Sofya V Lushchekina

List of Publications by Citations

100 papers	1,234 citations	20 h-index	30 g-index
107 ext. papers	1,493 ext. citations	3.7 avg, IF	4.62 L-index

#	Paper	IF	Citations
100	Characterization of a complete cycle of acetylcholinesterase catalysis by ab initio QM/MM modeling. *Journal of Molecular Modeling*, **2008**, 14, 409-16	2	64
99	Conjugates of β-Carbolines and Phenothiazine as new selective inhibitors of butyrylcholinesterase and blockers of NMDA receptors for Alzheimer Disease. *Scientific Reports*, **2015**, 5, 13164	4.9	59
98	Optimization of Cholinesterase-Based Catalytic Bioscavengers Against Organophosphorus Agents. *Frontiers in Pharmacology*, **2018**, 9, 211	5.6	52
97	Synthesis, molecular docking and biological evaluation of N,N-disubstituted 2-aminothiazolines as a new class of butyrylcholinesterase and carboxylesterase inhibitors. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 1050-62	3.4	47
96	New evidence for dual binding site inhibitors of acetylcholinesterase as improved drugs for treatment of Alzheimer's disease. *Neuropharmacology*, **2019**, 155, 131-141	5.5	46
95	Esterase profiles of organophosphorus compounds in vitro predict their behavior in vivo. *Chemico-Biological Interactions*, **2016**, 259, 332-342	5	46
94	Novel conjugates of aminoadamantanes with carbazole derivatives as potential multitarget agents for AD treatment. *Scientific Reports*, **2017**, 7, 45627	4.9	42
93	Effects of viscosity and osmotic stress on the reaction of human butyrylcholinesterase with cresyl saligenin phosphate, a toxicant related to aerotoxic syndrome: kinetic and molecular dynamics studies. *Biochemical Journal*, **2013**, 454, 387-99	3.8	42
92	Slow-binding inhibition of acetylcholinesterase by an alkylammonium derivative of 6-methyluracil: mechanism and possible advantages for myasthenia gravis treatment. *Biochemical Journal*, **2016**, 473, 1225-36	3.8	33
91	Mixed implicit/explicit solvation models in quantum mechanical calculations of binding enthalpy for protein–ligand complexes. *International Journal of Quantum Chemistry*, **2006**, 106, 1943-1963	2.1	31
90	Computer-designed active human butyrylcholinesterase double mutant with a new catalytic triad. *Chemico-Biological Interactions*, **2019**, 306, 138-146	5	30
89	Emergence of catalytic bioscavengers against organophosphorus agents. *Chemico-Biological Interactions*, **2016**, 259, 319-326	5	30
88	9-Substituted acridine derivatives as acetylcholinesterase and butyrylcholinesterase inhibitors possessing antioxidant activity for Alzheimer's disease treatment. *Bioorganic and Medicinal Chemistry*, **2017**, 25, 5981-5994	3.4	28
87	Quantum chemical modelling in the research of molecular mechanisms of enzymatic catalysis. *Russian Chemical Reviews*, **2012**, 81, 1011-1025	6.8	26
86	Characterization of a novel BCHE "silent" allele: point mutation (p.Val204Asp) causes loss of activity and prolonged apnea with suxamethonium. *PLoS ONE*, **2014**, 9, e101552	3.7	26
85	6-Methyluracil Derivatives as Bifunctional Acetylcholinesterase Inhibitors for the Treatment of Alzheimer's Disease. *ChemMedChem*, **2015**, 10, 1863-74	3.7	25
84	Cholinesterase and carboxylesterase inhibitors as pharmacological agents. *Russian Chemical Bulletin*, **2019**, 68, 967-984	1.7	23

83	Slow-binding inhibition of cholinesterases, pharmacological and toxicological relevance. *Archives of Biochemistry and Biophysics*, **2016**, 593, 60-8	4.1	23
82	Characterization of a novel butyrylcholinesterase point mutation (p.Ala34Val), "silent" with mivacurium. *Biochemical Pharmacology*, **2014**, 92, 476-83	6	23
81	Overview of novel multifunctional agents based on conjugates of β-carbolines, carbazoles, tetrahydrocarbazoles, phenothiazines, and aminoadamantanes for treatment of Alzheimer's disease. *Chemico-Biological Interactions*, **2019**, 308, 224-234	5	22
80	Focused design of polypharmacophoric neuroprotective compounds: Conjugates of β-carbolines with carbazole derivatives and tetrahydrocarbazole. *Pure and Applied Chemistry*, **2017**, 89, 1167-1184	2.1	20
79	Conjugates of tacrine and 1,2,4-thiadiazole derivatives as new potential multifunctional agents for Alzheimer's disease treatment: Synthesis, quantum-chemical characterization, molecular docking, and biological evaluation. *Bioorganic Chemistry*, **2020**, 94, 103387	5.1	20
78	Modeling the Complete Catalytic Cycle of Aspartoacylase. *Journal of Physical Chemistry B*, **2016**, 120, 4221-31	3.4	20
77	Molecular modeling of butyrylcholinesterase inhibition by cresyl saligenin phosphate. *Russian Chemical Bulletin*, **2013**, 62, 2527-2537	1.7	17
76	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
75	Synthesis, molecular docking, and biological activity of 2-vinyl chromones: Toward selective butyrylcholinesterase inhibitors for potential Alzheimer's disease therapeutics. *Bioorganic and Medicinal Chemistry*, **2018**, 26, 4716-4725	3.4	16
74	Role of Acetylcholinesterase in Aβ-Amyloid Aggregation Studied by Accelerated Molecular Dynamics. *BioNanoScience*, **2017**, 7, 396-402	3.4	16
73	Computation of hydration free energies of organic solutes with an implicit water model. *Journal of Computational Chemistry*, **2006**, 27, 552-70	3.5	16
72	Characterization of butyrylcholinesterase in bovine serum. *Chemico-Biological Interactions*, **2017**, 266, 17-27	5	15
71	Synthesis, molecular docking, and biological activity of polyfluoroalkyl dihydroazolo[5,1-c][1,2,4]triazines as selective carboxylesterase inhibitors. *Bioorganic and Medicinal Chemistry*, **2017**, 25, 3997-4007	3.4	15
70	3D structure of the natural tetrameric form of human butyrylcholinesterase as revealed by cryoEM, SAXS and MD. *Biochimie*, **2019**, 156, 196-205	4.6	15
69	Synthesis, molecular docking, and biological evaluation of 3-oxo-2-tolylhydrazinylidene-4,4,4-trifluorobutanoates bearing higher and natural alcohol moieties as new selective carboxylesterase inhibitors. *Bioorganic Chemistry*, **2019**, 91, 103097	5.1	14
68	On quantum mechanical--molecular mechanical (QM/MM) approaches to model hydrolysis of acetylcholine by acetylcholinesterase. *Chemico-Biological Interactions*, **2013**, 203, 51-6	5	14
67	Alkyl 2-arylhydrazinylidene-3-oxo-3-polyfluoroalkylpropionates as new effective and selective inhibitors of carboxylesterase. *Doklady Biochemistry and Biophysics*, **2015**, 465, 381-5	0.8	14
66	Molecular modeling evidence for His438 flip in the mechanism of butyrylcholinesterase hysteretic behavior. *Journal of Molecular Neuroscience*, **2014**, 52, 434-45	3.3	13

65	Three Faces of N-Acetylaspartate: Activator, Substrate, and Inhibitor of Human Aspartoacylase. *Journal of Physical Chemistry B*, **2017**, 121, 9389-9397	3.4	12
64	Conjugates of methylene blue with -carboline derivatives as new multifunctional agents for the treatment of neurodegenerative diseases. *Scientific Reports*, **2019**, 9, 4873	4.9	11
63	Modeling reactivation of the phosphorylated human butyrylcholinesterase by QM(DFTB)/MM calculations. *Journal of Theoretical and Computational Chemistry*, **2015**, 14, 1550051	1.8	11
62	New Infestin-4 Mutants with Increased Selectivity against Factor XIIa. *PLoS ONE*, **2015**, 10, e0144940	3.7	11
61	New Hybrids of 4-Amino-2,3-polymethylene-quinoline and -Tolylsulfonamide as Dual Inhibitors of Acetyl- and Butyrylcholinesterase and Potential Multifunctional Agents for Alzheimer's Disease Treatment. *Molecules*, **2020**, 25,	4.8	11
60	New Multifunctional Agents Based on Conjugates of 4-Amino-2,3-polymethylenequinoline and Butylated Hydroxytoluene for Alzheimer's Disease Treatment. *Molecules*, **2020**, 25,	4.8	10
59	Catalytic bioscavengers against organophosphorus agents: mechanistic issues of self-reactivating cholinesterases. *Toxicology*, **2018**, 409, 91-102	4.4	10
58	Research on cholinesterases in the Soviet Union and Russia: a historical perspective. *Chemico-Biological Interactions*, **2013**, 203, 3-9	5	10
57	Slow-binding inhibitors of acetylcholinesterase of medical interest. *Neuropharmacology*, **2020**, 177, 108236	5.5	10
56	Macrocyclic derivatives of 6-methyluracil as ligands of the peripheral anionic site of acetylcholinesterase. *MedChemComm*, **2014**, 5, 1729-1735	5	9
55	Bi-functional sterically hindered phenol lipid-based delivery systems as potential multi-target agents against Alzheimer's disease via an intranasal route. *Nanoscale*, **2020**, 12, 13757-13770	7.7	8
54	Interactions outside the proteinase-binding loop contribute significantly to the inhibition of activated coagulation factor XII by its canonical inhibitor from corn. *Journal of Biological Chemistry*, **2014**, 289, 14109-20	5.4	8
53	Time-course of human cholinesterases-catalyzed competing substrate kinetics. *Chemico-Biological Interactions*, **2019**, 310, 108702	5	7
52	C-547, a 6-methyluracil derivative with long-lasting binding and rebinding on acetylcholinesterase: Pharmacokinetic and pharmacodynamic studies. *Neuropharmacology*, **2018**, 131, 304-315	5.5	7
51	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
50	Modeling chemical transformations at the active sites of cholinesterases by quantum-based simulations. *Moscow University Chemistry Bulletin*, **2015**, 70, 274-277	0.5	7
49	6-Methyluracil derivatives as acetylcholinesterase inhibitors for treatment of Alzheimer's disease. *International Journal of Risk and Safety in Medicine*, **2015**, 27 Suppl 1, S69-71	1.6	6
48	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

47	Structural basis of diversity and homodimerization specificity of zinc-finger-associated domains in Drosophila. *Nucleic Acids Research*, **2021**, 49, 2375-2389	20.1	6
46	Steady-State Kinetics of Enzyme-Catalyzed Hydrolysis of Echothiophate, a P-S Bonded Organophosphorus as Monitored by Spectrofluorimetry. *Molecules*, **2020**, 25,	4.8	5
45	Arachidonoylcholine and Other Unsaturated Long-Chain Acylcholines Are Endogenous Modulators of the Acetylcholine Signaling System. *Biomolecules*, **2020**, 10,	5.9	5
44	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
43	Prebiotic synthesis and selection of macromolecules: Thermal cycling as a condition for synthesis and combinatorial selection. *Geochemistry International*, **2014**, 52, 1197-1206	0.8	5
42	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
41	Computation of entropy contribution to protein-ligand binding free energy. *Biochemistry (Moscow)*, **2007**, 72, 785-92	2.9	5
40	ORGANOPHOSPHORUS NEUROTOXINS **2020**,		5
39	A new sensitive spectrofluorimetric method for measurement of activity and kinetic study of cholinesterases. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2020**, 1868, 140270	4	5
38	6-Methyluracil derivatives as peripheral site ligand-hydroxamic acid conjugates: Reactivation for paraoxon-inhibited acetylcholinesterase. *European Journal of Medicinal Chemistry*, **2020**, 185, 111787	6.8	5
37	Conjugates of Tacrine and Its Cyclic Homologues with p-Toluenesulfonamide as Novel Acetylcholinesterase and Butyrylcholinesterase Inhibitors. *Doklady Biochemistry and Biophysics*, **2018**, 483, 369-373	0.8	5
36	Amiridine-piperazine hybrids as cholinesterase inhibitors and potential multitarget agents for Alzheimer's disease treatment. *Bioorganic Chemistry*, **2021**, 112, 104974	5.1	5
35	Synthesis of 2-arylhydrazinylidene-3-oxo-4,4,4-trifluorobutanoic acids as new selective carboxylesterase inhibitors and radical scavengers. *Bioorganic and Medicinal Chemistry Letters*, **2019**, 29, 126716	2.9	4
34	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
33	Water-soluble betaines and amines based on thiacalix[4]arene scaffold as new cholinesterase inhibitors. *Bioorganic Chemistry*, **2020**, 94, 103455	5.1	4
32	Conjugation of Aminoadamantane and β-Carboline Pharmacophores Gives Rise to Unexpected Properties of Multifunctional Ligands. *Molecules*, **2021**, 26,	4.8	4
31	Computational Exploration of Reactivity of 6-Methyluracil/Imidazole-2-Carbaldehyde Oxime Conjugate. *BioNanoScience*, **2017**, 7, 229-232	3.4	3
30	Bis-β-carbolines as new potential multitarget agents for Alzheimer's disease. *Pure and Applied Chemistry*, **2020**, 92, 1057-1080	2.1	3

29	1-(3--Butylphenyl)-2,2,2-Trifluoroethanone as a Potent Transition-State Analogue Slow-Binding Inhibitor of Human Acetylcholinesterase: Kinetic, MD and QM/MM Studies. *Biomolecules*, **2020**, 10,	5.9	3
28	Novel potent bifunctional carboxylesterase inhibitors based on a polyfluoroalkyl-2-imino-1,3-dione scaffold. *European Journal of Medicinal Chemistry*, **2021**, 218, 113385	6.8	3
27	Influence of the β-carboline and carbazole pharmacophore moieties on anticholinesterase and antiradical activity of multifunctional agents for the treatment of neurodegenerative diseases. *Russian Chemical Bulletin*, **2018**, 67, 1724-1731	1.7	3
26	Water structure changes in oxime-mediated reactivation process of phosphorylated human acetylcholinesterase. *Bioscience Reports*, **2018**, 38,	4.1	3
25	The four-helix bundle in cholinesterase dimers: Structural and energetic determinants of stability. *Chemico-Biological Interactions*, **2019**, 309, 108699	5	2
24	Computer simulation in molecular medicine and drug design. *Herald of the Russian Academy of Sciences*, **2016**, 86, 185-192	0.7	2
23	Human butyrylcholinesterase polymorphism: Molecular modeling. *International Journal of Risk and Safety in Medicine*, **2015**, 27 Suppl 1, S80-1	1.6	2
22	Supercomputer Modeling of Dual-Site Acetylcholinesterase (AChE) Inhibition. *Supercomputing Frontiers and Innovations*, **2018**, 5,	7.2	2
21	Novel Acetylcholinesterase Inhibitors Based on Uracil Moiety for Possible Treatment of Alzheimer Disease. *Molecules*, **2020**, 25,	4.8	2
20	Synthesis of new efficient and selective carboxylesterase inhibitors based on adamantyl and citronellyl 4,4,4-trifluoro-2-arylhydrazonylidene-3-oxobutanoates. *Russian Chemical Bulletin*, **2021**, 70, 567-572	1.7	2
19	Supercomputer simulation of the covalent inhibition of the main protease of SARS-CoV-2.. *Russian Chemical Bulletin*, **2021**, 70, 2084-2089	1.7	2
18	Kinetics and mechanism of inhibition of serine esterases by fluorinated carbethoxy 1-aminophosphonates. *Doklady Biochemistry and Biophysics*, **2013**, 451, 203-6	0.8	1
17	Quantum mechanical/molecular mechanical analysis of mechanisms of enzyme action. Human acetylcholinesterase. *Russian Chemical Bulletin*, **2011**, 60, 2196-2204	1.7	1
16	Impact of Sucrose as Osmolyte on Molecular Dynamics of Mouse Acetylcholinesterase. *Biomolecules*, **2020**, 10,	5.9	1
15	Conjugates of Tacrine with Salicylamide as Promising Multitarget Agents for Alzheimer's Disease.. *ChemMedChem*, **2022**, e202200080	3.7	1
14	Steady-state kinetic analysis of human cholinesterases over wide concentration ranges of competing substrates. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2022**, 1870, 140733	4	0
13	α-tocopherol, a slow-binding inhibitor of acetylcholinesterase. *Chemico-Biological Interactions*, **2021**, 348, 109646	5	0
12	Catalytic bioscavengers: the second generation of bioscavenger-based medical countermeasures **2020**, 1199-1229		

List of Publications

11	Analysis of Apparent Catalytic Parameters of Multiple Molecular Forms of Human Plasma Butyrylcholinesterase by Activity Gel-Scanning Following Non-denaturing Electrophoresis. *BioNanoScience*, **2018**, 8, 367-372	3.4
10	Synthesis of new N-(pyridin-3-ylmethyl)-2-aminothiazoline derivatives possessing anticholinesterase and antiradical activity as potential multifunctional agents for the treatment of neurodegenerative diseases. *Russian Chemical Bulletin*, **2017**, 66, 1897-1904	1.7
9	Molecular modeling of mechanism of action of anti-myasthenia gravis slow-binding inhibitor of acetylcholinesterase. *International Journal of Risk and Safety in Medicine*, **2015**, 27 Suppl 1, S74-5	1.6
8	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
7	Study and modeling of mechanisms of cholinesterasis reactions in order to improve their catalytic properties in the neutralization reactions of organophosphorous compounds **2020**, 134-174	
6	Research on cholinesterases in the Soviet Union and Russia **2020**, 35-43	
5	Study and modeling of mechanisms of cholinesterasis reactions in order to improve their catalytic properties in the neutralization reactions of organophosphorus compounds **2020**, 140-180	
4	Research on cholinesterases in the Soviet Union and Russia **2020**, 29-37	
3	Human cholinesterases **2020**, 69-126	
2	Human cholinesterases **2020**, 63-120	
1	Mechanisms of the Aspartoacylase Catalytic Activity Regulation According to the Computer Modeling Results. *Moscow University Chemistry Bulletin*, **2018**, 73, 152-154	0.5