Lalith Perera

List of Publications by Year in Descending Order

125 papers	19,738 citations	39 h-index	131 g-index
131 ext. papers	22,356 ext. citations	6.8 avg, IF	6.23 L-index

#	Paper	IF	Citations
125	Pharmacophore optimization of imidazole chalcones to modulate microtubule dynamics.. *Bioorganic Chemistry*, **2022**, 122, 105700	5.1	
124	A structural expos□of noncanonical molecular reactivity within the protein tyrosine phosphatase WPD loop.. *Nature Communications*, **2022**, 13, 2231	17.4	0
123	A post-transcriptional regulon controlled by TtpA, the single tristetraprolin family member expressed in Dictyostelium discoideum. *Nucleic Acids Research*, **2021**, 49, 11920-11937	20.1	2
122	The humanized nanobody RBD-1-2G tolerates the spike N501Y mutation to neutralize SARS-CoV-2 **2021**,		1
121	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,	11.5	3
120	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,	6.6	2
119	Phosphopeptide interactions of the Nbs1 N-terminal FHA-BRCT1/2 domains. *Scientific Reports*, **2021**, 11, 9046	4.9	2
118	Potential SARS-CoV-2 main protease inhibitors. *Drug Discovery Today*, **2021**, 26, 804-816	8.8	52
117	Structural basis for proficient oxidized ribonucleotide insertion in double strand break repair. *Nature Communications*, **2021**, 12, 5055	17.4	0
116	Characterization of SARS2 Nsp15 nuclease activity reveals it's mad about U. *Nucleic Acids Research*, **2021**, 49, 10136-10149	20.1	8
115	A new class of cytotoxic agents targets tubulin and disrupts microtubule dynamics. *Bioorganic Chemistry*, **2021**, 116, 105297	5.1	1
114	Mechanisms of SSBP1 variants in mitochondrial disease: Molecular dynamics simulations reveal stable tetramers with altered DNA binding surfaces. *DNA Repair*, **2021**, 107, 103212	4.3	2
113	Cryo-EM structures of the SARS-CoV-2 endoribonuclease Nsp15 reveal insight into nuclease specificity and dynamics. *Nature Communications*, **2021**, 12, 636	17.4	28
112	Preferential DNA Polymerase ‡Reverse Reaction with Imidodiphosphate. *ACS Omega*, **2020**, 5, 15317-15324	3.7	
111	Cryo-EM Structures of the SARS-CoV-2 Endoribonuclease Nsp15 **2020**,		2
110	ESR1 Mutations Associated With Estrogen Insensitivity Syndrome Change Conformation of Ligand-Receptor Complex and Altered Transcriptome Profile. *Endocrinology*, **2020**, 161,	4.8	4
109	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	3.7	23

108	The tandem zinc finger RNA binding domain of members of the tristetraprolin protein family. *Wiley Interdisciplinary Reviews RNA*, **2019**, 10, e1531	9.3	10
107	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	11.5	2
106	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**,	4.4	36
105	A ubiquitin-like domain is required for stabilizing the N-terminal ATPase module of human SMCHD1. *Communications Biology*, **2019**, 2, 255	6.7	6
104	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	12.9	13
103	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	7.5	11
102	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,	0.4	78
101	Structural and functional consequences of SMCHD1 mutations associated with arhinia and muscular dystrophy. *FASEB Journal*, **2019**, 33, 493.5	0.9	
100	Hydrophobic ligands influence the structure, stability, and processing of the major cockroach allergen Bla g 1. *Scientific Reports*, **2019**, 9, 18294	4.9	6
99	Ligand induced dissociation of the AR homodimer precedes AR monomer translocation to the nucleus. *Scientific Reports*, **2019**, 9, 16734	4.9	7
98	Probing Dominant Negative Behavior of Glucocorticoid Receptor through a Hybrid Structural and Biochemical Approach. *Molecular and Cellular Biology*, **2018**, 38,	4.8	4
97	GATA3 zinc finger 2 mutations reprogram the breast cancer transcriptional network. *Nature Communications*, **2018**, 9, 1059	17.4	45
96	A Bioactive Resveratrol Trimer from the Stem Bark of the Sri Lankan Endemic Plant Vateria copallifera. *Journal of Natural Products*, **2018**, 81, 1693-1700	4.9	5
95	Identification of the effector domain of biglycan that facilitates BMP-2 osteogenic function. *Scientific Reports*, **2018**, 8, 7022	4.9	15
94	Differential Biological Action, Coregulator Interactions, and Molecular Dynamic Analysis of Bisphenol A (BPA), BPAF, and BPS Ligand-ER Complexes. *Environmental Health Perspectives*, **2018**, 126, 017012	8.4	51
93	An Ancient Family of RNA-Binding Proteins: Still Important!. *Trends in Biochemical Sciences*, **2017**, 42, 285-296	10.3	37
92	Phosphorylated Nuclear Receptor CAR Forms a Homodimer To Repress Its Constitutive Activity for Ligand Activation. *Molecular and Cellular Biology*, **2017**, 37,	4.8	25
91	Hiding in Plain Sight: The Bimetallic Magnesium Covalent Bond in Enzyme Active Sites. *Inorganic Chemistry*, **2017**, 56, 313-320	5.1	8

90	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	3.6	31
89	Identification of drivers for the metamorphic transition of HIV-1 reverse transcriptase. *Biochemical Journal*, **2017**, 474, 3321-3338	3.8	5
88	Revealing the role of the product metal in DNA polymerase ╫catalysis. *Nucleic Acids Research*, **2017**, 45, 2736-2745	20.1	22
87	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	8.3	23
86	Serological, genomic and structural analyses of the major mite allergen Der p 23. *Clinical and Experimental Allergy*, **2016**, 46, 365-76	4.1	52
85	GATA3-dependent cellular reprogramming requires activation-domain dependent recruitment of a chromatin remodeler. *Genome Biology*, **2016**, 17, 36	18.3	74
84	Reversal of DNA damage induced Topoisomerase 2 DNA-protein crosslinks by Tdp2. *Nucleic Acids Research*, **2016**, 44, 3829-44	20.1	17
83	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	11.5	44
82	Uncovering the polymerase-induced cytotoxicity of an oxidized nucleotide. *Nature*, **2015**, 517, 635-9	50.4	102
81	Functional equivalence of an evolutionarily conserved RNA binding module. *Journal of Biological Chemistry*, **2015**, 290, 24413-23	5.4	14
80	Asymmetric conformational maturation of HIV-1 reverse transcriptase. *ELife*, **2015**, 4,	8.9	16
79	Characterization of an anti-Bla g 1 scFv: epitope mapping and cross-reactivity. *Molecular Immunology*, **2014**, 59, 200-7	4.3	6
78	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	3.5	30
77	Mutational and structural analysis of the tandem zinc finger domain of tristetraprolin. *Journal of Biological Chemistry*, **2014**, 289, 565-80	5.4	17
76	Synthesis and biological evaluation of largazole analogues with modified surface recognition cap groups. *European Journal of Medicinal Chemistry*, **2014**, 86, 528-41	6.8	13
75	Molecular mechanism of substrate specificity for heparan sulfate 2-O-sulfotransferase. *Journal of Biological Chemistry*, **2014**, 289, 13407-18	5.4	33
74	The Drosophila Tis11 protein and its effects on mRNA expression in flies. *Journal of Biological Chemistry*, **2014**, 289, 35042-60	5.4	14
73	Molecular mechanisms for the regulation of histone mRNA stem-loop-binding protein by phosphorylation. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, E2937-46	11.5	22

72	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	5.3	5
71	Unusual fragmentation pathways in collagen glycopeptides. *Journal of the American Society for Mass Spectrometry*, **2013**, 24, 1072-81	3.5	12
70	Phenobarbital indirectly activates the constitutive active androstane receptor (CAR) by inhibition of epidermal growth factor receptor signaling. *Science Signaling*, **2013**, 6, ra31	8.8	138
69	Amino acid substitution in the active site of DNA polymerase explains the energy barrier of the nucleotidyl transfer reaction. *Journal of the American Chemical Society*, **2013**, 135, 8078-88	16.4	36
68	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, 2344-58	3.9	14
67	HPAM: Hirshfeld Partitioned Atomic Multipoles. *Computer Physics Communications*, **2012**, 183, 390-397	4.2	13
66	Solution structure of the Dickerson DNA dodecamer containing a single ribonucleotide. *Biochemistry*, **2012**, 51, 2407-16	3.2	45
65	Modeling of the DNA-binding site of yeast Pms1 by mass spectrometry. *DNA Repair*, **2011**, 10, 454-65	4.3	11
64	A finite field method for calculating molecular polarizability tensors for arbitrary multipole rank. *Journal of Computational Chemistry*, **2011**, 32, 3283-95	3.5	22
63	Molecular insights into DNA polymerase deterrents for ribonucleotide insertion. *Journal of Biological Chemistry*, **2011**, 286, 31650-60	5.4	38
62	Conformational dependence of 13C shielding and coupling constants for methionine methyl groups. *Journal of Biomolecular NMR*, **2010**, 48, 31-47	3	24
61	Atomic forces for geometry-dependent point multipole and gaussian multipole models. *Journal of Computational Chemistry*, **2010**, 31, 2702-13	3.5	13
60	Dephosphorylation of threonine 38 is required for nuclear translocation and activation of human xenobiotic receptor CAR (NR1I3). *Journal of Biological Chemistry*, **2009**, 284, 34785-92	5.4	102
59	Template strand scrunching during DNA gap repair synthesis by human polymerase lambda. *Nature Structural and Molecular Biology*, **2009**, 16, 967-72	17.6	45
58	Reaction mechanism of the epsilon 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, 1550-6	16.4	52
57	Structural characterization of the conformational change in calbindin-D28k upon calcium binding using differential surface modification analyzed by mass spectrometry. *Biochemistry*, **2009**, 48, 8603-14	3.2	6
56	Cooperative damage recognition by UvrA and UvrB: identification of UvrA residues that mediate DNA binding. *DNA Repair*, **2008**, 7, 392-404	4.3	28
55	Catalytic mechanism of human DNA polymerase lambda with Mg2+ and Mn2+ from ab initio quantum mechanical/molecular mechanical studies. *DNA Repair*, **2008**, 7, 1824-34	4.3	50

54	Transmembrane domain interactions and residue proline 378 are essential for proper structure, especially disulfide bond formation, in the human vitamin K-dependent gamma-glutamyl carboxylase. *Biochemistry*, **2008**, 47, 6301-10	3.2	9
53	Plasminogen alleles influence susceptibility to invasive aspergillosis. *PLoS Genetics*, **2008**, 4, e1000101	6	131
52	Proposed structural models of human factor Va and prothrombinase. *Journal of Thrombosis and Haemostasis*, **2008**, 6, 83-9	15.4	21
51	Simple Formulas for Improved Point-Charge Electrostatics in Classical Force Fields and Hybrid Quantum Mechanical/Molecular Mechanical Embedding. *International Journal of Quantum Chemistry*, **2008**, 108, 1905-1912	2.1	51
50	Total synthesis and selective activity of a new class of conformationally restrained epothilones. *Chemistry - A European Journal*, **2008**, 14, 570-81	4.8	11
49	Computational study of the putative active form of protein Z (PZa): sequence design and structural modeling. *Protein Science*, **2008**, 17, 1354-61	6.3	6
48	Binuclear manganese(II) complexes in biological systems. *Molecular Physics*, **2007**, 105, 2893-2898	1.7	13
47	Binding of 5-phospho-D-arabinonohydroxamate and 5-phospho-D-arabinonate inhibitors to zinc phosphomannose isomerase from Candida albicans studied by polarizable molecular mechanics and quantum mechanics. *Journal of Computational Chemistry*, **2007**, 28, 938-57	3.5	40
46	A proposed structural model of human protein Z. *Journal of Thrombosis and Haemostasis*, **2007**, 5, 1558-61	15.4	9
45	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, 169-80	1.9	19
44	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	3.9	163
43	What causes the enhancement of activity of factor VIIa by tissue factor?. *Journal of Thrombosis and Haemostasis*, **2006**, 4, 2726-9	15.4	11
42	A reconsideration of the evidence for structural reorganization in FVII zymogen. *Journal of Thrombosis and Haemostasis*, **2005**, 3, 1543-5	15.4	5
41	Surface solvation for an ion in a water cluster. *Journal of Chemical Physics*, **2005**, 122, 024513	3.9	74
40	Early Unfolding Response of a Stable Protein Domain to Environmental Changes *Journal of Physical Chemistry A*, **2004**, 108, 9834-9840	2.8	
39	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, 2577-88	15.4	22
38	Explicit water near the catalytic I helix Thr in the predicted solution structure of CYP2A4. *Biophysical Journal*, **2003**, 84, 57-68	2.9	14
37	Predicted solution structure of zymogen human coagulation FVII. *Journal of Computational Chemistry*, **2002**, 23, 35-47	3.5	13

36	Molecular Dynamics Simulations of Sodium Dodecyl Sulfate Micelle in Water: The Behavior of Water. *Journal of Physical Chemistry B*, **2002**, 106, 10902-10907	3.4	161
35	Molecular Dynamics Simulation of Sodium Dodecyl Sulfate Micelle in Water: Micellar Structural Characteristics and Counterion Distribution. *Journal of Physical Chemistry B*, **2002**, 106, 3788-3793	3.4	293
34	Structure and dynamics of zymogen human blood coagulation factor X. *Biophysical Journal*, **2002**, 82, 1190-206	2.9	63
33	Four loops of the catalytic domain of factor viia mediate the effect of the first EGF-like domain substitution on factor viia catalytic activity. *Journal of Molecular Biology*, **2001**, 307, 1503-17	6.5	20
32	Modeling Human Zymogen Factor IX. *Thrombosis and Haemostasis*, **2001**, 85, 596-603	7	20
31	Heparan sulfate biosynthesis: a theoretical study of the initial sulfation step by N-deacetylase/N-sulfotransferase. *Biophysical Journal*, **2000**, 79, 2909-17	2.9	17
30	Modeling zymogen protein C. *Biophysical Journal*, **2000**, 79, 2925-43	2.9	29
29	New tricks for modelers from the crystallography toolkit: the particle mesh Ewald algorithm and its use in nucleic acid simulations. *Structure*, **1999**, 7, R55-60	5.2	497
28	Probing the structural changes in the light chain of human coagulation factor VIIa due to tissue factor association. *Biophysical Journal*, **1999**, 77, 99-113	2.9	11
27	Engineering of betabellin-15D: a 64 residue beta sheet protein that forms long narrow multimeric fibrils. *Protein Science*, **1998**, 7, 1545-54	6.3	26
26	Trans-cis isomerization of proline 22 in bovine prothrombin fragment 1: a surprising result of structural characterization. *Biochemistry*, **1998**, 37, 10920-7	3.2	16
25	Thermally Induced Structural Changes in F-(H2O)11 and Cl-(H2O)11 Clusters: Molecular Dynamics Computer Simulations. *The Journal of Physical Chemistry*, **1996**, 100, 1350-1356		38
24	Role of Water in the Hydration Force Acting between Lipid Bilayers. *Langmuir*, **1996**, 12, 2625-2629	4	69
23	The solvation of Cl□Br□and I□n acetonitrile clusters: Photoelectron spectroscopy and molecular dynamics simulations. *Journal of Chemical Physics*, **1996**, 105, 2675-2685	3.9	95
22	Cube to cage transitions in (H2O)n (n=12, 16, and 20). *Journal of Chemical Physics*, **1996**, 105, 3715-3721	3.9	61
21	Effect of the treatment of long-range forces on the dynamics of ions in aqueous solutions. *Journal of Chemical Physics*, **1995**, 102, 450-456	3.9	139
20	The structure of water at platinum/water interfaces Molecular dynamics computer simulations. *Surface Science*, **1995**, 335, 401-415	1.8	51
19	A smooth particle mesh Ewald method. *Journal of Chemical Physics*, **1995**, 103, 8577-8593	3.9	14532

18	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	4	110
17	Molecular Dynamics Computer Simulations of Aqueous Solution/Platinum Interface **1994**, 101-118		1
16	Structures of Cl(H2O)n and F(H2O)n (n=2,3,...,15) clusters. Molecular dynamics computer simulations. *Journal of Chemical Physics*, **1994**, 100, 3085-3093	3.9	146
15	Enthalpies of formation and stabilization energies of Br(H2O)n (n=1,2, 15) clusters. Comparisons between molecular dynamics computer simulations and experiment. *Chemical Physics Letters*, **1994**, 218, 377-382	2.5	63
14	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		30
13	Mobility of stretched water. *Journal of Chemical Physics*, **1993**, 98, 9859-9862	3.9	24
12	Stabilization energies of Cl Br and I ions in water clusters. *Journal of Chemical Physics*, **1993**, 99, 4222-4224	3.9	96
11	Ion solvation in water clusters. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1993**, 26, 166-168		22
10	Solvation Dynamics in a Stockmayer Fluid **1993**, 461-483		
9	Structure and dynamics of Cl(H2O)20 clusters: The effect of the polarizability and the charge of the ion. *Journal of Chemical Physics*, **1992**, 96, 8288-8294	3.9	112
8	Dynamics of ion solvation in a Stockmayer fluid. *Journal of Chemical Physics*, **1992**, 96, 3092-3101	3.9	100
7	Ultrafast solvation dynamics in a Stockmayer fluid. *Journal of Chemical Physics*, **1992**, 97, 5253-5254	3.9	35
6	Energetics and structure in I 2 (CO2) n clusters. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1991**, 20, 173-175		37
5	Many-body effects in molecular dynamics simulations of Na+(H2O)n and Cl(H2O)n clusters. *Journal of Chemical Physics*, **1991**, 95, 1954-1963	3.9	300
4	Spectral shifts and structural classes in microsolutions of rare gas clusters containing a molecular chromophore. *Journal of Chemical Physics*, **1990**, 93, 4884-4897	3.9	88
3	Charge localization in negative ion dynamics: Effect on caging of Br 2 in Arn and (CO2)n clusters. *Journal of Chemical Physics*, **1989**, 90, 7354-7368	3.9	76
2	A smooth particle mesh Ewald method		1
1	Characterization of SARS2 Nsp15 Nuclease Activity Reveals its Mad About U		1