Maria G Khrenova

List of Publications by Year
in descending order

108	1,310	331259	454577
papers	citations	21 h-index	30 g-index

111	111	111	1358
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	State-of-the-art of computational green chemistry in leading universities in Russia. , 2022, , 55-77.		0
2	Drug Repurposing of the Unithiol: Inhibition of Metallo-Î²-Lactamases for the Treatment of Carbapenem-Resistant Gram-Negative Bacterial Infections. International Journal of Molecular Sciences, 2022, 23, 1834.	1.8	5
3	Complex of HIV-1 Integrase with Cellular Ku Protein: Interaction Interface and Search for Inhibitors. International Journal of Molecular Sciences, 2022, 23, 2908.	1.8	4
4	<scp>Ketoâ€enol</scp> tautomerism from the electron delocalization perspective. Journal of Computational Chemistry, 2022, , .	1.5	6
5	A Puzzling Protein from Variovorax paradoxus Has a PLP Fold Type IV Transaminase Structure and Binds PLP without Catalytic Lysine. Crystals, 2022, 12, 619.	1.0	0
6	Ketoâ€enol tautomerism of the 4,5â€dimethylâ€2â€(2â€²â€hydroxyphenyl)imidazole in water solution: Modeling equilibrium between neutral forms and accurate assignment of the absorption bands. International Journal of Quantum Chemistry, 2021, 121, e26577.	1.0	1
7	Benchmark studies of hydrogen bond governing reactivity of cephalosporins in <scp>L1</scp> metalloâ€Î²â€lactamase: Efficient and reliable <scp>QSPR</scp> equations. International Journal of Quantum Chemistry, 2021, 121, e26451.	1.0	3
8	Light-Induced Change of Arginine Conformation Modulates the Rate of Adenosine Triphosphate to Cyclic Adenosine Monophosphate Conversion in the Optogenetic System Containing Photoactivated Adenylyl Cyclase. Journal of Chemical Information and Modeling, 2021, 61, 1215-1225.	2.5	13
9	The explicit role of electron exchange in the hydrogen bonded molecular complexes. Journal of Computational Chemistry, 2021, 42, 870-882.	1.5	11
10	Molecular mechanism of the cesium and rubidium selective binding to the calix[4]arene revealed by Bornâ€“Oppenheimer molecular dynamics simulation and electron density analysis. Mendeleev Communications, 2021, 31, 185-187.	0.6	3
11	Boronic Acids as Prospective Inhibitors of Metallo-Î²-Lactamases: Efficient Chemical Reaction in the Enzymatic Active Site Revealed by Molecular Modeling. Molecules, 2021, 26, 2026.	1.7	11
12	The O to S substitution in urea brings inhibition activity against thiocyanate dehydrogenase. Mendeleev Communications, 2021, 31, 373-375.	0.6	1
13	The O to S substitution in urea brings inhibition activity against thiocyanate dehydrogenase. Mendeleev Communications, 2021, 31, 373-375.	0.6	0
14	Mechanism of Guanosine Triphosphate Hydrolysis by the Visual Proteins Arl3-RP2: Free Energy Reaction Profiles Computed with Ab Initio Type QM/MM Potentials. Molecules, 2021, 26, 3998.	1.7	7
15	Molecular Modeling Reveals the Mechanism of Ran-RanGAP-Catalyzed Guanosine Triphosphate Hydrolysis without an Arginine Finger. ACS Catalysis, 2021, 11, 8985-8998.	5.5	10
16	The Uncommon Active Site of D-Amino Acid Transaminase from Haliscomenobacter hydrossis: Biochemical and Structural Insights into the New Enzyme. Molecules, 2021, 26, 5053.	1.7	14
17	Metallo-Î²-Lactamases: Influence of the Active Site Structure on the Mechanisms of Antibiotic Resistance and Inhibition. Biochemistry (Moscow), 2021, 86, S24-S37.	0.7	1
18	Computer Modeling of Structures of Reversibly Switchable Fluorescent Proteins with LOV Domains. Crystallography Reports, 2021, 66, 815-818.	0.1	1

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19	Two Sides of Quantum-Based Modeling of Enzyme-Catalyzed Reactions: Mechanistic and Electronic Structure Aspects of the Hydrolysis by Glutamate Carboxypeptidase. Molecules, 2021, 26, 6280.	1.7	4
20	Modeling Spectral Tuning in Red Fluorescent Proteins Using the Dipole Moment Variation upon Excitation. Journal of Chemical Information and Modeling, 2021, 61, 5125-5132.	2.5	2
21	LSSmScarlet, dCyRFP2s, dCyOFP2s and CRISPRed2s, Genetically Encoded Red Fluorescent Proteins with a Large Stokes Shift. International Journal of Molecular Sciences, 2021, 22, 12887.	1.8	9
22	Discrimination of enzymeâ€“substrate complexes by reactivity using the electron density analysis: peptide bond hydrolysis by the matrix metalloproteinase-2. Mendeleev Communications, 2020, 30, 583-585.	0.6	10
23	Dipole Moment Variation Clears Up Electronic Excitations in the Ï€-Stacked Complexes of Fluorescent Protein Chromophores. Journal of Chemical Information and Modeling, 2020, 60, 6288-6297.	2.5	5
24	Dynamical properties of enzymeâ€“substrate complexes disclose substrate specificity of the SARS-CoV-2 main protease as characterized by the electron density descriptors. Physical Chemistry Chemical Physics, 2020, 22, 19069-19079.	1.3	29
25	Intermediates of the Autocatalytic Reaction of the Formation of a Chromophore in a Green Fluorescent Protein. Russian Journal of Physical Chemistry B, 2020, 14, 457-461.	0.2	4
26	Molecular Mechanism of Stereospecificity toward D-Leucine of the Transaminase from Desulfohalobium retbaense Revealed by Molecular Dynamic Simulations. Moscow University Chemistry Bulletin, 2020, 75, 167-171.	0.2	0
27	Proof of concept for poor inhibitor binding and efficient formation of covalent adducts of KRAS^{G12C} and ARS compounds. Organic and Biomolecular Chemistry, 2020, 18, 3069-3081.	1.5	16
28	Trinuclear copper biocatalytic center forms an active site of thiocyanate dehydrogenase. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 5280-5290.	3.3	19
29	The common trends for the halogen, chalcogen, and pnictogen bonds via sorting principles and local bonding properties. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	20
30	Revealing electronic features governing hydrolysis of cephalosporins in the active site of the L1 metallo-Î²-lactamase. RSC Advances, 2020, 10, 8664-8676.	1.7	9
31	Electronic Steric Factors in the Active Site of Metallo-Î²-Lactamase and Reactivity of Cephalosporin Antibiotics. Moscow University Chemistry Bulletin, 2019, 74, 106-110.	0.2	4
32	The NÂ·Â·Â·H hydrogen bond strength in the transition state at the limiting step determines the reactivity of cephalosporins in the active site of L1 metallo-Î²-lactamase. Mendeleev Communications, 2019, 29, 492-494.	0.6	13
33	Molecular Modeling of Photophysical Properties of Components of FÃ¶rster Resonance Energy Transfer Pairs Containing Flavin-Based Fluorescent Proteins and Their Analogs. Russian Journal of Physical Chemistry B, 2019, 13, 389-393.	0.2	1
34	Reconstructing the Electron Density of Intermediates of the Hydrolysis of N-Acetylaspartate by Aspartoacylase. Russian Journal of Physical Chemistry A, 2019, 93, 1873-1879.	0.1	0
35	Novel flavin-based fluorescent proteins with red-shifted emission bands: a computational study. Photochemical and Photobiological Sciences, 2019, 18, 177-189.	1.6	13
36	Computational Challenges in Modeling of Representative Bioimaging Proteins: GFP-Like Proteins, Flavoproteins, and Phytochromes. Journal of Physical Chemistry B, 2019, 123, 6133-6149.	1.2	38

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37	The QM/MM-QTAIM approach reveals the nature of the different reactivity of cephalosporins in the active site of L1 metallo-Î²-lactamase. New Journal of Chemistry, 2019, 43, 7329-7338.	1.4	25
38	Origin of the Ï€-stacking induced shifts in absorption spectral bands of the green fluorescent protein chromophore. Chemical Physics, 2019, 522, 32-38.	0.9	15
39	Structure and dynamics of photoactivatable adenylyl cyclase. Russian Chemical Bulletin, 2019, 68, 1991-1996.	0.4	1
40	Allosteric Control of N-Acetyl-Aspartate Hydrolysis by the Y231C and F295S Mutants of Human Aspartoacylase. Journal of Chemical Information and Modeling, 2019, 59, 2299-2308.	2.5	6
41	Aspartoacylase: a central nervous system enzyme. Structure, catalytic activity and regulation mechanisms. Russian Chemical Reviews, 2019, 88, 1-26.	2.5	7
42	Effect of solvation water shells on enzyme active sites in zinc-dependent hydrolases. Structural Chemistry, 2019, 30, 481-488.	1.0	4
43	Modeling the Transient Kinetics of the L1 Metallo-Î²-Lactamase. Journal of Physical Chemistry B, 2018, 122, 1378-1386.	1.2	19
44	Towards first-principles calculation of electronic excitations in the ring of the protein-bound bacteriochlorophylls. Chemical Physics, 2018, 505, 34-39.	0.9	6
45	Detection of protease activity by fluorescent protein FRET sensors: from computer simulation to live cells. Methods and Applications in Fluorescence, 2018, 6, 022001.	1.1	18
46	Monomerization of the photoconvertible fluorescent protein SAASoti by rational mutagenesis of single amino acids. Scientific Reports, 2018, 8, 15542.	1.6	8
47	Mechanisms of the Aspartoacylase Catalytic Activity Regulation According to the Computer Modeling Results. Moscow University Chemistry Bulletin, 2018, 73, 152-154.	0.2	0
48	Simulation of Spectra of Red Fluorescent Protein Mutants. Moscow University Chemistry Bulletin, 2018, 73, 212-215.	0.2	4
49	Mechanism of Metallo-Î²-Lactamase Inhibition by Oxacephalosporin Antibiotic. Moscow University Chemistry Bulletin, 2018, 73, 155-157.	0.2	1
50	Competition between two cysteines in covalent binding of biliverdin to phytochrome domains. Organic and Biomolecular Chemistry, 2018, 16, 7518-7529.	1.5	12
51	Amideâ€“imide tautomerization in the glutamine side chain in enzymatic and photochemical reactions in proteins. Physical Chemistry Chemical Physics, 2018, 20, 23827-23836.	1.3	25
52	Molecular mechanism of the dark-state recovery in BLUF photoreceptors. Chemical Physics Letters, 2017, 676, 25-31.	1.2	11
53	Molecular mechanism of interactions between MMP-2 and its oligopeptide-based inhibitors. Mendeleev Communications, 2017, 27, 157-159.	0.6	2
54	Mutants of the Flavoprotein iLOV as Prospective Red-Shifted Fluorescent Markers. Journal of Physical Chemistry B, 2017, 121, 10018-10025.	1.2	25

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55	Three Faces of N-Acetylaspartate: Activator, Substrate, and Inhibitor of Human Aspartoacylase. Journal of Physical Chemistry B, 2017, 121, 9389-9397.	1.2	13
56	Testing the ability of rhodanine and 2, 4-thiazolidinedione to interact with the human pancreatic alpha-amylase: electron-density descriptors complement molecular docking, QM, and QM/MM dynamics calculations. Journal of Molecular Modeling, 2017, 23, 252.	0.8	7
57	Improving the Design of the Triple-Decker Motif in Red Fluorescent Proteins. Journal of Physical Chemistry B, 2017, 121, 10602-10609.	1.2	8
58	Evaluation of the Q y absorption band maximum in a light-harvesting complex of the bacterial photosynthetic center Thermochromatium tepidum. Moscow University Chemistry Bulletin, 2017, 72, 111-114.	0.2	0
59	Supercomputer technologies for structural-kinetic study of mechanisms of enzyme catalysis: A quantum-chemical description of aspartoacylase catalysis. Doklady Physical Chemistry, 2017, 474, 89-92.	0.2	6
60	Spectroscopy of Flavin-Containing Proteins: Theoretical Insights. Springer Series in Chemical Physics, 2017, , 185-188.	0.2	0
61	Methodological aspects of the calculation of the free energy profile of guanosine triphosphate hydrolysis by Ras-GAP protein complex. Moscow University Chemistry Bulletin, 2016, 71, 283-286.	0.2	0
62	Oxoethylene derivative of the natural substrate as an inhibitor of matrix metalloproteinase MMP-2. Mendeleev Communications, 2016, 26, 207-208.	0.6	1
63	Reaction mechanism of matrix metalloproteinases with a catalytically active zinc ion studied by the QM(DFTB)/MM simulations. Mendeleev Communications, 2016, 26, 209-211.	0.6	12
64	Reaction Mechanism of Guanosine Triphosphate Hydrolysis by the Vision-Related Protein Complex Arl3â€“RP2. Journal of Physical Chemistry B, 2016, 120, 3873-3879.	1.2	6
65	Computational characterization of the all-atom structure and the calcium binding sites of the LH1â€“RC core complex from Thermochromatium tepidum. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650020.	1.8	2
66	Modeling the Complete Catalytic Cycle of Aspartoacylase. Journal of Physical Chemistry B, 2016, 120, 4221-4231.	1.2	25
67	Modeling GTP hydrolysis in RasGAP protein complex. Moscow University Chemistry Bulletin, 2016, 71, 21-24.	0.2	0
68	Methodological aspects of QM/MM calculations: A case study on matrix metalloproteinaseâ€2. Journal of Computational Chemistry, 2016, 37, 1801-1809.	1.5	21
69	Theoretical vibrational spectroscopy of intermediates and the reaction mechanism of the guanosine triphosphate hydrolysis by the protein complex Ras-GAP. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 166, 68-72.	2.0	8
70	Mechanism of proteolysis in matrix metalloproteinase-2 revealed by QM/MM modeling. Journal of Computational Chemistry, 2015, 36, 1621-1630.	1.5	36
71	Why does mutation of <scp>G</scp>ln61 in Ras by the nitro analog <scp>NG</scp>ln maintain activity of <scp>R</scp>asâ€<scp>GAP</scp> in hydrolysis of guanosine triphosphate?. Proteins: Structure, Function and Bioinformatics, 2015, 83, 2091-2099.	1.5	9
72	Genetically Encoded FRET-Sensor Based on Terbium Chelate and Red Fluorescent Protein for Detection of Caspase-3 Activity. International Journal of Molecular Sciences, 2015, 16, 16642-16654.	1.8	3

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73	Hydrolysis of Guanosine Triphosphate (GTP) by the RasÂ·GAP Protein Complex: Reaction Mechanism and Kinetic Scheme. Journal of Physical Chemistry B, 2015, 119, 12838-12845.	1.2	50
74	Estimating Orientation Factors in the FRET Theory of Fluorescent Proteins: The TagRFP-KFP Pair and Beyond. Biophysical Journal, 2015, 108, 126-132.	0.2	28
75	On Quantum Chemistry Code Adaptation for RSC PetaStream Architecture. Lecture Notes in Computer Science, 2015, , 113-121.	1.0	4
76	A Light-Induced Reaction with Oxygen Leads to Chromophore Decomposition and Irreversible Photobleaching in GFP-Type Proteins. Journal of Physical Chemistry B, 2015, 119, 5444-5452.	1.2	28
77	Computational characterization of the chemical step in the GTP hydrolysis by Ras-GAP for the wild-type and G13V mutated Ras. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1046-1053.	1.5	19
78	Theoretical Characterization of the Flavin-Based Fluorescent Protein iLOV and its Q489K Mutant. Journal of Physical Chemistry B, 2015, 119, 5176-5183.	1.2	40
79	Computer modeling of properties of complex molecular systems. AIP Conference Proceedings, 2015, , .	0.3	0
80	The photoreaction mechanism in the bacterial blue light receptor BLUF according to metadynamics modeling. Moscow University Chemistry Bulletin, 2014, 69, 149-151.	0.2	2
81	Computer modeling of components of photoreceptor systems. Russian Chemical Bulletin, 2014, 63, 1703-1709.	0.4	1
82	Optical transitions in the light-harvesting complexes of bacterial photosynthetic centers. Moscow University Chemistry Bulletin, 2014, 69, 152-154.	0.2	2
83	Exploration of the Zinc Finger Motif in Controlling Activity of Matrix Metalloproteinases. Journal of Physical Chemistry B, 2014, 118, 13505-13512.	1.2	15
84	Modeling the Role of G12V and G13V Ras Mutations in the Ras-GAP-Catalyzed Hydrolysis Reaction of Guanosine Triphosphate. Biochemistry, 2014, 53, 7093-7099.	1.2	40
85	All-atom structures and calcium binding sites of the bacterial photosynthetic LH1-RC core complex from Thermochromatium tepidum. Journal of Molecular Modeling, 2014, 20, 2287.	0.8	7
86	Catalytic Cycle of Penicillin Acylase from Escherichia coli: QM/MM Modeling of Chemical Transformations in the Enzyme Active Site upon Penicillin G Hydrolysis. ACS Catalysis, 2014, 4, 2521-2529.	5.5	24
87	The structure of the enzyme-substrate complex of the phosphodiesterase catalytic domain with cyclic diguanosine monophosphate. Moscow University Chemistry Bulletin, 2014, 69, 1-4.	0.2	1
88	Computational Characterization of Ketoneâ€“Ketal Transformations at the Active Site of Matrix Metalloproteinases. Journal of Physical Chemistry B, 2014, 118, 4345-4350.	1.2	5
89	Quantum chemical modeling of components of dye-sensitized solar cells. Moscow University Chemistry Bulletin, 2013, 68, 77-79.	0.2	2
90	Molecular model of LH1 light-harvesting complex of the photosynthetic center of Thermochromatium tepidum bacteria. Moscow University Chemistry Bulletin, 2013, 68, 80-82.	0.2	2

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91	Quantum chemistry in studies of fluorescent and photosensing proteins. International Journal of Quantum Chemistry, 2013, 113, 1828-1832.	1.0	2
92	Thermal Isomerization of the Chromoprotein asFP595 and Its Kindling Mutant A143G: QM/MM Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2013, 117, 13507-13514.	1.2	10
93	Molecular modeling of the FÃ¶rster resonance energy transfer between FusionRed and Dedushka(eqFP670) fluorescent proteins. , 2013, , .		1
94	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.	1.2	50
95	Minimum energy reaction profiles for the hydrolysis reaction of the cyclic guanosine monophosphate in water: Comparison of the results of two QM/MM approaches. Computational and Theoretical Chemistry, 2012, 983, 88-94.	1.1	8
96	FLIM-FRET Imaging of Caspase-3 Activity in Live Cells Using Pair of Red Fluorescent Proteins. Theranostics, 2012, 2, 215-226.	4.6	35
97	Effect of Protein Environment on Electronically Excited and Ionized States of the Green Fluorescent Protein Chromophore. Journal of Physical Chemistry B, 2011, 115, 8296-8303.	1.2	87
98	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.	1.3	26
99	Modeling the mechanism of hydrolysis of cyclic guanosine monophosphates in aqueous solution. Moscow University Chemistry Bulletin, 2011, 66, 229-231.	0.2	2
100	Coupling between the BLUF and EAL domains in the blue light-regulated phosphodiesterase BlrP1. Journal of Molecular Modeling, 2011, 17, 1579-1586.	0.8	17
101	Algorithms of the flexible effective fragment method used for modeling of transformations in enzyme active sites. Moscow University Chemistry Bulletin, 2010, 65, 355-357.	0.2	2
102	Quantum Chemistry Calculations Provide Support to the Mechanism of the Light-Induced Structural Changes in the Flavin-Binding Photoreceptor Proteins. Journal of Chemical Theory and Computation, 2010, 6, 2293-2302.	2.3	38
103	Modeling reaction routes from rhodopsin to bathorhodopsin. Proteins: Structure, Function and Bioinformatics, 2010, 78, 614-622.	1.5	19
104	Studies on the conformational state of the chromophore group (11-cis-retinal) in rhodopsin by computer molecular simulation methods. Biophysics (Russian Federation), 2009, 54, 465-470.	0.2	1
105	Screen-printed ion-selective electrodes covered with membranes containing ionic liquids. Mendeleev Communications, 2008, 18, 88-89.	0.6	28
106	Ionic liquid based on a quaternary phosphonium cation as a plasticizer and an electrode-active component of ion-selective electrode membranes. Moscow University Chemistry Bulletin, 2007, 62, 48-51.	0.2	3
107	Ionic Liquids Plasticize and Bring Ion-Sensing Ability to Polymer Membranes of Selective Electrodes. Electroanalysis, 2006, 18, 1416-1421.	1.5	75
108	Interplay between the Enamine and Imine Forms of the Hydrolyzed Imipenem in the Active Sites of Metallo-Î²-lactamases and in Water Solution. Journal of Chemical Information and Modeling, 0, , .	2.5	3