Alexander V Nemukhin

List of Publications by Citations

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	Photoinduced Chemistry in Fluorescent Proteins: Curse or Blessing?. *Chemical Reviews*, **2017**, 117, 758-795	55.1	154
206	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
205	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
204	Molecular models predict light-induced glutamine tautomerization in BLUF photoreceptors. *Biophysical Journal*, **2008**, 94, 3872-9	2.9	103
203	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
202	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
201	Intermolecular complexes of HXeOH with water: stabilization and destabilization effects. *Journal of the American Chemical Society*, **2002**, 124, 10706-11	16.4	86
200	QM/MM modeling the Ras-GAP catalyzed hydrolysis of guanosine triphosphate. *Proteins: Structure, Function and Bioinformatics*, **2005**, 60, 495-503	4.2	84
199	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
198	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
197	Characterization of a complete cycle of acetylcholinesterase catalysis by ab initio QM/MM modeling. *Journal of Molecular Modeling*, **2008**, 14, 409-16	2	64
196	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
195	Flexible effective fragment QM/MM method: validation through the challenging tests. *Journal of Computational Chemistry*, **2003**, 24, 1410-20	3.5	61
194	Modeling of Biomolecular Systems with the Quantum Mechanical and Molecular Mechanical Method Based on the Effective Fragment Potential Technique: Proposal of Flexible Fragments. *Journal of Physical Chemistry A*, **2002**, 106, 10663-10672	2.8	60
193	Mechanism of triphosphate hydrolysis in aqueous solution: QM/MM simulations in water clusters. *Journal of Physical Chemistry B*, **2006**, 110, 4407-12	3.4	56
192	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
191	Molecular Dynamics of Surface-Moving Thermally Driven Nanocars. *Journal of Chemical Theory and Computation*, **2008**, 4, 652-6	6.4	55

190	Optimization of Cholinesterase-Based Catalytic Bioscavengers Against Organophosphorus Agents. *Frontiers in Pharmacology*, **2018**, 9, 211	5.6	52
189	Gas phase absorption studies of photoactive yellow protein chromophore derivatives. *Journal of Physical Chemistry A*, **2009**, 113, 9442-9	2.8	52
188	Electronic Excitations of the Chromophore from the Fluorescent Protein asFP595 in Solutions. *Journal of Chemical Theory and Computation*, **2006**, 2, 292-9	6.4	44
187	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
186	Quantum chemical modeling of the GTP hydrolysis by the RAS-GAP protein complex. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2004**, 1700, 125-36	4	40
185	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
184	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
183	A QM/MM approach with effective fragment potentials applied to the dipeptide□water structures. *Computational and Theoretical Chemistry*, **2002**, 581, 167-175		37
182	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
181	Modeling of serine protease prototype reactions with the flexible effective fragment potential quantum mechanical/molecular mechanical method. *Theoretical Chemistry Accounts*, **2004**, 111, 36-48	1.9	36
180	On the Origin of Potential Barrier for the Reaction OH- + CO2 -lHCO3- in Water: Studies by Using Continuum and Cluster Solvation Methods. *Journal of Physical Chemistry B*, **2002**, 106, 1734-1740	3.4	32
179	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
178	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
177	Rigid-Body Molecular Dynamics of Fullerene-Based Nanocars on Metallic Surfaces. *Journal of Chemical Theory and Computation*, **2010**, 6, 2581-90	6.4	31
176	Computer-designed active human butyrylcholinesterase double mutant with a new catalytic triad. *Chemico-Biological Interactions*, **2019**, 306, 138-146	5	30
175	Conformation-dependent chemical reaction of formic acid with an oxygen atom. *Journal of Physical Chemistry A*, **2009**, 113, 8143-6	2.8	30
174	Modeling photoabsorption of the asFP595 chromophore. *Journal of Physical Chemistry A*, **2008**, 112, 8804-10	2.8	30
173	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

172	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
171	Ground-state structures and vertical excitations for the kindling fluorescent protein asFP595. *Journal of Physical Chemistry B*, **2006**, 110, 18635-40	3.4	29
170	Mechanism of proteolysis in matrix metalloproteinase-2 revealed by QM/MM modeling. *Journal of Computational Chemistry*, **2015**, 36, 1621-30	3.5	28
169	FLIM-FRET Imaging of Caspase-3 Activity in Live Cells Using Pair of Red Fluorescent Proteins. *Theranostics*, **2012**, 2, 215-26	12.1	28
168	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
167	Quantum chemical modelling in the research of molecular mechanisms of enzymatic catalysis. *Russian Chemical Reviews*, **2012**, 81, 1011-1025	6.8	26
166	Hybrid DIM-based QM/MM approach applied to vibrational spectra and trapping site structures of HArF in solid argon. *Chemical Physics Letters*, **2005**, 405, 165-171	2.5	26
165	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
164	Triple-Decker Motif for Red-Shifted Fluorescent Protein Mutants. *Journal of Physical Chemistry Letters*, **2013**, 4, 1743-7	6.4	25
163	Minimum energy reaction profiles for ATP hydrolysis in myosin. *Journal of Molecular Graphics and Modelling*, **2011**, 31, 1-4	2.8	24
162	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
161	Hybrid diatomics-in-molecules-based quantum mechanical/molecular mechanical approach applied to the modeling of structures and spectra of mixed molecular clusters Arn(HCl)m and Arn(HF)m. *Journal of Chemical Physics*, **2004**, 120, 3732-43	3.9	24
160	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
159	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
158	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
157	Matrix-isolation study of the phenol–water complex and phenol dimer. *Chemical Physics Letters*, **2011**, 517, 9-15	2.5	22
156	Quantum chemical modeling of reaction mechanism for 2-oxoglutarate dependent enzymes: effect of substitution of iron by nickel and cobalt. *Journal of Physical Chemistry A*, **2006**, 110, 4223-8	2.8	22
155	trans and cis Chromophore structures in the kindling fluorescent protein asFP595. *Chemical Physics Letters*, **2006**, 424, 184-188	2.5	21

154	On photoabsorption of the neutral form of the green fluorescent protein chromophore. *Biophysical Chemistry*, **2009**, 145, 1-6	3.5	20
153	Quantum Chemical Simulations of the Proton Transfer in Water Wires Attached to Molecular Walls. *Journal of Physical Chemistry B*, **2003**, 107, 2958-2965	3.4	20
152	Modeling the Complete Catalytic Cycle of Aspartoacylase. *Journal of Physical Chemistry B*, **2016**, 120, 4221-31	3.4	20
151	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
150	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
149	Computational strategy for tuning spectral properties of red fluorescent proteins. *Biophysical Chemistry*, **2011**, 158, 91-5	3.5	18
148	On the nature of oxoiron (IV) intermediate in dioxygen activation by non-heme enzymes. *Theoretical Chemistry Accounts*, **2006**, 115, 348-353	1.9	18
147	Interactions of Azodicarbonamide (ADA) Species with the Model Zinc Finger Site: Theoretical Support of the Zinc Finger Domain Destruction in the HIV-1 Nucleocapsid Protein (NCp7) by ADA. *Journal of Physical Chemistry B*, **2001**, 105, 11341-11350	3.4	18
146	Methodological aspects of QM/MM calculations: A case study on matrix metalloproteinase-2. *Journal of Computational Chemistry*, **2016**, 37, 1801-9	3.5	17
145	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
144	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
143	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
142	Mutants of the Flavoprotein iLOV as Prospective Red-Shifted Fluorescent Markers. *Journal of Physical Chemistry B*, **2017**, 121, 10018-10025	3.4	16
141	Hydrogen bonding at the diatomics-in-molecules level: Water clusters. *Journal of Chemical Physics*, **2000**, 113, 2638-2647	3.9	16
140	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
139	Modeling the Transient Kinetics of the L1 Metallo-β-Lactamase. *Journal of Physical Chemistry B*, **2018**, 122, 1378-1386	3.4	15
138	Coupling between the BLUF and EAL domains in the blue light-regulated phosphodiesterase BlrP1. *Journal of Molecular Modeling*, **2011**, 17, 1579-86	2	15
137	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

136	Modeling dioxygen binding to the non-heme iron-containing enzymes. *International Journal of Quantum Chemistry*, **2006**, 106, 2184-2190	2.1	15
135	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
134	On quantum mechanical--molecular mechanical (QM/MM) approaches to model hydrolysis of acetylcholine by acetylcholinesterase. *Chemico-Biological Interactions*, **2013**, 203, 51-6	5	14
133	Modeling spectral tuning in monomeric teal fluorescent protein mTFP1. *Biophysical Chemistry*, **2010**, 149, 78-82	3.5	14
132	Molecular modeling evidence for His438 flip in the mechanism of butyrylcholinesterase hysteretic behavior. *Journal of Molecular Neuroscience*, **2014**, 52, 434-45	3.3	13
131	Theoretical Investigation of the Reactivity of Copper Atoms with Carbon Disulfide. *Journal of Physical Chemistry A*, **2003**, 107, 2711-2715	2.8	13
130	Quantum chemical modeling of the reduction of cis-diammineplatinum(IV) tetrachloride [Pt(NH3)2Cl4] by methyl thiolate anion. *Journal of Computational Chemistry*, **2005**, 26, 865-70	3.5	13
129	Diatomics-in-ionic-systems and ab initio predictions for the stationary points on potential energy surfaces of the (HF)n clusters (n=3). *Journal of Chemical Physics*, **1999**, 111, 4442-4452	3.9	13
128	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
127	Three Faces of N-Acetylaspartate: Activator, Substrate, and Inhibitor of Human Aspartoacylase. *Journal of Physical Chemistry B*, **2017**, 121, 9389-9397	3.4	12
126	Interaction of phenol with xenon and nitrogen: spectroscopic and computational characterization. *Journal of Chemical Physics*, **2012**, 137, 134305	3.9	12
125	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
124	Hindered rotation of HArF in solid argon: Infrared spectroscopy and a theoretical model. *Physical Review B*, **2008**, 77,	3.3	12
123	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
122	Synthesis, crystal structures and theoretical study of mixed ligand complexes of lanthanides acetylacetonates with o-phenanthroline and 2,2?-dipyridyl: The unexpected inverted electrostatic trend in stability. *Journal of Molecular Structure*, **2006**, 789, 187-194	3.4	12
121	Quantum Chemical Studies of Reactions of the Cyclic Disulfides with the Zinc Finger Domains in the HIV-1 Nucleocapsid Protein (NCp7). *Journal of the American Chemical Society*, **2000**, 122, 7087-7094	16.4	12
120	Modeling structure and excitation of biliverdin-binding domains in infrared fluorescent proteins. *Chemical Physics Letters*, **2018**, 710, 59-63	2.5	12
119	Modeling reactivation of the phosphorylated human butyrylcholinesterase by QM(DFTB)/MM calculations. *Journal of Theoretical and Computational Chemistry*, **2015**, 14, 1550051	1.8	11

118	Exploration of the zinc finger motif in controlling activity of matrix metalloproteinases. *Journal of Physical Chemistry B*, **2014**, 118, 13505-12	3.4	11
117	On the Mechanism of Carborane Diffusion on a Hydrated Silica Surface. *Journal of Physical Chemistry C*, **2011**, 115, 108-111	3.8	11
116	Conformational partitioning in pH-induced fluorescence of the kindling fluorescent protein (KFP). *Journal of Physical Chemistry B*, **2011**, 115, 9195-201	3.4	11
115	The nature of biomimetically relevant rate enhancement of hydrolysis in a coordination sphere of square-planar metal complexes suggested by an X-ray structural study of a,b-h,g-[Pt{o-C6H4C(Me)NOC(O)Me}(□Cl)]2. *Mendeleev Communications*, **1997**, 7, 159-162	1.9	11
114	Novel flavin-based fluorescent proteins with red-shifted emission bands: a computational study. *Photochemical and Photobiological Sciences*, **2019**, 18, 177-189	4.2	10
113	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
112	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
111	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
110	Structures of the Peptide□Water Complexes Studied by the Hybrid Quantum Mechanical□Molecular Mechanical (QM/MM) Technique. *Structural Chemistry*, **2004**, 15, 3-9	1.8	10
109	Theoretical Modeling of the Structures and Properties of Lanthanum Complexes with Substituted Acetylacetones. *Doklady Chemistry*, **2003**, 389, 87-91	0.8	10
108	Computational study of a transition state analog of phosphoryl transfer in the Ras-RasGAP complex: AlF(x) versus MgF3-. *Journal of Molecular Modeling*, **2005**, 11, 503-8	2	10
107	Origin of the □-stacking induced shifts in absorption spectral bands of the green fluorescent protein chromophore. *Chemical Physics*, **2019**, 522, 32-38	2.3	10
106	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
105	Impact of pyrophosphate and O-ethyl-substituted pyrophosphate groups on DNA structure. *Journal of Physical Chemistry B*, **2007**, 111, 432-8	3.4	9
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100	The molecular spectra and structure of the oxides of boron and aluminium. *Russian Chemical Reviews*, **1993**, 62, 527-538	6.8	9
99	The molecular structure and computed vibrational spectrum of B2O3. *Computational and Theoretical Chemistry*, **1981**, 85, 195-205		9
98	Competition between two cysteines in covalent binding of biliverdin to phytochrome domains. *Organic and Biomolecular Chemistry*, **2018**, 16, 7518-7529	3.9	9
97	Molecular mechanism of the dark-state recovery in BLUF photoreceptors. *Chemical Physics Letters*, **2017**, 676, 25-31	2.5	8
96	Implementation of the replica-exchange molecular dynamics method for rigid bodies. *International Journal of Quantum Chemistry*, **2006**, 106, 2208-2213	2.1	8
95	Theoretical modeling of the heterobimetallic complex [La(pta)3Cu(salen)] and its precursors. *Journal of Alloys and Compounds*, **2004**, 374, 335-338	5.7	8
94	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
93	Frontiers in Multiscale Modeling of Photoreceptor Proteins. *Photochemistry and Photobiology*, **2021**, 97, 243-269	3.6	8
92	Role of zwitterions in kindling fluorescent protein photochemistry. *Journal of Physical Chemistry B*, **2015**, 119, 2467-74	3.4	7
91	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
90	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
89	Towards quantum-based modeling of enzymatic reaction pathways: Application to the acetylholinesterase catalysis. *Chemical Physics Letters*, **2013**, 556, 251-255	2.5	7
88	Modeling chemical transformations at the active sites of cholinesterases by quantum-based simulations. *Moscow University Chemistry Bulletin*, **2015**, 70, 274-277	0.5	7
87	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
86	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
85	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
84	A new hybrid approach for modeling reactions in molecular clusters: Application for the hydrogen bonded systems. *Journal of Chemical Physics*, **2000**, 112, 513-521	3.9	7
83	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

82	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
81	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
80	Modeling of the glycine tripeptide cyclization in the Ser65Gly/Tyr66Gly mutant of green fluorescent protein. *Mendeleev Communications*, **2019**, 29, 187-189	1.9	6
79	Improving the Design of the Triple-Decker Motif in Red Fluorescent Proteins. *Journal of Physical Chemistry B*, **2017**, 121, 10602-10609	3.4	6
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76	Interaction of lanthanide atoms with 4-pentyl-4′-cyanobiphenyl in low-temperature condensates. *Mendeleev Communications*, **2005**, 15, 10-11	1.9	6
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73	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
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71	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
70	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
69	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
68	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
67	On the potential-energy surface of the Mg + CO2 (C2v) system. *Mendeleev Communications*, **2001**, 11, 150-151	1.9	5
66	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
65	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

64	Aspartoacylase: a central nervous system enzyme. Structure, catalytic activity and regulation mechanisms. *Russian Chemical Reviews*, **2019**, 88, 1-26	6.8	5
63	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
62	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
61	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
60	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
59	Simulated 18O kinetic isotope effects in enzymatic hydrolysis of guanosine triphosphate. *Biochemistry (Moscow)*, **2009**, 74, 1044-8	2.9	4
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56	Theoretical characterization of the 1,3-diazaazulene molecule and its derivatives. *Computational and Theoretical Chemistry*, **2008**, 855, 40-44		4
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49	QM/MM modeling of the structures and properties of the β-diketonate-based lanthanide complexes. *International Journal of Quantum Chemistry*, **2005**, 104, 203-213	2.1	3
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