. Biophysical Journal, 1999, 77, 99-113.	0.2	13
89	Total Synthesis and Selective Activity of a New Class of Conformationally Restrained Epothilones. Chemistry - A European Journal, 2008, 14, 570-581.	1.7	13
90	Transmembrane Domain Interactions and Residue Proline 378 Are Essential for Proper Structure, Especially Disulfide Bond Formation, in the Human Vitamin K-Dependent Î³-Glutamyl Carboxylase. Biochemistry, 2008, 47, 6301-6310.	1.2	13

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91	Modeling of the DNA-binding site of yeast Pms1 by mass spectrometry. DNA Repair, 2011, 10, 454-465.	1.3	13
92	The mosquito protein AEG12 displays both cytolytic and antiviral properties via a common lipid transfer mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	13
93	What causes the enhancement of activity of factor VIIa by tissue factor?. Journal of Thrombosis and Haemostasis, 2006, 4, 2726-2729.	1.9	11
94	Ligand induced dissociation of the AR homodimer precedes AR monomer translocation to the nucleus. Scientific Reports, 2019, 9, 16734.	1.6	11
95	A proposed structural model of human protein Z. Journal of Thrombosis and Haemostasis, 2007, 5, 1558-1561.	1.9	10
96	Hiding in Plain Sight: The Bimetallic Magnesium Covalent Bond in Enzyme Active Sites. Inorganic Chemistry, 2017, 56, 313-320.	1.9	10
97	Structural basis for proficient oxidized ribonucleotide insertion in double strand break repair. Nature Communications, 2021, 12, 5055.	5.8	10
98	NCX-4040, a Unique Nitric Oxide Donor, Induces Reversal of Drug-Resistance in Both ABCB1- and ABCG2-Expressing Multidrug Human Cancer Cells. Cancers, 2021, 13, 1680.	1.7	9
99	Structural Characterization of the Conformational Change in Calbindin-D28k upon Calcium Binding Using Differential Surface Modification Analyzed by Mass Spectrometry. Biochemistry, 2009, 48, 8603-8614.	1.2	8
100	Probing Dominant Negative Behavior of Glucocorticoid Receptor Î² through a Hybrid Structural and Biochemical Approach. Molecular and Cellular Biology, 2018, 38, .	1.1	8
101	A ubiquitin-like domain is required for stabilizing the N-terminal ATPase module of human SMCHD1. Communications Biology, 2019, 2, 255.	2.0	8
102	Identification of drivers for the metamorphic transition of HIV-1 reverse transcriptase. Biochemical Journal, 2017, 474, 3321-3338.	1.7	7
103	A Bioactive Resveratrol Trimer from the Stem Bark of the Sri Lankan Endemic Plant Vateria copallifera. Journal of Natural Products, 2018, 81, 1693-1700.	1.5	7
104	ESR1 Mutations Associated With Estrogen Insensitivity Syndrome Change Conformation of Ligand-Receptor Complex and Altered Transcriptome Profile. Endocrinology, 2020, 161, .	1.4	7
105	Phosphopeptide interactions of the Nbs1 N-terminal FHA-BRCT1/2 domains. Scientific Reports, 2021, 11, 9046.	1.6	7
106	Probing the mechanisms of two exonuclease domain mutators of DNA polymerase Ïµ. Nucleic Acids Research, 2022, 50, 962-974.	6.5	7
107	A structural exposÃ© of noncanonical molecular reactivity within the protein tyrosine phosphatase WPD loop. Nature Communications, 2022, 13, 2231.	5.8	7
108	Computational study of the putative active form of protein Z (PZa): Sequence design and structural modeling. Protein Science, 2008, 17, 1354-1361.	3.1	6

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109	Characterization of an anti-Bla g 1 scFv: Epitope mapping and cross-reactivity. Molecular Immunology, 2014, 59, 200-207.	1.0	6
110	A new class of cytotoxic agents targets tubulin and disrupts microtubule dynamics. Bioorganic Chemistry, 2021, 116, 105297.	2.0	6
111	A reconsideration of the evidence for structural reorganization in FVII zymogen. Journal of Thrombosis and Haemostasis, 2005, 3, 1543-1545.	1.9	5
112	Applications of Quantum Mechanical/Molecular Mechanical Methods to the Chemical Insertion Step of DNA and RNA Polymerization. Advances in Protein Chemistry and Structural Biology, 2014, 97, 83-113.	1.0	5
113	Mechanisms of SSBP1 variants in mitochondrial disease: Molecular dynamics simulations reveal stable tetramers with altered DNA binding surfaces. DNA Repair, 2021, 107, 103212.	1.3	4
114	A post-transcriptional regulon controlled by TtpA, the single tristetraprolin family member expressed in Dictyostelium discoideum. Nucleic Acids Research, 2021, 49, 11920-11937.	6.5	3
115	Pharmacophore optimization of imidazole chalcones to modulate microtubule dynamics. Bioorganic Chemistry, 2022, 122, 105700.	2.0	3
116	Influence of Hydrophobic Cargo Binding on the Structure, Stability, and Allergenicity of the Cockroach Allergen Bla g 1. Journal of Allergy and Clinical Immunology, 2019, 143, AB213.	1.5	2
117	Molecular Dynamics Computer Simulations of Aqueous Solution/Platinum Interface. , 1994, , 101-118.		1
118	Structural, Serological, and Genomic Analyses of the Major Mite Allergen Der p 23. Journal of Allergy and Clinical Immunology, 2016, 137, AB267.	1.5	1
119	A smooth particle mesh Ewald method. , 0, .		1
120	Early Unfolding Response of a Stable Protein Domain to Environmental Changesâ€. Journal of Physical Chemistry A, 2004, 108, 9834-9840.	1.1	0
121	Preferential DNA Polymerase Î² Reverse Reaction with Imidodiphosphate. ACS Omega, 2020, 5, 15317-15324.	1.6	0
122	Solvation Dynamics in a Stockmayer Fluid. , 1993, , 461-483.		0
123	Abstract 964: GATA3 modulates chromatin structure to establish active enhancers in breast cancer cells. , 2015, , .		0
124	SAT-205 ESR1 Q375H and R394H Mutants Associated with Estrogen Insensitivity Syndrome Mediate Genome-Wide Genetic and Epigenetic Aberrances. Journal of the Endocrine Society, 2019, 3, .	0.1	0
125	Structural and functional consequences of SMCHD1 mutations associated with arhinia and muscular dystrophy. FASEB Journal, 2019, 33, 493.5.	0.2	0