Tatiana Domratcheva

List of Publications by Year
in descending order

36	1,927	257450 24	345221 36
papers	citations	h-index	g-index

41	41	41	1797
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Crystal Structure and Mechanism of a DNA (6â€4) Photolyase. Angewandte Chemie - International Edition, 2008, 47, 10076-10080.	13.8	174
2	Crystal Structures of the AppA BLUF Domain Photoreceptor Provide Insights into Blue Light-mediated Signal Transduction. Journal of Molecular Biology, 2006, 362, 717-732.	4.2	157
3	Structure of a bacterial BLUF photoreceptor: Insights into blue light-mediated signal transduction. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 12350-12355.	7.1	155
4	Three-dimensional view of ultrafast dynamics in photoexcited bacteriorhodopsin. Nature Communications, 2019, 10, 3177.	12.8	121
5	Molecular Models Predict Light-Induced Glutamine Tautomerization in BLUF Photoreceptors. Biophysical Journal, 2008, 94, 3872-3879.	0.5	118
6	X-ray and NMR Crystallography in an Enzyme Active Site: The Indoline Quinonoid Intermediate in Tryptophan Synthase. Journal of the American Chemical Society, 2011, 133, 4-7.	13.7	101
7	Decrypting Cryptochrome: Revealing the Molecular Identity of the Photoactivation Reaction. Journal of the American Chemical Society, 2012, 134, 18046-18052.	13.7	98
8	Mechanism and dynamics of fatty acid photodecarboxylase. Science, 2021, 372, .	12.6	93
9	Ultrafast Infrared Spectroscopy of Riboflavin: Dynamics, Electronic Structure, and Vibrational Mode Analysis. Journal of Physical Chemistry B, 2008, 112, 13424-13432.	2.6	79
10	Primary Reactions of the LOV2 Domain of Phototropin Studied with Ultrafast Mid-Infrared Spectroscopy and Quantum Chemistry. Biophysical Journal, 2009, 97, 227-237.	0.5	79
11	Separation of photo-induced radical pair in cryptochrome to a functionally critical distance. Scientific Reports, 2014, 4, 3845.	3.3	65
12	Evidence for Tautomerisation of Glutamine in BLUF Blue Light Receptors by Vibrational Spectroscopy and Computational Chemistry. Scientific Reports, 2016, 6, 22669.	3.3	64
13	Electronic Structure of (6â^'4) DNA Photoproduct Repair Involving a Non-Oxetane Pathway. Journal of the American Chemical Society, 2009, 131, 17793-17799.	13.7	51
14	Structure and Mechanistic Implications of a Tryptophan Synthase Quinonoid Intermediate. ChemBioChem, 2008, 9, 1024-1028.	2.6	50
15	Photoinduced Electron Transfer Facilitates Tautomerization of the Conserved Signaling Glutamine Side Chain in BLUF Protein Light Sensors. Journal of Physical Chemistry B, 2013, 117, 2369-2377.	2.6	50
16	Photoreaction in BLUF Receptors: Protonâ€coupled Electron Transfer in the Flavinâ€Glnâ€Tyr System^{â€}. Photochemistry and Photobiology, 2011, 87, 554-563.	2.5	45
17	Analysis of the Primary Photocycle Reactions Occurring in the Light, Oxygen, and Voltage Blue-Light Receptor by Multiconfigurational Quantum-Chemical Methods. Journal of Chemical Theory and Computation, 2006, 2, 1565-1574.	5.3	43
18	Glutamine Rotamers in BLUF Photoreceptors: A Mechanistic Reappraisal. Journal of Physical Chemistry B, 2013, 117, 2888-2897.	2.6	42

#	Article	IF	Citations
19	Neutral Histidine and Photoinduced Electron Transfer in DNA Photolyases. Journal of the American Chemical Society, 2011, 133, 18172-18182.	13.7	40
20	Theoretical Characterization of the Flavin-Based Fluorescent Protein iLOV and its Q489K Mutant. Journal of Physical Chemistry B, 2015, 119, 5176-5183.	2.6	40
21	Onset of the Electronic Absorption Spectra of Isolated and Ï€-Stacked Oligomers of 5,6-Dihydroxyindole: An Ab Initio Study of the Building Blocks of Eumelanin. Journal of Physical Chemistry B, 2016, 120, 3493-3502.	2.6	37
22	Single Hydrogen Bond Donation from Flavin N₅ to Proximal Asparagine Ensures FAD Reduction in DNA Photolyase. Journal of the American Chemical Society, 2016, 138, 4368-4376.	13.7	29
23	Computational Characterization of Reaction Intermediates in the Photocycle of the Sensory Domain of the AppA Blue Light Photoreceptor^{â€}. Photochemistry and Photobiology, 2011, 87, 564-573.	2.5	26
24	Frontiers in Multiscale Modeling of Photoreceptor Proteins. Photochemistry and Photobiology, 2021, 97, 243-269.	2.5	26
25	Î²Q114N and Î²T110V Mutations Reveal a Critically Important Role of the Substrate Î±-Carboxylate Site in the Reaction Specificity of Tryptophan Synthase. Biochemistry, 2007, 46, 14100-14116.	2.5	25
26	Role of the Molecular Environment in Flavoprotein Color and Redox Tuning: QM Cluster versus QM/MM Modeling. Journal of Chemical Theory and Computation, 2015, 11, 3878-3894.	5.3	25
27	Coupling between the BLUF and EAL domains in the blue light-regulated phosphodiesterase BlrP1. Journal of Molecular Modeling, 2011, 17, 1579-1586.	1.8	17
28	Vibrational Mode Analysis of Isotope-Labeled Electronically Excited Riboflavin. Journal of Physical Chemistry B, 2011, 115, 7621-7628.	2.6	16
29	Challenges in Computing Electron-Transfer Energies of DNA Repair Using Hybrid QM/MM Models. Journal of Chemical Theory and Computation, 2013, 9, 4644-4652.	5.3	12
30	Molecular mechanism of the dark-state recovery in BLUF photoreceptors. Chemical Physics Letters, 2017, 676, 25-31.	2.6	11
31	Indications of 5â€² to 3â€² Interbase Electron Transfer as the First Step of Pyrimidine Dimer Formation Probed by a Dinucleotide Analog. Chemistry - A European Journal, 2017, 23, 7526-7537.	3.3	8
32	CHARMM Force-Field Parameters for Morphine, Heroin, and Oliceridine, and Conformational Dynamics of Opioid Drugs. Journal of Chemical Information and Modeling, 2021, 61, 3964-3977.	5.4	8
33	Computational Spectroscopy, Dynamics, and Photochemistry of Photosensory Flavoproteins. Methods in Molecular Biology, 2014, 1146, 191-228.	0.9	6
34	Four resonance structures elucidate double-bond isomerisation of a biological chromophore. Physical Chemistry Chemical Physics, 2020, 22, 8535-8544.	2.8	5
35	Protonation States of Molecular Groups in the Chromophore-Binding Site Modulate Properties of the Reversibly Switchable Fluorescent Protein rsEGFP2. Journal of Physical Chemistry Letters, 2021, 12, 8263-8271.	4.6	5
36	Spiers Memorial Lecture : Introductory lecture: the impact of structure on photoinduced processes in nucleic acids and proteins. Faraday Discussions, 2018, 207, 9-26.	3.2	2