Stacey D Wetmore

List of Publications by Year
in descending order

128	2,550	186209 28	289141 40
papers	citations	h-index	g-index

131	131	131	1837
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Effects of a Second Local DNA Damage Event on the Toxicity of the Human Carcinogen 4-Aminobiphenyl: A Molecular Dynamics Study of a Damaged DNA Structure. Chemical Research in Toxicology, 2022, 35, 499-511.	1.7	3
2	Multiscale computational investigations of the translesion synthesis bypass of tobacco-derived DNA adducts: critical insights that complement experimental biochemical studies. Physical Chemistry Chemical Physics, 2022, 24, 10667-10683.	1.3	2
3	Posttranscriptional modifications at the 37th position in the anticodon stemâ€“loop of tRNA: structural insights from MD simulations. Rna, 2021, 27, 202-220.	1.6	8
4	Anatomy of noncovalent interactions between the nucleobases or ribose and Ï€-containing amino acids in RNAâ€“protein complexes. Nucleic Acids Research, 2021, 49, 2213-2225.	6.5	18
5	Chalcogen versus Dative Bonding in [SF₃]⁺ Lewis Acidâ€“Base Adducts: [SF₃(NCCH₃)₂]⁺, [SF₃(NC₅H₅)₂]⁺, and [SF₃(phen)]⁺ (phen = 1,10-phenanthroline). Inorganic Chemistry, 2021, 60, 3893-3901.	1.9	5
6	Structural Rationalization for the Nonmutagenic and Mutagenic Bypass of the Tobacco-Derived O4-4-(3-Pyridyl)-4-oxobut-1-yl-thymine Lesion by Human Polymerase Î·: A Multiscale Computational Study. Chemical Research in Toxicology, 2021, 34, 1619-1629.	1.7	3
7	Impact of DNA Adduct Size, Number, and Relative Position on the Toxicity of Aromatic Amines: A Molecular Dynamics Case Study of ^{AN}dG- and ^{AP}dG-Containing DNA Duplexes. Journal of Chemical Information and Modeling, 2021, 61, 2313-2327.	2.5	9
8	Stabilisation of [W V F 4] + by Nâ€•and Pâ€Donor Ligands: Secondâ€Order Jahnâ€Teller Effects in Octacoordinate d 1 Complexes. Chemistry - A European Journal, 2021, 27, 11335-11343.	1.7	2
9	Assessment of the Accuracy of DFT-Predicted Li⁺â€“Nucleic Acid Binding Energies. Journal of Chemical Theory and Computation, 2021, 17, 5392-5408.	2.3	4
10	Established and Emerging Regulatory Roles of Eukaryotic Translation Initiation Factor 5B (eIF5B). Frontiers in Genetics, 2021, 12, 737433.	1.1	13
11	Role of Stacking Interactions in the Stability of Primitive Genetics: A Quantum Chemical View. Journal of Chemical Information and Modeling, 2021, 61, 4321-4330.	2.5	1
12	Donorâ€Stabilised [SbF4]+: SbF5 as a Fluoideâ€Ion Donor. Chemistry - A European Journal, 2021, 27, 16334-16337.	1.7	5
13	Lewis Acid Behavior of MoF5 and MoOF4: Syntheses and Characterization of MoF5(NCCH3), MoF5(NC5H5)n, and MoOF4(NC5H5)n (n = 1, 2). Inorganic Chemistry, 2021, 60, 15695-15711.	1.9	0
14	Structure of an Unusual Tetracyclic Deoxyguanosine Adduct: Implications for Frameshift Mutagenicity of ortho-Cyano Nitroanilines. Chemical Research in Toxicology, 2020, 33, 584-593.	1.7	4
15	Replication of the Aristolochic Acid I Adenine Adduct (ALI-N⁶-A) by a Model Translesion Synthesis DNA Polymerase: Structural Insights on the Induction of Transversion Mutations from Molecular Dynamics Simulations. Chemical Research in Toxicology, 2020, 33, 2573-2583.	1.7	7
16	Insights into the Direct Oxidative Repair of Etheno Lesions: MD and QM/MM Study on the Substrate Scope of ALKBH2 and AlkB. DNA Repair, 2020, 96, 102944.	1.3	9
17	Can modified DNA base pairs with chalcogen bonding expand the genetic alphabet? A combined quantum chemical and molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2020, 22, 23754-23765.	1.3	6
18	Reactions of Molybdenum and Tungsten Oxide Tetrafluoride with Sulfur(IV) Lewis Bases: Structure and Bonding in [WOF₄]₄, MOF₄(OSO), and [SF₃][M₂O₂F₉] (M = Mo, W). Inorganic Chemistry, 2020, 59, 17544-17554.	1.9	5

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19	Lighting Up the Thrombin-Binding Aptamer G-Quadruplex with an Internal Cyanine-Indole-Quinolinium Nucleobase Surrogate. Direct Fluorescent Intensity Readout for Thrombin Binding without Topology Switching. Bioconjugate Chemistry, 2020, 31, 2596-2606.	1.8	11
20	Computational studies of DNA repair: Insights into the function of monofunctional DNA glycosylases in the base excision repair pathway. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1471.	6.2	7
21	DFT Study on the Deglycosylation of Methylated, Oxidized, and Canonical Pyrimidine Nucleosides in Water: Implications for Epigenetic Regulation and DNA Repair. Journal of Physical Chemistry B, 2020, 124, 2392-2400.	1.2	3
22	Stabilisation of [WF₅]⁺ and WF₅ by Pyridine: Facile Access to [WF₅(NC₅H₅)₃]⁺ and WF₅(NC₅H₅)₂. Chemistry - A European Journal, 2020, 26, 6879-6886.	1.7	3
23	Impact of the Position of the Chemically Modified 5-Furyl-2â€²-Deoxyuridine Nucleoside on the Thrombin DNA Aptamerâ€“Protein Complex: Structural Insights into Aptamer Response from MD Simulations. Molecules, 2019, 24, 2908.	1.7	10
24	Stabilization of [WF₅]⁺ by Bidentate Nâ€Donor Ligands. Angewandte Chemie, 2019, 131, 13169-13172.	1.6	2
25	Stabilization of [WF₅]⁺ by Bidentate Nâ€Donor Ligands. Angewandte Chemie - International Edition, 2019, 58, 13035-13038.	7.2	5
26	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. Journal of Physical Chemistry B, 2019, 123, 6980-6989.	1.2	7
27	DFT and MD Studies of Formaldehyde-Derived DNA Adducts: Molecular-Level Insights into the Differential Mispairing Potentials of the Adenine, Cytosine, and Guanine Lesions. Journal of Physical Chemistry A, 2019, 123, 6229-6240.	1.1	9
28	Uncovering a unique approach for damaged DNA replication: A computational investigation of a mutagenic tobacco-derived thymine lesion. Nucleic Acids Research, 2019, 47, 1871-1879.	6.5	8
29	Computational Insight into the Differential Mutagenic Patterns of O-Methylthymine Lesions. Chemical Research in Toxicology, 2019, 32, 2107-2117.	1.7	4
30	Acceptor Influence on Thiolate Sensing by Hemicyanine Dyes. Journal of Organic Chemistry, 2019, 84, 2261-2268.	1.7	13
31	Exploring the Identity of the General Base for a DNA Polymerase Catalyzed Reaction Using QM/MM: The Case Study of Human Translesion Synthesis Polymerase Î·. ACS Catalysis, 2019, 9, 2543-2551.	5.5	17
32	Can Cyanuric Acid and 2,4,6-Triaminopyrimidine Containing Ribonucleosides be Components of Prebiotic RNA? Insights from QM Calculations and MD Simulations. ChemPhysChem, 2019, 20, 1415-1415.	1.0	0
33	DNA repair enzymes ALKBH2, ALKBH3,Âand AlkB oxidize 5-methylcytosine to 5-hydroxymethylcytosine, 5-formylcytosine and 5-carboxylcytosine in vitro. Nucleic Acids Research, 2019, 47, 5522-5529.	6.5	51
34	Synthesis, Characterization, and Lewis Acid Behavior of [W(NC₆F₅)F₄]_x and Computational Study of W(NR)F₄ (R = H, F, CH₃, CF₃,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 142 Td (C<sub>6<	1.9	5
35	W(NC₆F₅)F₄(NCCH₃), and W(NC₆F₅)F₄(NC₅H₅)_n Can Cyanuric Acid and 2,4,6â€Triaminopyrimidine Containing Ribonucleosides be Components of Prebiotic RNA? Insights from QM Calculations and MD Simulations. ChemPhysChem, 2019, 20, 1425-1436.	1.0	10
36	Unveiling a Single-Metal-Mediated Phosphodiester Bond Cleavage Mechanism for Nucleic Acids: A Multiscale Computational Investigation of a Human DNA Repair Enzyme. Journal of the American Chemical Society, 2019, 141, 8646-8656.	6.6	33

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37	Quantum Chemical Studies of the Structure and Stability of N-Methylated DNA Nucleobase Dimers: Insights into the Mutagenic Base Pairing of Damaged DNA. Journal of Physical Chemistry A, 2018, 122, 410-419.	1.1	9
38	Structural Insight into the Discrimination between 8-Oxoguanine Glycosidic Conformers by DNA Repair Enzymes: A Molecular Dynamics Study of Human Oxoguanine Glycosylase 1 and Formamidopyrimidine-DNA Glycosylase. Biochemistry, 2018, 57, 1144-1154.	1.2	4
39	Manipulation of a DNA aptamerâ€“protein binding site through arylation of internal guanine residues. Organic and Biomolecular Chemistry, 2018, 16, 3831-3840.	1.5	11
40	Conformational Preference and Fluorescence Response of a C-Linked C8-Biphenyl-Guanine Lesion in the NarI Mutational Hotspot: Evidence for Enhanced Syn Adduct Formation. Chemical Research in Toxicology, 2018, 31, 37-47.	1.7	7
41	Computational insights into the mutagenicity of two tobacco-derived carcinogenic DNA lesions. Nucleic Acids Research, 2018, 46, 11858-11868.	6.5	9
42	Structural explanation for the tunable substrate specificity of an E. coli nucleoside hydrolase: insights from molecular dynamics simulations. Journal of Computer-Aided Molecular Design, 2018, 32, 1375-1388.	1.3	0
43	Fluorescent Nucleobase Analogues with Extended Pi Surfaces Stabilize <scp>DNA</scp> Duplexes Containing O⁶â€Alkylguanine Adducts. Helvetica Chimica Acta, 2018, 101, e1800066.	1.0	4
44	Molecular Dynamics Simulations of Mismatched DNA Duplexes Associated with the Major C⁸-Linked 2â€²-Deoxyguanosine Adduct of the Food Mutagen Ochratoxin A: Influence of Opposing Base, Adduct Ionization State, and Sequence on the Structure of Damaged DNA. Chemical Research in Toxicology, 2018, 31, 712-720.	1.7	7
45	Effect of Size and Shape of Nitrogen-Containing Aromatics on Conformational Preferences of DNA Containing Damaged Guanine. Journal of Chemical Information and Modeling, 2018, 58, 1415-1425.	2.5	6
46	DNA base sequence effects on bulky lesion-induced conformational heterogeneity during DNA replication. Nucleic Acids Research, 2018, 46, 6356-6370.	6.5	10
47	Syntheses, characterisation, and computational studies of tungsten hexafluoride adducts with pyridine and its derivatives. Journal of Fluorine Chemistry, 2018, 215, 1-9.	0.9	9
48	Combining crystallographic and quantum chemical data to understand DNA-protein Ï€-interactions in nature. Structural Chemistry, 2017, 28, 1487-1500.	1.0	12
49	How do hydrophobic nucleobases differ from natural DNA nucleobases? Comparison of structural features and duplex properties from QM calculations and MD simulations. Physical Chemistry Chemical Physics, 2017, 19, 16365-16374.	1.3	24
50	Molecular Insights into the Translesion Synthesis of Benzyl-Guanine from Molecular Dynamics Simulations: Structural Evidence of Mutagenic and Nonmutagenic Replication. Biochemistry, 2017, 56, 1841-1853.	1.2	6
51	Mutagenicity of Ochratoxin A: Role for a Carbon-Linked C8â€“Deoxyguanosine Adduct?. Journal of Agricultural and Food Chemistry, 2017, 65, 7097-7105.	2.4	17
52	Syntheses and Characterization of W(NC₆F₅)F₅^{â€“} and W₂(NC₆F₅)₂F₉^{â€“} Salts and Computational Studies of the W(NR)F₅^{â€“} (R = H, F, CH₃,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 W₂(NC₆F₅)₂F₉^{â€“} Anions. Inorganic Chemistry, 2017, 56, 12581-12593.	1.9	4
53	Conformational Flexibility of the Benzyl-Guanine Adduct in a Bypass Polymerase Active Site Permits Replication: Insights from Molecular Dynamics Simulations. Chemical Research in Toxicology, 2017, 30, 2013-2022.	1.7	8
54	Molecular Modeling of the Major DNA Adduct Formed from Food Mutagen Ochratoxin A inNarI Two-Base Deletion Duplexes: Impact of Sequence Context and Adduct Ionization on Conformational Preference and Mutagenicity. Chemical Research in Toxicology, 2017, 30, 1582-1591.	1.7	8

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55	QM/MM Study of the Reaction Catalyzed by Alkyladenine DNA Glycosylase: Examination of the Substrate Specificity of a DNA Repair Enzyme. Journal of Physical Chemistry B, 2017, 121, 11096-11108.	1.2	14
56	Solidâ€State Structure of Protonated Ketones and Aldehydes. Angewandte Chemie - International Edition, 2017, 56, 16380-16384.	7.2	21
57	Structural and electronic properties of barbituric acid and melamine-containing ribonucleosides as plausible components of prebiotic RNA: implications for prebiotic self-assembly. Physical Chemistry Chemical Physics, 2017, 19, 30762-30771.	1.3	20
58	Conformational flexibility and base-pairing tendency of the tobacco carcinogen O6-[4-oxo-4-(3-pyridyl)butyl]guanine. Biophysical Chemistry, 2017, 228, 25-37.	1.5	5
59	Understanding the Mutagenicity of O-Linked and C-Linked Guanine DNA Adducts: A Combined Experimental and Computational Approach. Chemical Research in Toxicology, 2017, 30, 177-188.	1.7	8
60	Computational Evaluation of Nucleotide Insertion Opposite Expanded and Widened DNA by the Translesion Synthesis Polymerase Dpo4. Molecules, 2016, 21, 822.	1.7	2
61	Hydrolytic Glycosidic Bond Cleavage in RNA Nucleosides: Effects of the 2â€²-Hydroxy Group and Acidâ€“Base Catalysis. Journal of Physical Chemistry B, 2016, 120, 12795-12806.	1.2	12
62	Optimization of fluorescent 8-heteroaryl-guanine probes for monitoring protein-mediated duplex â†' G-quadruplex exchange. Organic and Biomolecular Chemistry, 2016, 14, 4409-4419.	1.5	17
63	C-Linked 8-aryl guanine nucleobase adducts: biological outcomes and utility as fluorescent probes. Chemical Science, 2016, 7, 3482-3493.	3.7	31
64	Evaluating the Substrate Selectivity of Alkyladenine DNA Glycosylase: The Synergistic Interplay of Active Site Flexibility and Water Reorganization. Biochemistry, 2016, 55, 798-808.	1.2	17
65	Photophysical properties of pushâ€“pull 8-aryl-deoxyguanosine probes within duplex and G-quadruplex structures. Journal of Materials Chemistry C, 2016, 4, 2915-2924.	2.7	19
66	Topology of RNAâ€“protein nucleobaseâ€“amino acid Ï€â€“Ï€ interactions and comparison to analogous DNAâ€–protein Ï€â€“Ï€ contacts. Rna, 2016, 22, 696-708.	1.6	40
67	DNA Distortion Caused by Uracil-Containing Intrastrand Cross-Links. Journal of Physical Chemistry B, 2016, 120, 1195-1204.	1.2	10
68	Effect of base sequence context on the conformational heterogeneity of aristolactam-I adducted DNA: structural and energetic insights into sequence-dependent repair and mutagenicity. Toxicology Research, 2016, 5, 197-209.	0.9	5
69	Landscape ofÏ€â€“Ï€and sugarâ€“Ï€contacts in DNAâ€“protein interactions. Journal of Biomolecular Structure and Dynamics, 2016, 34, 184-200.	2.0	18
70	Enhancing Bulge Stabilization through Linear Extension of C8-Aryl-Guanine Adducts to Promote Polymerase Blockage or Strand Realignment to Produce a C:C Mismatch. Chemical Research in Toxicology, 2015, 28, 1647-1658.	1.7	22
71	Adenine versus guanine DNA adducts of aristolochic acids: role of the carcinogenâ€“purine linkage in the differential global genomic repair propensity. Nucleic Acids Research, 2015, 43, 7388-7397.	6.5	16
72	Influence of the Linkage Type and Functional Groups in the Carcinogenic Moiety on the Conformational Preferences of Damaged DNA: Structural and Energetic Characterization of Carbon- and Oxygen-Linked C8-Phenolic-Guanine Adducts. Chemical Research in Toxicology, 2015, 28, 782-796.	1.7	12

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73	Chlorine Functionalization of a Model Phenolic C8-Guanine Adduct Increases Conformational Rigidity and Blocks Extension by a Y-Family DNA Polymerase. Chemical Research in Toxicology, 2015, 28, 1346-1356.	1.7	13
74	An ONIOM and MD Investigation of Possible Monofunctional Activity of Human 8-Oxoguanineâ€“DNA Glycosylase (hOgg1). Journal of Physical Chemistry B, 2015, 119, 8013-8023.	1.2	20
75	Conformational Preferences of DNA following Damage by Aristolochic Acids: Structural and Energetic Insights into the Different Mutagenic Potential of the ALI and ALII-N⁶-dA Adducts. Biochemistry, 2015, 54, 2414-2428.	1.2	16
76	Quantum mechanical study of the Î²- and Î´-lyase reactions during the base excision repair process: application to FPG. Physical Chemistry Chemical Physics, 2015, 17, 24696-24706.	1.3	9
77	Glycosidic Bond Cleavage in DNA Nucleosides: Effect of Nucleobase Damage and Activation on the Mechanism and Barrier. Journal of Physical Chemistry B, 2015, 119, 15601-15612.	1.2	14
78	Structural and energetic characterization of the major DNA adduct formed from the food mutagen ochratoxin A in the NarI hotspot sequence: influence of adduct ionization on the conformational preferences and implications for the NER propensity. Nucleic Acids Research, 2014, 42, 11831-11845.	6.5	27
79	Computational Investigation of Glycosylase and Î²-Lyase Activity Facilitated by Proline: Applications to FPG and Comparisons to hOgg1. Journal of Physical Chemistry B, 2014, 118, 14566-14577.	1.2	16
80	Structural and biochemical impact of C8-aryl-guanine adducts within the NarI recognition DNA sequence: influence of aryl ring size on targeted and semi-targeted mutagenicity. Nucleic Acids Research, 2014, 42, 13405-13421.	6.5	39
81	DNAâ€“protein Ï€-interactions in nature: abundance, structure, composition and strength of contacts between aromatic amino acids and DNA nucleobases or deoxyribose sugar. Nucleic Acids Research, 2014, 42, 6726-6741.	6.5	126
82	Electronic tuning of fluorescent 8-aryl-guanine probes for monitoring DNA duplexâ€“quadruplex exchange. Chemical Science, 2014, 5, 788-796.	3.7	28
83	Complex Conformational Heterogeneity of the Highly Flexible O6-Benzyl-guanine DNA Adduct. Chemical Research in Toxicology, 2014, 27, 1310-1325.	1.7	12
84	Influence of Chlorine Substitution on the Hydrolytic Stability of Biaryl Ether Nucleoside Adducts Produced by Phenolic Toxins. Journal of Organic Chemistry, 2013, 78, 7176-7185.	1.7	10
85	Significant Strength of Charged DNAâ€“Protein Ï€â€“Ï€ Interactions: A Preliminary Study of Cytosine. Journal of Physical Chemistry B, 2013, 117, 10462-10474.	1.2	26
86	Hydrolysis of the damaged deoxythymidine glycol nucleoside and comparison to canonical DNA. Physical Chemistry Chemical Physics, 2013, 15, 19343.	1.3	5
87	Standard Role for a Conserved Aspartate or More Direct Involvement in Deglycosylation? An ONIOM and MD Investigation of Adenineâ€“DNA Glycosylase. Biochemistry, 2013, 52, 8753-8765.	1.2	15
88	Exploring the limits of nucleobase expansion: computational design of naphthohomologated (xx-) purines and comparison to the natural and xDNA purines. Physical Chemistry Chemical Physics, 2013, 15, 15538.	1.3	22
89	yDNA versus yyDNA pyrimidines: computational analysis of the effects of unidirectional ring expansion on the preferred sugarâ€“base orientation, hydrogen-bonding interactions and stacking abilities. Physical Chemistry Chemical Physics, 2013, 15, 2435.	1.3	23
90	Selecting DFT methods for use in optimizations of enzyme active sites: applications to ONIOM treatments of DNA glycosylases. Canadian Journal of Chemistry, 2013, 91, 559-572.	0.6	16

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91	Structural Influence of C8-Phenoxy-Guanine in the NarI Recognition DNA Sequence. Chemical Research in Toxicology, 2013, 26, 1397-1408.	1.7	21
92	Modeling the Conformational Preference of the Carbon-Bonded Covalent Adduct Formed upon Exposure of 2â€²-Deoxyguanosine to Ochratoxin A. Chemical Research in Toxicology, 2013, 26, 803-816.	1.7	26
93	C8-linked bulky guanosine DNA adducts: experimental and computational insights into adduct conformational preferences and resulting mutagenicity. Future Medicinal Chemistry, 2012, 4, 1981-2007.	1.1	27
94	Glycosidic Bond Cleavage in Deoxynucleotides: Effects of Solvent and the DNA Phosphate Backbone in the Computational Model. Journal of Physical Chemistry B, 2012, 116, 14275-14284.	1.2	19
95	Combined Effects of Ï€â€“Ï€ Stacking and Hydrogen Bonding on the (N1) Acidity of Uracil and Hydrolysis of 2â€²-Deoxyuridine. Journal of Physical Chemistry B, 2012, 116, 2622-2632.	1.2	15
96	Mechanistic and Conformational Flexibility of the Covalent Linkage Formed during Î²-Lyase Activity on an AP-Site: Application to hOgg1. Journal of Physical Chemistry B, 2012, 116, 10786-10797.	1.2	18
97	C⁸-Heteroaryl-2â€²-deoxyguanosine Adducts as Conformational Fluorescent Probes in the NarI Recognition Sequence. Journal of Organic Chemistry, 2012, 77, 10498-10508.	1.7	34
98	Effects of Extending the Computational Model on DNAâ€“Protein T-shaped Interactions: The Case of Adenineâ€“Histidine Dimers. Journal of Physical Chemistry A, 2011, 115, 12646-12658.	1.1	14
99	Conformational Flexibility of C8-Phenoxylguanine Adducts in Deoxydinucleoside Monophosphates. Journal of Physical Chemistry B, 2011, 115, 12993-13002.	1.2	12
100	Evaluating How Discrete Water Molecules Affect Proteinâ€“DNA Ï€â€“Ï€ and Ï€+â€“Ï€ Stacking and T-Shaped Interactions: The Case of Histidine-Adenine Dimers. Journal of Physical Chemistry B, 2011, 115, 10990-11003.	1.2	24
101	A QM/QM Investigation of the hUNG2 Reaction Surface: The Untold Tale of a Catalytic Residue. Biochemistry, 2011, 50, 4218-4227.	1.2	27
102	Modeling the Chemical Step Utilized by Human Alkyladenine DNA Glycosylase: A Concerted Mechanism Aids in Selectively Excising Damaged Purines. Journal of the American Chemical Society, 2011, 133, 16258-16269.	6.6	39
103	The assessment of density functionals for DNAâ€“protein stacked and T-shaped complexes. Canadian Journal of Chemistry, 2010, 88, 815-830.	0.6	36
104	Effect of Watsonâ^'Crick and Hoogsteen Base Pairing on the Conformational Stability of C8-Phenoxyl-2â€²-deoxyguanosine Adducts. Journal of Physical Chemistry B, 2010, 114, 12995-13004.	1.2	17
105	Effects of the biological backbone on stacking interactions at DNAâ€“protein interfaces: the interplay between the backboneâ‹¯Ï€ and Ï€â‹¯Ï€ components. Physical Chemistry Chemical Physics, 2010, 12, 14515.	1.3	43
106	Conformational Flexibility of C8-Phenoxyl-2â€²-deoxyguanosine Nucleotide Adducts. Journal of Physical Chemistry B, 2010, 114, 4373-4382.	1.2	36
107	Modeling the Dissociative Hydrolysis of the Natural DNA Nucleosides. Journal of Physical Chemistry B, 2010, 114, 1104-1113.	1.2	27
108	Effects of Nucleophile, Oxidative Damage, and Nucleobase Orientation on the Glycosidic Bond Cleavage in Deoxyguanosine. Journal of Physical Chemistry B, 2010, 114, 2319-2326.	1.2	27

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109	A Preliminary Investigation of the Additivity of Ï€â^Ï€ or Ï€⁺â^Ï€ Stacking and T-Shaped Interactions between Natural or Damaged DNA Nucleobases and Histidine. Journal of Physical Chemistry B, 2010, 114, 3355-3367.	1.2	33
110	Noncovalent Interactions Involving Histidine: The Effect of Charge on Ï€â^Ï€ Stacking and T-Shaped Interactions with the DNA Nucleobases. Journal of Physical Chemistry B, 2009, 113, 16046-16058.	1.2	80
111	Designing an Appropriate Computational Model for DNA Nucleoside Hydrolysis: A Case Study of 2â€²-Deoxyuridine. Journal of Physical Chemistry B, 2009, 113, 6533-6542.	1.2	35
112	Evidence for Stabilization of DNA/RNAâ^'Protein Complexes Arising from Nucleobaseâ^'Amino Acid Stacking and T-Shaped Interactions. Journal of Chemical Theory and Computation, 2009, 5, 1400-1410.	2.3	72
113	Concerning the Hydrolytic Stability of 8-Aryl-2â€²-deoxyguanosine Nucleoside Adducts: Implications for Abasic Site Formation at Physiological pH. Journal of Organic Chemistry, 2009, 74, 5793-5802.	1.7	28
114	Computational comparison of the stacking interactions between the aromatic amino acids and the natural or (cationic) methylated nucleobases. Physical Chemistry Chemical Physics, 2008, 10, 2801.	1.3	42
115	Remarkably Strong T-Shaped Interactions between Aromatic Amino Acids and Adenine: Their Increase upon Nucleobase Methylation and a Comparison to Stacking. Journal of Chemical Theory and Computation, 2008, 4, 1768-1780.	2.3	38
116	yDNA versus xDNA Pyrimidine Nucleobases: Computational Evidence for Dependence of Duplex Stability on Spacer Location. Journal of Physical Chemistry B, 2008, 112, 12526-12536.	1.2	19
117	Computational and Experimental Evidence for the Structural Preference of Phenolic C-8 Purine Adducts. Journal of Physical Chemistry A, 2008, 112, 3742-3753.	1.1	40
118	How Do Size-Expanded DNA Nucleobases Enhance Duplex Stability? Computational Analysis of the Hydrogen-Bonding and Stacking Ability of xDNA Bases. Journal of Physical Chemistry B, 2007, 111, 2999-3009.	1.2	38
119	Environmental Effects on the Enhancement in Natural and Damaged DNA Nucleobase Acidity Because of Discrete Hydrogen-Bonding Interactions. Journal of Physical Chemistry A, 2007, 111, 1933-1942.	1.1	13
120	Effects of Hydrogen-Bonding and Stacking Interactions with Amino Acids on the Acidity of Uracil. Journal of Physical Chemistry B, 2007, 111, 1858-1871.	1.2	31
121	A Kinetic and Thermodynamic Study of the Glycosidic Bond Cleavage in Deoxyuridine. Journal of Physical Chemistry B, 2007, 111, 3800-3812.	1.2	35
122	A computational characterization of the hydrogen-bonding and stacking interactions of hypoxanthine. Physical Chemistry Chemical Physics, 2007, 9, 497-509.	1.3	36
123	Characterization of the stacking interactions between DNA or RNA nucleobases and the aromatic amino acids. Chemical Physics Letters, 2007, 444, 167-175.	1.2	92
124	Characterization of Nucleobaseâ^'Amino Acid Stacking Interactions Utilized by a DNA Repair Enzyme. Journal of Physical Chemistry B, 2006, 110, 19652-19663.	1.2	76
125	Nitrosubstituted aromatic molecules as universal nucleobases: Computational analysis of stacking interactions. Chemical Physics Letters, 2006, 428, 157-166.	1.2	29
126	Effects of Hydrogen Bonding on the Acidity of Adenine, Guanine, and Their 8-Oxo Derivatives. Journal of Physical Chemistry A, 2005, 109, 6351-6362.	1.1	41

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127	Effects of Hydrogen Bonding on the Acidity of Uracil Derivatives. Journal of Physical Chemistry A, 2004, 108, 7709-7718.	1.1	48
128	Effects of Hydrogen Bonding on the Acidity of Uracil. Journal of Physical Chemistry A, 2003, 107, 10406-10413.	1.1	54