Alexander V Nemukhin

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

207 papers	3,595 citations	31 h-index	49 g-index
223 ext. papers	3,933 ext. citations	4 avg, IF	5.53 L-index

#	Paper	IF	Citations
207	Spontaneous Reactivation of OPC-Inhibited BChE Mutants: Modeling of Mechanisms. *Russian Journal of Physical Chemistry B*, **2022**, 16, 103-108	1.2	0
206	Two Sides of Quantum-Based Modeling of Enzyme-Catalyzed Reactions: Mechanistic and Electronic Structure Aspects of the Hydrolysis by Glutamate Carboxypeptidase. *Molecules*, **2021**, 26,	4.8	1
205	Modeling Spectral Tuning in Red Fluorescent Proteins Using the Dipole Moment Variation upon Excitation. *Journal of Chemical Information and Modeling*, **2021**, 61, 5125-5132	6.1	0
204	QM/MM Approaches Shed Light on GFP Puzzles. *Challenges and Advances in Computational Chemistry and Physics*, **2021**, 271-292	0.7	2
203	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,	4.8	2
202	Molecular Modeling Reveals the Mechanism of Ran-RanGAP-Catalyzed Guanosine Triphosphate Hydrolysis without an Arginine Finger. *ACS Catalysis*, **2021**, 11, 8985-8998	13.1	3
201	Stalling chromophore synthesis of the fluorescent protein Venus reveals the molecular basis of the final oxidation step. *Chemical Science*, **2021**, 12, 7735-7745	9.4	5
200	Model of the RNA Polymerase Complex of the SARS-CoV-2 Virus with Favipiravir. *Russian Journal of Physical Chemistry B*, **2021**, 15, 103-107	1.2	1
199	Interplay between Locally Excited and Charge Transfer States Governs the Photoswitching Mechanism in the Fluorescent Protein Dreiklang. *Journal of Physical Chemistry B*, **2021**, 125, 757-770	3.4	5
198	Modeling photophysical properties of the bacteriophytochrome-based fluorescent protein IFP1.4. *Journal of Chemical Physics*, **2021**, 154, 065101	3.9	1
197	Frontiers in Multiscale Modeling of Photoreceptor Proteins. *Photochemistry and Photobiology*, **2021** , 97, 243-269	3.6	8
196	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	6.1	5
195	Tuning Electrostatic Gating of Semiconducting Carbon Nanotubes by Controlling Protein Orientation in Biosensing Devices. *Angewandte Chemie - International Edition*, **2021**, 60, 20184-20189	16.4	3
194	Tuning Electrostatic Gating of Semiconducting Carbon Nanotubes by Controlling Protein Orientation in Biosensing Devices. *Angewandte Chemie*, **2021**, 133, 20346-20351	3.6	0
193	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	6.4	1
192	Supercomputer simulation of the covalent inhibition of the main protease of SARS-CoV-2.. *Russian Chemical Bulletin*, **2021**, 70, 2084-2089	1.7	2
191	Theoretical characterization of the photochemical reaction CO2 + O(3P) -lCO + O2 related to experiments in solid krypton. *Chemical Physics Letters*, **2020**, 746, 137303	2.5	1

190	Structure of the Brain -Acetylaspartate Biosynthetic Enzyme NAT8L Revealed by Computer Modeling. *ACS Chemical Neuroscience*, **2020**, 11, 2296-2302	5.7	1
189	Proof of concept for poor inhibitor binding and efficient formation of covalent adducts of KRAS and ARS compounds. *Organic and Biomolecular Chemistry*, **2020**, 18, 3069-3081	3.9	10
188	Mechanisms of ATP to cAMP Conversion Catalyzed by the Mammalian Adenylyl Cyclase: A Role of Magnesium Coordination Shells and Proton Wires. *Journal of Physical Chemistry B*, **2020**, 124, 451-460	3.4	7
187	Discrimination of enzyme–substrate complexes by reactivity using the electron density analysis: peptide bond hydrolysis by the matrix metalloproteinase-2. *Mendeleev Communications*, **2020**, 30, 583-585	1.9	7
186	Dipole Moment Variation Clears Up Electronic Excitations in the π-Stacked Complexes of Fluorescent Protein Chromophores. *Journal of Chemical Information and Modeling*, **2020**, 60, 6288-6297	6.1	1
185	Dynamical properties of enzyme-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	3.6	13
184	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	1.2	2
183	Molecular Modeling of Photophysical Properties of Components of Förster Resonance Energy Transfer Pairs Containing Flavin-Based Fluorescent Proteins and Their Analogs. *Russian Journal of Physical Chemistry B*, **2019**, 13, 389-393	1.2	1
182	Novel flavin-based fluorescent proteins with red-shifted emission bands: a computational study. *Photochemical and Photobiological Sciences*, **2019**, 18, 177-189	4.2	10
181	Diversity of mechanisms in Ras-GAP catalysis of guanosine triphosphate hydrolysis revealed by molecular modeling. *Organic and Biomolecular Chemistry*, **2019**, 17, 4879-4891	3.9	10
180	Computer-designed active human butyrylcholinesterase double mutant with a new catalytic triad. *Chemico-Biological Interactions*, **2019**, 306, 138-146	5	30
179	Computational Challenges in Modeling of Representative Bioimaging Proteins: GFP-Like Proteins, Flavoproteins, and Phytochromes. *Journal of Physical Chemistry B*, **2019**, 123, 6133-6149	3.4	25
178	Modeling of the glycine tripeptide cyclization in the Ser65Gly/Tyr66Gly mutant of green fluorescent protein. *Mendeleev Communications*, **2019**, 29, 187-189	1.9	6
177	Computational Modeling Reveals the Mechanism of Fluorescent State Recovery in the Reversibly Photoswitchable Protein Dreiklang. *Journal of Physical Chemistry B*, **2019**, 123, 8901-8909	3.4	5
176	Origin of the π-stacking induced shifts in absorption spectral bands of the green fluorescent protein chromophore. *Chemical Physics*, **2019**, 522, 32-38	2.3	10
175	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	6.1	5
174	Aspartoacylase: a central nervous system enzyme. Structure, catalytic activity and regulation mechanisms. *Russian Chemical Reviews*, **2019**, 88, 1-26	6.8	5
173	Effect of solvation water shells on enzyme active sites in zinc-dependent hydrolases. *Structural Chemistry*, **2019**, 30, 481-488	1.8	3

172	Modeling the Transient Kinetics of the L1 Metallo-β-Lactamase. *Journal of Physical Chemistry B*, **2018**, 122, 1378-1386	3.4	15
171	Towards first-principles calculation of electronic excitations in the ring of the protein-bound bacteriochlorophylls. *Chemical Physics*, **2018**, 505, 34-39	2.3	3
170	Optimization of Cholinesterase-Based Catalytic Bioscavengers Against Organophosphorus Agents. *Frontiers in Pharmacology*, **2018**, 9, 211	5.6	52
169	Mechanisms of the Aspartoacylase Catalytic Activity Regulation According to the Computer Modeling Results. *Moscow University Chemistry Bulletin*, **2018**, 73, 152-154	0.5	
168	Simulation of Spectra of Red Fluorescent Protein Mutants. *Moscow University Chemistry Bulletin*, **2018**, 73, 212-215	0.5	3
167	Mechanism of Metallo-β-Lactamase Inhibition by Oxacephalosporin Antibiotic. *Moscow University Chemistry Bulletin*, **2018**, 73, 155-157	0.5	0
166	Competition between two cysteines in covalent binding of biliverdin to phytochrome domains. *Organic and Biomolecular Chemistry*, **2018**, 16, 7518-7529	3.9	9
165	Modeling structure and excitation of biliverdin-binding domains in infrared fluorescent proteins. *Chemical Physics Letters*, **2018**, 710, 59-63	2.5	12
164	Amide-imide tautomerization in the glutamine side chain in enzymatic and photochemical reactions in proteins. *Physical Chemistry Chemical Physics*, **2018**, 20, 23827-23836	3.6	17
163	Molecular mechanism of the dark-state recovery in BLUF photoreceptors. *Chemical Physics Letters*, **2017**, 676, 25-31	2.5	8
162	Mutants of the Flavoprotein iLOV as Prospective Red-Shifted Fluorescent Markers. *Journal of Physical Chemistry B*, **2017**, 121, 10018-10025	3.4	16
161	Three Faces of N-Acetylaspartate: Activator, Substrate, and Inhibitor of Human Aspartoacylase. *Journal of Physical Chemistry B*, **2017**, 121, 9389-9397	3.4	12
160	Role of Protein Dimeric Interface in Allosteric Inhibition of N-Acetyl-Aspartate Hydrolysis by Human Aspartoacylase. *Journal of Chemical Information and Modeling*, **2017**, 57, 1999-2008	6.1	17
159	Improving the Design of the Triple-Decker Motif in Red Fluorescent Proteins. *Journal of Physical Chemistry B*, **2017**, 121, 10602-10609	3.4	6
158	Molecular Modeling Clarifies the Mechanism of Chromophore Maturation in the Green Fluorescent Protein. *Journal of the American Chemical Society*, **2017**, 139, 10239-10249	16.4	31
157	Photoinduced Chemistry in Fluorescent Proteins: Curse or Blessing?. *Chemical Reviews*, **2017**, 117, 758-795	53.1	154
156	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	0.5	
155	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	0.8	5

154	Computer simulation in molecular medicine and drug design. *Herald of the Russian Academy of Sciences*, **2016**, 86, 185-192	0.7	2
153	Modeling hydrolysis of the cyclic dimeric guanosine monophosphate by phosphodiesterases. *Moscow University Chemistry Bulletin*, **2016**, 71, 12-15	0.5	1
152	Methodological aspects of QM/MM calculations: A case study on matrix metalloproteinase-2. *Journal of Computational Chemistry*, **2016**, 37, 1801-9	3.5	17
151	Understanding the non-catalytic behavior of human butyrylcholinesterase silent variants: Comparison of wild-type enzyme, catalytically active Ala328Cys mutant, and silent Ala328Asp variant. *Chemico-Biological Interactions*, **2016**, 259, 223-232	5	7
150	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	4.4	6
149	Molecular polymorphism of human enzymes as the basis of individual sensitivity to drugs. Supercomputer-assisted modeling as a tool for analysis of structural changes and enzymatic activity of proteins. *Russian Chemical Bulletin*, **2016**, 65, 1592-1607	1.7	6
148	Reaction mechanism of matrix metalloproteinases with a catalytically active zinc ion studied by the QM(DFTB)/MM simulations. *Mendeleev Communications*, **2016**, 26, 209-211	1.9	8
147	Reaction Mechanism of Guanosine Triphosphate Hydrolysis by the Vision-Related Protein Complex Arl3-RP2. *Journal of Physical Chemistry B*, **2016**, 120, 3873-9	3.4	5
146	Computational characterization of the all-atom structure and the calcium binding sites of the LH1-RC core complex from Thermochromatium tepidum. *Journal of Theoretical and Computational Chemistry*, **2016**, 15, 1650020	1.8	2
145	Modeling the Complete Catalytic Cycle of Aspartoacylase. *Journal of Physical Chemistry B*, **2016**, 120, 4221-31	3.4	20
144	Analysis of proton wires in the enzyme active site suggests a mechanism of c-di-GMP hydrolysis by the EAL domain phosphodiesterases. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 1670-1680	4.2	4
143	A Light-Induced Reaction with Oxygen Leads to Chromophore Decomposition and Irreversible Photobleaching in GFP-Type Proteins. *Journal of Physical Chemistry B*, **2015**, 119, 5444-52	3.4	23
142	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, 1046-53	4.2	14
141	Theoretical Characterization of the Flavin-Based Fluorescent Protein iLOV and its Q489K Mutant. *Journal of Physical Chemistry B*, **2015**, 119, 5176-83	3.4	29
140	Modeling reactivation of the phosphorylated human butyrylcholinesterase by QM(DFTB)/MM calculations. *Journal of Theoretical and Computational Chemistry*, **2015**, 14, 1550051	1.8	11
139	Toward molecular mechanism of xenon anesthesia: a link to studies of xenon complexes with small aromatic molecules. *Journal of Physical Chemistry A*, **2015**, 119, 2517-21	2.8	10
138	Interaction of aromatic compounds with xenon: spectroscopic and computational characterization for the cases of p-cresol and toluene. *Journal of Physical Chemistry A*, **2015**, 119, 2587-93	2.8	15
137	Role of zwitterions in kindling fluorescent protein photochemistry. *Journal of Physical Chemistry B*, **2015**, 119, 2467-74	3.4	7

136	Mechanism of proteolysis in matrix metalloproteinase-2 revealed by QM/MM modeling. *Journal of Computational Chemistry*, **2015**, 36, 1621-30	3.5	28
135	Why does mutation of Gln61 in Ras by the nitro analog NGln maintain activity of Ras-GAP in hydrolysis of guanosine triphosphate?. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 2091-9	4.2	9
134	Modeling chemical transformations at the active sites of cholinesterases by quantum-based simulations. *Moscow University Chemistry Bulletin*, **2015**, 70, 274-277	0.5	7
133	Hydrolysis of Guanosine Triphosphate (GTP) by the Ras-GAP Protein Complex: Reaction Mechanism and Kinetic Scheme. *Journal of Physical Chemistry B*, **2015**, 119, 12838-45	3.4	37
132	Estimating orientation factors in the FRET theory of fluorescent proteins: the TagRFP-KFP pair and beyond. *Biophysical Journal*, **2015**, 108, 126-32	2.9	19
131	Molecular modeling evidence for His438 flip in the mechanism of butyrylcholinesterase hysteretic behavior. *Journal of Molecular Neuroscience*, **2014**, 52, 434-45	3.3	13
130	Exploration of the zinc finger motif in controlling activity of matrix metalloproteinases. *Journal of Physical Chemistry B*, **2014**, 118, 13505-12	3.4	11
129	Modeling the role of G12V and G13V Ras mutations in the Ras-GAP-catalyzed hydrolysis reaction of guanosine triphosphate. *Biochemistry*, **2014**, 53, 7093-9	3.2	31
128	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	2	5
127	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	13.1	19
126	The structure of the enzyme-substrate complex of the phosphodiesterase catalytic domain with cyclic diguanosine monophosphate. *Moscow University Chemistry Bulletin*, **2014**, 69, 1-4	0.5	1
125	Computational characterization of ketone-ketal transformations at the active site of matrix metalloproteinases. *Journal of Physical Chemistry B*, **2014**, 118, 4345-50	3.4	5
124	The photoreaction mechanism in the bacterial blue light receptor BLUF according to metadynamics modeling. *Moscow University Chemistry Bulletin*, **2014**, 69, 149-151	0.5	2
123	Computer modeling of components of photoreceptor systems. *Russian Chemical Bulletin*, **2014**, 63, 1703-1709	1.7	1
122	Optical transitions in the light-harvesting complexes of bacterial photosynthetic centers. *Moscow University Chemistry Bulletin*, **2014**, 69, 152-154	0.5	2
121	First-principles characterization of the energy landscape and optical spectra of green fluorescent protein along the A-I-B proton transfer route. *Journal of the American Chemical Society*, **2013**, 135, 11541-9	16.4	55
120	Quantum chemical modeling of components of dye-sensitized solar cells. *Moscow University Chemistry Bulletin*, **2013**, 68, 77-79	0.5	2
119	Molecular model of LH1 light-harvesting complex of the photosynthetic center of Thermochromatium tepidum bacteria. *Moscow University Chemistry Bulletin*, **2013**, 68, 80-82	0.5	2

118	On quantum mechanical--molecular mechanical (QM/MM) approaches to model hydrolysis of acetylcholine by acetylcholinesterase. *Chemico-Biological Interactions*, **2013**, 203, 51-6	5	14
117	Quantum chemistry in studies of fluorescent and photosensing proteins. *International Journal of Quantum Chemistry*, **2013**, 113, 1828-1832	2.1	2
116	Thermal isomerization of the chromoprotein asFP595 and its kindling mutant A143G: QM/MM molecular dynamics simulations. *Journal of Physical Chemistry B*, **2013**, 117, 13507-14	3.4	7
115	Towards quantum-based modeling of enzymatic reaction pathways: Application to the acetylholinesterase catalysis. *Chemical Physics Letters*, **2013**, 556, 251-255	2.5	7
114	Molecular modeling of the Förster resonance energy transfer between FusionRed and Dedushka(eqFP670) fluorescent proteins **2013**,		1
113	Unusual emitting states of the kindling fluorescent protein: appearance of the cationic chromophore in the GFP family. *Journal of Physical Chemistry B*, **2013**, 117, 7228-34	3.4	12
112	Triple-Decker Motif for Red-Shifted Fluorescent Protein Mutants. *Journal of Physical Chemistry Letters*, **2013**, 4, 1743-7	6.4	25
111	Photoinduced electron transfer facilitates tautomerization of the conserved signaling glutamine side chain in BLUF protein light sensors. *Journal of Physical Chemistry B*, **2013**, 117, 2369-77	3.4	39
110	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	2	7
109	Interaction of phenol with xenon and nitrogen: spectroscopic and computational characterization. *Journal of Chemical Physics*, **2012**, 137, 134305	3.9	12
108	Quantum chemistry behind bioimaging: insights from ab initio studies of fluorescent proteins and their chromophores. *Accounts of Chemical Research*, **2012**, 45, 265-75	24.3	114
107	FLIM-FRET Imaging of Caspase-3 Activity in Live Cells Using Pair of Red Fluorescent Proteins. *Theranostics*, **2012**, 2, 215-26	12.1	28
106	Exploring structural and optical properties of fluorescent proteins by squeezing: modeling high-pressure effects on the mStrawberry and mCherry red fluorescent proteins. *Journal of Physical Chemistry B*, **2012**, 116, 12426-40	3.4	26
105	Quantum chemical modelling in the research of molecular mechanisms of enzymatic catalysis. *Russian Chemical Reviews*, **2012**, 81, 1011-1025	6.8	26
104	Modeling absorption of the kindling fluorescent protein with the neutral form of the chromophore. *International Journal of Quantum Chemistry*, **2012**, 112, 2947-2951	2.1	7
103	Toward Molecular-Level Characterization of Photoinduced Decarboxylation of the Green Fluorescent Protein: Accessibility of the Charge-Transfer States. *Journal of Chemical Theory and Computation*, **2012**, 8, 1912-20	6.4	22
102	On the Mechanism of Carborane Diffusion on a Hydrated Silica Surface. *Journal of Physical Chemistry C*, **2011**, 115, 108-111	3.8	11
101	Quantum mechanical/molecular mechanical analysis of mechanisms of enzyme action. Human acetylcholinesterase. *Russian Chemical Bulletin*, **2011**, 60, 2196-2204	1.7	1

100	Effect of protein environment on electronically excited and ionized states of the green fluorescent protein chromophore. *Journal of Physical Chemistry B*, **2011**, 115, 8296-303	3.4	82
99	Computational characterization of reaction intermediates in the photocycle of the sensory domain of the AppA blue light photoreceptor. *Photochemistry and Photobiology*, **2011**, 87, 564-73	3.6	23
98	Minimum energy reaction profiles for ATP hydrolysis in myosin. *Journal of Molecular Graphics and Modelling*, **2011**, 31, 1-4	2.8	24
97	Matrix-isolation study of the phenol–water complex and phenol dimer. *Chemical Physics Letters*, **2011**, 517, 9-15	2.5	22
96	Conformational partitioning in pH-induced fluorescence of the kindling fluorescent protein (KFP). *Journal of Physical Chemistry B*, **2011**, 115, 9195-201	3.4	11
95	Modeling of calcium binding in the light-harvesting complex of photosynthetic reaction center of the Thermochromatium tepidum bacterium. *Moscow University Chemistry Bulletin*, **2011**, 66, 80-82	0.5	4
94	Modeling the mechanism of hydrolysis of cyclic guanosine monophosphates in aqueous solution. *Moscow University Chemistry Bulletin*, **2011**, 66, 229-231	0.5	2
93	Coupling between the BLUF and EAL domains in the blue light-regulated phosphodiesterase BlrP1. *Journal of Molecular Modeling*, **2011**, 17, 1579-86	2	15
92	The origin of radiationless conversion of the excited state in the kindling fluorescent protein (KFP): femtosecond studies and quantum modeling. *Laser Physics Letters*, **2011**, 8, 469-474	1.5	7
91	Computational strategy for tuning spectral properties of red fluorescent proteins. *Biophysical Chemistry*, **2011**, 158, 91-5	3.5	18
90	Modeling Structures and Spectra of Trapped Species in Low-Temperature Matrices **2011**, 447-468		
89	Free Energy Barriers for the N-Terminal Asparagine to Succinimide Conversion: Quantum Molecular Dynamics Simulations for the Fully Solvated Model. *Journal of Chemical Theory and Computation*, **2010**, 6, 184-9	6.4	17
88	Rigid-Body Molecular Dynamics of Fullerene-Based Nanocars on Metallic Surfaces. *Journal of Chemical Theory and Computation*, **2010**, 6, 2581-90	6.4	31
87	Potential Energy Landscape of the Electronic States of the GFP Chromophore in Different Protonation Forms: Electronic Transition Energies and Conical Intersections. *Journal of Chemical Theory and Computation*, **2010**, 6, 2377-87	6.4	95
86	Diffusion of fullerene-based nanocars on the surface of a gold crystal. *Moscow University Chemistry Bulletin*, **2010**, 65, 219-220	0.5	6
85	Algorithms of the flexible effective fragment method used for modeling of transformations in enzyme active sites. *Moscow University Chemistry Bulletin*, **2010**, 65, 355-357	0.5	1
84	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, 2293-302	6.4	36
83	Modeling spectral tuning in monomeric teal fluorescent protein mTFP1. *Biophysical Chemistry*, **2010** , 149, 78-82	3.5	14

82	Modeling of the mechanism of hydrolysis of succinylcholine in the active site of native and modified (Asp70Gly) human butyrylcholinesterase. *Russian Chemical Bulletin*, **2010**, 59, 55-60	1.7	5
81	Correlation between the substrate structure and the rate of acetylcholinesterase hydrolysis modeled with the combined quantum mechanical/molecular mechanical studies. *Chemico-Biological Interactions*, **2010**, 187, 59-63	5	4
80	Modeling negative ion defect migration through the gramicidin A channel. *Journal of Molecular Modeling*, **2009**, 15, 1009-12	2	2
79	On photoabsorption of the neutral form of the green fluorescent protein chromophore. *Biophysical Chemistry*, **2009**, 145, 1-6	3.5	20
78	Simulated 18O kinetic isotope effects in enzymatic hydrolysis of guanosine triphosphate. *Biochemistry (Moscow)*, **2009**, 74, 1044-8	2.9	4
77	Quantum chemical justification of the specificity of enzyme catalysis: Correlations between the rate of enzyme catalysis by acetylcholinesterase and substrate structure. *Doklady Physical Chemistry*, **2009**, 426, 98-100	0.8	
76	Gas phase absorption studies of photoactive yellow protein chromophore derivatives. *Journal of Physical Chemistry A*, **2009**, 113, 9442-9	2.8	52
75	Conformation-dependent chemical reaction of formic acid with an oxygen atom. *Journal of Physical Chemistry A*, **2009**, 113, 8143-6	2.8	30
74	Quantum Chemical Benchmark Studies of the Electronic Properties of the Green Fluorescent Protein Chromophore: 2. Cis-Trans Isomerization in Water. *Journal of Chemical Theory and Computation*, **2009**, 5, 1907-14	6.4	42
73	Quantum Chemical Benchmark Studies of the Electronic Properties of the Green Fluorescent Protein Chromophore. 1. Electronically Excited and Ionized States of the Anionic Chromophore in the Gas Phase. *Journal of Chemical Theory and Computation*, **2009**, 5, 1895-906	6.4	104
72	Opening the Arg-Glu salt bridge in myosin: computational study. *Physical Chemistry Chemical Physics*, **2009**, 11, 4804-7	3.6	6
71	Molecular models predict light-induced glutamine tautomerization in BLUF photoreceptors. *Biophysical Journal*, **2008**, 94, 3872-9	2.9	103
70	Molecular Dynamics of Surface-Moving Thermally Driven Nanocars. *Journal of Chemical Theory and Computation*, **2008**, 4, 652-6	6.4	55
69	Modeling photoabsorption of the asFP595 chromophore. *Journal of Physical Chemistry A*, **2008**, 112, 8804-10	2.8	30
68	Hindered rotation of HArF in solid argon: Infrared spectroscopy and a theoretical model. *Physical Review B*, **2008**, 77,	3.3	12
67	Conformation dependence of pKa's of the chromophores from the purple asFP595 and yellow zFP538 fluorescent proteins. *Computational and Theoretical Chemistry*, **2008**, 863, 39-43		12
66	Characterization of a complete cycle of acetylcholinesterase catalysis by ab initio QM/MM modeling. *Journal of Molecular Modeling*, **2008**, 14, 409-16	2	64
65	Theoretical characterization of the 1,3-diazaazulene molecule and its derivatives. *Computational and Theoretical Chemistry*, **2008**, 855, 40-44		4

64	Mechanisms of enzymatic hydrolysis of nucleoside triphosphates by quantum and molecular mechanics. *Russian Journal of General Chemistry*, **2008**, 78, 696-703	0.7	
63	Modeling of the structure and electronic spectra of green fluorescent protein chromophore. *Russian Journal of Physical Chemistry B*, **2008**, 2, 671-675	1.2	24
62	Simulation of proton transport in the gramicidin A channel. *Moscow University Chemistry Bulletin*, **2008**, 63, 241-244	0.5	
61	Structure of the enzyme-substrate complex for guanosine triphosphate hydrolysis by elongation factor EF-Tu: Comparison of quantum mechanics/molecular mechanics and molecular dynamics results. *Moscow University Chemistry Bulletin*, **2008**, 63, 321-323	0.5	1
60	Impact of pyrophosphate and O-ethyl-substituted pyrophosphate groups on DNA structure. *Journal of Physical Chemistry B*, **2007**, 111, 432-8	3.4	9
59	Photochemical synthesis of H2O2 from the H2O...O(3P) van der Waals complex: experimental observations in solid krypton and theoretical modeling. *Journal of Physical Chemistry A*, **2007**, 111, 11444-9	2.8	15
58	Performance of the spin-flip and multireference methods for bond breaking in hydrocarbons: a benchmark study. *Journal of Physical Chemistry A*, **2007**, 111, 13264-71	2.8	30
57	Experimental and theoretical studies of the products of reaction between Ln(hfa)3 and Cu(acac)2 (Ln=La, Y; acac=acetylacetonate, hfa=hexafluoroacetylacetonate). *Journal of Molecular Structure*, **2007**, 831, 46-54	3.4	4
56	Mixed-ligand complexes based on asymmetric gadolinium β-diketonates: Synthesis, crystal structure, and theoretical modeling. *Russian Journal of Inorganic Chemistry*, **2007**, 52, 1365-1377	1.5	1
55	The role of magnesium in hydrolysis of triphosphates in water: Quantum mechanical/molecular mechanical modeling. *Moscow University Chemistry Bulletin*, **2007**, 62, 123-127	0.5	1
54	Implementation of a molecular dynamics approach with rigid fragments to simulation of chemical reactions in biomolecular systems. *Moscow University Chemistry Bulletin*, **2007**, 62, 177-179	0.5	2
53	Mechanism of the myosin catalyzed hydrolysis of ATP as rationalized by molecular modeling. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 7057-61	11.5	64
52	Investigation of matrix-isolated species: spectroscopy and molecular modelling. *Russian Chemical Reviews*, **2007**, 76, 1085-1092	6.8	4
51	An opsin shift in rhodopsin: retinal S0-S1 excitation in protein, in solution, and in the gas phase. *Journal of the American Chemical Society*, **2007**, 129, 13035-42	16.4	90
50	Mechanisms of guanosine triphosphate hydrolysis by Ras and Ras-GAP proteins as rationalized by ab initio QM/MM simulations. *Proteins: Structure, Function and Bioinformatics*, **2007**, 66, 456-66	4.2	76
49	Accurate modeling of the S 0 -S 1 photo-absorption in biological chromophores **2007**,		6
48	On the nature of oxoiron (IV) intermediate in dioxygen activation by non-heme enzymes. *Theoretical Chemistry Accounts*, **2006**, 115, 348-353	1.9	18
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