Lalith Perera

List of Publications by Year
in descending order

125 papers	24,371 citations	71102 41 h-index	19190 118 g-index
131 all docs	131 docs citations	131 times ranked	25582 citing authors

#	Article	IF	Citations
1	Probing the mechanisms of two exonuclease domain mutators of DNA polymerase Ïµ. Nucleic Acids Research, 2022, 50, 962-974.	14.5	7
2	Pharmacophore optimization of imidazole chalcones to modulate microtubule dynamics. Bioorganic Chemistry, 2022, 122, 105700.	4.1	3
3	A structural exposÃ© of noncanonical molecular reactivity within the protein tyrosine phosphatase WPD loop. Nature Communications, 2022, 13, 2231.	12.8	7
4	Potential SARS-CoV-2 main protease inhibitors. Drug Discovery Today, 2021, 26, 804-816.	6.4	128
5	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, .	7.1	13
6	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.	3.7	9
7	Phosphopeptide interactions of the Nbs1 N-terminal FHA-BRCT1/2 domains. Scientific Reports, 2021, 11, 9046.	3.3	7
8	Structural basis for proficient oxidized ribonucleotide insertion in double strand break repair. Nature Communications, 2021, 12, 5055.	12.8	10
9	Characterization of SARS2 Nsp15 nuclease activity reveals it's mad about U. Nucleic Acids Research, 2021, 49, 10136-10149.	14.5	44
10	A new class of cytotoxic agents targets tubulin and disrupts microtubule dynamics. Bioorganic Chemistry, 2021, 116, 105297.	4.1	6
11	Mechanisms of SSBP1 variants in mitochondrial disease: Molecular dynamics simulations reveal stable tetramers with altered DNA binding surfaces. DNA Repair, 2021, 107, 103212.	2.8	4
12	Cryo-EM structures of the SARS-CoV-2 endoribonuclease Nsp15 reveal insight into nuclease specificity and dynamics. Nature Communications, 2021, 12, 636.	12.8	80
13	A post-transcriptional regulon controlled by TtpA, the single tristetraprolin family member expressed in Dictyostelium discoideum. Nucleic Acids Research, 2021, 49, 11920-11937.	14.5	3
14	Preferential DNA Polymerase Î² Reverse Reaction with Imidodiphosphate. ACS Omega, 2020, 5, 15317-15324.	3.5	0
15	ESR1 Mutations Associated With Estrogen Insensitivity Syndrome Change Conformation of Ligand-Receptor Complex and Altered Transcriptome Profile. Endocrinology, 2020, 161, .	2.8	7
16	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.	3.1	76
17	A ubiquitin-like domain is required for stabilizing the N-terminal ATPase module of human SMCHD1. Communications Biology, 2019, 2, 255.	4.4	8
18	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.	10.0	22

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19	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.	5.6	19
20	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.	2.5	32
21	The tandem zinc finger RNA binding domain of members of the tristetraprolin protein family. Wiley Interdisciplinary Reviews RNA, 2019, 10, e1531.	6.4	17
22	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.	2.9	2
23	Hydrophobic ligands influence the structure, stability, and processing of the major cockroach allergen Bla g 1. Scientific Reports, 2019, 9, 18294.	3.3	14
24	Ligand induced dissociation of the AR homodimer precedes AR monomer translocation to the nucleus. Scientific Reports, 2019, 9, 16734.	3.3	11
25	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, .	0.2	0
26	Structural and functional consequences of SMCHD1 mutations associated with arhinia and muscular dystrophy. FASEB Journal, 2019, 33, 493.5.	0.5	0
27	Probing Dominant Negative Behavior of Glucocorticoid Receptor Î² through a Hybrid Structural and Biochemical Approach. Molecular and Cellular Biology, 2018, 38, .	2.3	8
28	GATA3 zinc finger 2 mutations reprogram the breast cancer transcriptional network. Nature Communications, 2018, 9, 1059.	12.8	72
29	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.	6.0	74
30	A Bioactive Resveratrol Trimer from the Stem Bark of the Sri Lankan Endemic Plant Vateria copallifera. Journal of Natural Products, 2018, 81, 1693-1700.	3.0	7
31	Identification of the effector domain of biglycan that facilitates BMP-2 osteogenic function. Scientific Reports, 2018, 8, 7022.	3.3	23
32	An Ancient Family of RNA-Binding Proteins: Still Important!. Trends in Biochemical Sciences, 2017, 42, 285-296.	7.5	55
33	Phosphorylated Nuclear Receptor CAR Forms a Homodimer To Repress Its Constitutive Activity for Ligand Activation. Molecular and Cellular Biology, 2017, 37, .	2.3	31
34	Hiding in Plain Sight: The Bimetallic Magnesium Covalent Bond in Enzyme Active Sites. Inorganic Chemistry, 2017, 56, 313-320.	4.0	10
35	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.	2.4	44
36	Identification of drivers for the metamorphic transition of HIV-1 reverse transcriptase. Biochemical Journal, 2017, 474, 3321-3338.	3.7	7

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37	Revealing the role of the product metal in DNA polymerase Î² catalysis. Nucleic Acids Research, 2017, 45, gkw1363.	14.5	27
38	Serological, genomic and structural analyses of the major mite allergen Der p 23. Clinical and Experimental Allergy, 2016, 46, 365-376.	2.9	69
39	GATA3-dependent cellular reprogramming requires activation-domain dependent recruitment of a chromatin remodeler. Genome Biology, 2016, 17, 36.	8.8	121
40	Structural, Serological, and Genomic Analyses of the Major Mite Allergen Der p 23. Journal of Allergy and Clinical Immunology, 2016, 137, AB267.	2.9	1
41	Reversal of DNA damage induced Topoisomerase 2 DNAâ€“protein crosslinks by Tdp2. Nucleic Acids Research, 2016, 44, 3829-3844.	14.5	23
42	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.	6.4	29
43	Functional Equivalence of an Evolutionarily Conserved RNA Binding Module. Journal of Biological Chemistry, 2015, 290, 24413-24423.	3.4	15
44	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.	7.1	49
45	Uncovering the polymerase-induced cytotoxicity of an oxidized nucleotide. Nature, 2015, 517, 635-639.	27.8	133
46	Asymmetric conformational maturation of HIV-1 reverse transcriptase. ELife, 2015, 4, .	6.0	19
47	Abstract 964: GATA3 modulates chromatin structure to establish active enhancers in breast cancer cells. , 2015, , .		0
48	The Drosophila Tis11 Protein and Its Effects on mRNA Expression in Flies. Journal of Biological Chemistry, 2014, 289, 35042-35060.	3.4	16
49	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.	7.1	29
50	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.	2.3	5
51	Characterization of an anti-Bla g 1 scFv: Epitope mapping and cross-reactivity. Molecular Immunology, 2014, 59, 200-207.	2.2	6
52	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.	1.2	38
53	Mutational and Structural Analysis of the Tandem Zinc Finger Domain of Tristetraprolin. Journal of Biological Chemistry, 2014, 289, 565-580.	3.4	18
54	Synthesis and biological evaluation of largazole analogues with modified surface recognition cap groups. European Journal of Medicinal Chemistry, 2014, 86, 528-541.	5.5	16

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55	Molecular Mechanism of Substrate Specificity for Heparan Sulfate 2-O-Sulfotransferase. Journal of Biological Chemistry, 2014, 289, 13407-13418.	3.4	39
56	Unusual Fragmentation Pathways in Collagen Glycopeptides. Journal of the American Society for Mass Spectrometry, 2013, 24, 1072-1081.	2.8	16
57	Phenobarbital Indirectly Activates the Constitutive Active Androstane Receptor (CAR) by Inhibition of Epidermal Growth Factor Receptor Signaling. Science Signaling, 2013, 6, ra31.	3.6	163
58	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.	13.7	40
59	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.	2.5	18
60	Solution Structure of the Dickerson DNA Dodecamer Containing a Single Ribonucleotide. Biochemistry, 2012, 51, 2407-2416.	2.5	56
61	HPAM: Hirshfeld partitioned atomic multipoles. Computer Physics Communications, 2012, 183, 390-397.	7.5	15
62	Modeling of the DNA-binding site of yeast Pms1 by mass spectrometry. DNA Repair, 2011, 10, 454-465.	2.8	13
63	A finite field method for calculating molecular polarizability tensors for arbitrary multipole rank. Journal of Computational Chemistry, 2011, 32, 3283-3295.	3.3	24
64	Molecular Insights into DNA Polymerase Deterrents for Ribonucleotide Insertion. Journal of Biological Chemistry, 2011, 286, 31650-31660.	3.4	45
65	Conformational dependence of 13C shielding and coupling constants for methionine methyl groups. Journal of Biomolecular NMR, 2010, 48, 31-47.	2.8	35
66	Atomic forces for geometryâ€dependent point multipole and Gaussian multipole models. Journal of Computational Chemistry, 2010, 31, 2702-2713.	3.3	18
67	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.	3.4	117
68	Template strand scrunching during DNA gap repair synthesis by human polymerase Î». Nature Structural and Molecular Biology, 2009, 16, 967-972.	8.2	49
69	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.	13.7	64
70	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.	2.5	8
71	Proposed structural models of human factor Va and prothrombinase. Journal of Thrombosis and Haemostasis, 2008, 6, 83-89.	3.8	27
72	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.	2.0	53

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73	Total Synthesis and Selective Activity of a New Class of Conformationally Restrained Epothilones. Chemistry - A European Journal, 2008, 14, 570-581.	3.3	13
74	Computational study of the putative active form of protein Z (PZa): Sequence design and structural modeling. Protein Science, 2008, 17, 1354-1361.	7.6	6
75	Cooperative damage recognition by UvrA and UvrB: Identification of UvrA residues that mediate DNA binding. DNA Repair, 2008, 7, 392-404.	2.8	29
76	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.	2.8	52
77	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.	2.5	13
78	Plasminogen Alleles Influence Susceptibility to Invasive Aspergillosis. PLoS Genetics, 2008, 4, e1000101.	3.5	145
79	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.	1.5	20
80	Binuclear manganese(II) complexes in biological systems. Molecular Physics, 2007, 105, 2893-2898.	1.7	14
81	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.	3.3	44
82	A proposed structural model of human protein Z. Journal of Thrombosis and Haemostasis, 2007, 5, 1558-1561.	3.8	10
83	What causes the enhancement of activity of factor VIIa by tissue factor?. Journal of Thrombosis and Haemostasis, 2006, 4, 2726-2729.	3.8	11
84	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.	3.0	169
85	A reconsideration of the evidence for structural reorganization in FVII zymogen. Journal of Thrombosis and Haemostasis, 2005, 3, 1543-1545.	3.8	5
86	Surface solvation for an ion in a water cluster. Journal of Chemical Physics, 2005, 122, 024513.	3.0	78
87	Early Unfolding Response of a Stable Protein Domain to Environmental Changesâ€. Journal of Physical Chemistry A, 2004, 108, 9834-9840.	2.5	0
88	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.	3.8	27
89	Explicit Water Near the Catalytic I Helix Thr in the Predicted Solution Structure of CYP2A4. Biophysical Journal, 2003, 84, 57-68.	0.5	14
90	Molecular Dynamics Simulations of Sodium Dodecyl Sulfate Micelle in Water:â€‰ The Behavior of Water. Journal of Physical Chemistry B, 2002, 106, 10902-10907.	2.6	173

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91	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.	2.6	334
92	Structure and Dynamics of Zymogen Human Blood Coagulation Factor X. Biophysical Journal, 2002, 82, 1190-1206.	0.5	73
93	Predicted solution structure of zymogen human coagulation FVII. Journal of Computational Chemistry, 2002, 23, 35-47.	3.3	15
94	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.	4.2	20
95	Modeling Human Zymogen Factor IX. Thrombosis and Haemostasis, 2001, 85, 596-603.	3.4	22
96	Heparan Sulfate Biosynthesis: A Theoretical Study of the Initial Sulfation Step by N-Deacetylase/N-Sulfotransferase. Biophysical Journal, 2000, 79, 2909-2917.	0.5	21
97	Modeling Zymogen Protein C. Biophysical Journal, 2000, 79, 2925-2943.	0.5	31
98	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.	3.3	571
99	Probing the Structural Changes in the Light Chain of Human Coagulation Factor VIIa Due to Tissue Factor Association. Biophysical Journal, 1999, 77, 99-113.	0.5	13
100	Engineering of betabellinâ€15d: A 64 residue beta sheet protein that forms long narrow multimeric fibrils. Protein Science, 1998, 7, 1545-1554.	7.6	28
101	Transâ^'Cisisomerization of Proline 22 in Bovine Prothrombin Fragment 1:Â A Surprising Result of Structural Characterizationâ€. Biochemistry, 1998, 37, 10920-10927.	2.5	19
102	Role of Water in the Hydration Force Acting between Lipid Bilayers. Langmuir, 1996, 12, 2625-2629.	3.5	71
103	The solvation of Clâ^', Brâ^', and Iâ^' in acetonitrile clusters: Photoelectron spectroscopy and molecular dynamics simulations. Journal of Chemical Physics, 1996, 105, 2675-2685.	3.0	103
104	Cube to cage transitions in (H2O)n (n=12, 16, and 20). Journal of Chemical Physics, 1996, 105, 3715-3721.	3.0	63
105	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
106	Effect of the treatment of longâ€range forces on the dynamics of ions in aqueous solutions. Journal of Chemical Physics, 1995, 102, 450-456.	3.0	148
107	The structure of water at platinum/water interfaces Molecular dynamics computer simulations. Surface Science, 1995, 335, 401-415.	1.9	54
108	A smooth particle mesh Ewald method. Journal of Chemical Physics, 1995, 103, 8577-8593.	3.0	18,266

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109	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.	3.5	117
110	Molecular Dynamics Computer Simulations of Aqueous Solution/Platinum Interface. , 1994, , 101-118.		1
111	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.	3.0	154
112	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.	2.6	65
113	Ion solvation in water clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 166-168.	1.0	22
114	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
115	Mobility of stretched water. Journal of Chemical Physics, 1993, 98, 9859-9862.	3.0	25
116	Stabilization energies of Clâ^', Brâ^', and Iâ^' ions in water clusters. Journal of Chemical Physics, 1993, 99, 4222-4224.	3.0	100
117	Solvation Dynamics in a Stockmayer Fluid. , 1993, , 461-483.		0
118	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.	3.0	118
119	Dynamics of ion solvation in a Stockmayer fluid. Journal of Chemical Physics, 1992, 96, 3092-3101.	3.0	104
120	Ultrafast solvation dynamics in a Stockmayer fluid. Journal of Chemical Physics, 1992, 97, 5253-5254.	3.0	35
121	Manyâ€body effects in molecular dynamics simulations of Na+(H2O)n and Clâ^'(H2O)n clusters. Journal of Chemical Physics, 1991, 95, 1954-1963.	3.0	322
122	Energetics and structure in I 2 ? (CO2) n clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1991, 20, 173-175.	1.0	37
123	Spectral shifts and structural classes in microsolutions of rare gas clusters containing a molecular chromophore. Journal of Chemical Physics, 1990, 93, 4884-4897.	3.0	95
124	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.	3.0	79
125	A smooth particle mesh Ewald method. , 0, .		1