

Tatiana Domratcheva

List of Publications by Year in descending order

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36
papers

1,927
citations

257450

24
h-index

345221

36
g-index

41
all docs

41
docs citations

41
times ranked

1797
citing authors

#	ARTICLE	IF	CITATIONS
1	Frontiers in Multiscale Modeling of Photoreceptor Proteins. Photochemistry and Photobiology, 2021, 97, 243-269.	2.5	26
2	Mechanism and dynamics of fatty acid photodecarboxylase. Science, 2021, 372, .	12.6	93
3	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
4	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
5	Four resonance structures elucidate double-bond isomerisation of a biological chromophore. Physical Chemistry Chemical Physics, 2020, 22, 8535-8544.	2.8	5
6	Three-dimensional view of ultrafast dynamics in photoexcited bacteriorhodopsin. Nature Communications, 2019, 10, 3177.	12.8	121
7	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
8	Molecular mechanism of the dark-state recovery in BLUF photoreceptors. Chemical Physics Letters, 2017, 676, 25-31.	2.6	11
9	Indications of $5\pi\pi^*$ to $3\pi\pi^*$ 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
10	Evidence for Tautomerisation of Glutamine in BLUF Blue Light Receptors by Vibrational Spectroscopy and Computational Chemistry. Scientific Reports, 2016, 6, 22669.	3.3	64
11	Onset of the Electronic Absorption Spectra of Isolated and π -Stacked Oligomers of 5,6-Dihydroxyindole: An <i>Ab Initio</i> Study of the Building Blocks of Eumelanin. Journal of Physical Chemistry B, 2016, 120, 3493-3502.	2.6	37
12	Single Hydrogen Bond Donation from Flavin N ₅ to Proximal Asparagine Ensures FAD Reduction in DNA Photolyase. Journal of the American Chemical Society, 2016, 138, 4368-4376.	13.7	29
13	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
14	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
15	Separation of photo-induced radical pair in cryptochrome to a functionally critical distance. Scientific Reports, 2014, 4, 3845.	3.3	65
16	Computational Spectroscopy, Dynamics, and Photochemistry of Photosensory Flavoproteins. Methods in Molecular Biology, 2014, 1146, 191-228.	0.9	6
17	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
18	Glutamine Rotamers in BLUF Photoreceptors: A Mechanistic Reappraisal. Journal of Physical Chemistry B, 2013, 117, 2888-2897.	2.6	42

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19	Photoinduced Electron Transfer Facilitates Tautomerization of the Conserved Signaling Glutamine Side Chain in BLUF Protein Light Sensors. <i>Journal of Physical Chemistry B</i> , 2013, 117, 2369-2377.	2.6	50
20	Decrypting Cryptochrome: Revealing the Molecular Identity of the Photoactivation Reaction. <i>Journal of the American Chemical Society</i> , 2012, 134, 18046-18052.	13.7	98
21	Neutral Histidine and Photoinduced Electron Transfer in DNA Photolyases. <i>Journal of the American Chemical Society</i> , 2011, 133, 18172-18182.	13.7	40
22	Vibrational Mode Analysis of Isotope-Labeled Electronically Excited Riboflavin. <i>Journal of Physical Chemistry B</i> , 2011, 115, 7621-7628.	2.6	16
23	X-ray and NMR Crystallography in an Enzyme Active Site: The Indoline Quinonoid Intermediate in Tryptophan Synthase. <i>Journal of the American Chemical Society</i> , 2011, 133, 4-7.	13.7	101
24	Computational Characterization of Reaction Intermediates in the Photocycle of the Sensory Domain of the AppA Blue Light Photoreceptor. <i>Photochemistry and Photobiology</i> , 2011, 87, 564-573.	2.5	26
25	Photoreaction in BLUF Receptors: Proton-Coupled Electron Transfer in the Flavin-Gln-Tyr System. <i>Photochemistry and Photobiology</i> , 2011, 87, 554-563.	2.5	45
26	Coupling between the BLUF and EAL domains in the blue light-regulated phosphodiesterase BlrP1. <i>Journal of Molecular Modeling</i> , 2011, 17, 1579-1586.	1.8	17
27	Electronic Structure of (6 ⁺ 4) DNA Photoproduct Repair Involving a Non-Oxetane Pathway. <i>Journal of the American Chemical Society</i> , 2009, 131, 17793-17799.	13.7	51
28	Primary Reactions of the LOV2 Domain of Phototropin Studied with Ultrafast Mid-Infrared Spectroscopy and Quantum Chemistry. <i>Biophysical Journal</i> , 2009, 97, 227-237.	0.5	79
29	Structure and Mechanistic Implications of a Tryptophan Synthase Quinonoid Intermediate. <i>ChemBioChem</i> , 2008, 9, 1024-1028.	2.6	50
30	Crystal Structure and Mechanism of a DNA (6 ⁺ 4) Photolyase. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 10076-10080.	13.8	174
31	Molecular Models Predict Light-Induced Glutamine Tautomerization in BLUF Photoreceptors. <i>Biophysical Journal</i> , 2008, 94, 3872-3879.	0.5	118
32	Ultrafast Infrared Spectroscopy of Riboflavin: Dynamics, Electronic Structure, and Vibrational Mode Analysis. <i>Journal of Physical Chemistry B</i> , 2008, 112, 13424-13432.	2.6	79
33	Q114N and T110V Mutations Reveal a Critically Important Role of the Substrate \pm -Carboxylate Site in the Reaction Specificity of Tryptophan Synthase. <i>Biochemistry</i> , 2007, 46, 14100-14116.	2.5	25
34	Analysis of the Primary Photocycle Reactions Occurring in the Light, Oxygen, and Voltage Blue-Light Receptor by Multiconfigurational Quantum-Chemical Methods. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1565-1574.	5.3	43
35	Crystal Structures of the AppA BLUF Domain Photoreceptor Provide Insights into Blue Light-mediated Signal Transduction. <i>Journal of Molecular Biology</i> , 2006, 362, 717-732.	4.2	157
36	Structure of a bacterial BLUF photoreceptor: Insights into blue light-mediated signal transduction. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 12350-12355.	7.1	155