

# Purshotam Sharma

## List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	How do hydrophobic nucleobases differ from natural DNA nucleobases? Comparison of structural features and duplex properties from QM calculations and MD simulations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 16365-16374.	2.8	24
2	Structural and electronic properties of barbituric acid and melamine-containing ribonucleosides as plausible components of prebiotic RNA: implications for prebiotic self-assembly. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 30762-30771.	2.8	20
3	Structural Patterns and Stabilities of Hydrogen-Bonded Pairs Involving Ribonucleotide Bases and Arginine, Glutamic Acid, or Glutamine Residues of Proteins from Quantum Mechanical Calculations. <i>ACS Omega</i> , 2020, 5, 3612-3623.	3.5	11
4	Can Cyanuric Acid and 2,4,6-Triaminopyrimidine Containing Ribonucleosides be Components of Prebiotic RNA? Insights from QM Calculations and MD Simulations. <i>ChemPhysChem</i> , 2019, 20, 1425-1436.	2.1	10
5	Higher order structures involving post transcriptionally modified nucleobases in RNA. <i>RSC Advances</i> , 2017, 7, 35694-35703.	3.6	9
6	Could Purines Be Formed from Cyanamide and Cyanoacetylene in a Prebiotic Earth Environment?. <i>ACS Omega</i> , 2019, 4, 12771-12781.	3.5	9
7	Cyanoacetaldehyde as a building block for prebiotic formation of pyrimidines. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25886.	2.0	9
8	Pairing interactions between nucleobases and ligands in aptamer:ligand complexes of riboswitches: crystal structure analysis, classification, optimal structures, and accurate interaction energies. <i>Rna</i> , 2019, 25, 1274-1290.	3.5	8
9	Molecular Dynamics Simulations of Mismatched DNA Duplexes Associated with the Major C <sup>8</sup> -Linked 2-Deoxyguanosine Adduct of the Food Mutagen Ochratoxin A: Influence of Opposing Base, Adduct Ionization State, and Sequence on the Structure of Damaged DNA. <i>Chemical Research in Toxicology</i> , 2018, 31, 712-720.	3.3	7
10	Molecular Dynamics Study of One-Base Deletion Duplexes Containing the Major DNA Adduct Formed by Ochratoxin A: Effects of Sequence Context and Adduct Ionization State on Lesion Site Structure and Mutagenicity. <i>Journal of Physical Chemistry B</i> , 2019, 123, 6980-6989.	2.6	7
11	Replication of the Aristolochic Acid I Adenine Adduct (ALI-N <sup>6</sup> -A) by a Model Translesion Synthesis DNA Polymerase: Structural Insights on the Induction of Transversion Mutations from Molecular Dynamics Simulations. <i>Chemical Research in Toxicology</i> , 2020, 33, 2573-2583.	3.3	7
12	Radical pathways for the formation of non-canonical nucleobases in prebiotic environments. <i>RSC Advances</i> , 2019, 9, 36530-36538.	3.6	6
13	Can modified DNA base pairs with chalcogen bonding expand the genetic alphabet? A combined quantum chemical and molecular dynamics simulation study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 23754-23765.	2.8	6
14	Influence of the Number, Nature and Position of Methyl Posttranscriptional Modifications on Nucleobase Stacking in RNA. <i>ChemPhysChem</i> , 2021, 22, 1622-1630.	2.1	5
15	Molecular Dynamics Simulations of the Aptamer Domain of Guanidinium Ion Binding Riboswitch <i>ykKc</i> -III: Structural Insights into the Discrimination of Cognate and Alternate Ligands. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5243-5255.	5.4	3
16	Exploring the Nature of Hydrogen Bonding between RNA and Proteins: A Comprehensive Analysis of RNA-Protein Complexes. <i>ChemPhysChem</i> , 2022, 23, e202100731.	2.1	2
17	Role of Stacking Interactions in the Stability of Primitive Genetics: A Quantum Chemical View. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4321-4330.	5.4	1
18	Can Cyanuric Acid and 2,4,6-Triaminopyrimidine Containing Ribonucleosides be Components of Prebiotic RNA? Insights from QM Calculations and MD Simulations. <i>ChemPhysChem</i> , 2019, 20, 1415-1415.	2.1	0