Sofya V Lushchekina

List of Publications by Year
in descending order

102 papers	1,765 citations	257101 24 h-index	344852 36 g-index
107 all docs	107 docs citations	107 times ranked	1588 citing authors

#	Article	IF	Citations
1	Conjugates of Î³-Carbolines and Phenothiazine as new selective inhibitors of butyrylcholinesterase and blockers of NMDA receptors for Alzheimer Disease. Scientific Reports, 2015, 5, 13164.	1.6	76
2	Characterization of a complete cycle of acetylcholinesterase catalysis by ab initio QM/MM modeling. Journal of Molecular Modeling, 2008, 14, 409-416.	0.8	69
3	New evidence for dual binding site inhibitors of acetylcholinesterase as improved drugs for treatment of Alzheimer's disease. Neuropharmacology, 2019, 155, 131-141.	2.0	67
4	Optimization of Cholinesterase-Based Catalytic Bioscavengers Against Organophosphorus Agents. Frontiers in Pharmacology, 2018, 9, 211.	1.6	59
5	Esterase profiles of organophosphorus compounds inÂvitro predict their behavior inÂvivo. Chemico-Biological Interactions, 2016, 259, 332-342.	1.7	58
6	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, 1050-1062.	1.4	57
7	Novel conjugates of aminoadamantanes with carbazole derivatives as potential multitarget agents for AD treatment. Scientific Reports, 2017, 7, 45627.	1.6	54
8	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, 387-399.	1.7	53
9	Conjugates of tacrine and 1,2,4-thiadiazole derivatives as new potential multifunctional agents for Alzheimerâ€™s disease treatment: Synthesis, quantum-chemical characterization, molecular docking, and biological evaluation. Bioorganic Chemistry, 2020, 94, 103387.	2.0	44
10	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.	1.4	43
11	Emergence of catalytic bioscavengers against organophosphorus agents. Chemico-Biological Interactions, 2016, 259, 319-326.	1.7	40
12	Slow-binding inhibition of acetylcholinesterase by an alkylammonium derivative of 6-methyluracil: mechanism and possible advantages for myasthenia gravis treatment. Biochemical Journal, 2016, 473, 1225-1236.	1.7	39
13	Cholinesterase and carboxylesterase inhibitors as pharmacological agents. Russian Chemical Bulletin, 2019, 68, 967-984.	0.4	39
14	Overview of novel multifunctional agents based on conjugates of Î³-carbolines, carbazoles, tetrahydrocarbazoles, phenothiazines, and aminoadamantanes for treatment of Alzheimer's disease. Chemico-Biological Interactions, 2019, 308, 224-234.	1.7	36
15	Mixed implicit/explicit solvation models in quantum mechanical calculations of binding enthalpy for proteinâ€"ligand complexes. International Journal of Quantum Chemistry, 2006, 106, 1943-1963.	1.0	35
16	Characterization of a Novel BCHE â€œSilentâ€•Allele: Point Mutation (p.Val204Asp) Causes Loss of Activity and Prolonged Apnea with Suxamethonium. PLoS ONE, 2014, 9, e101552.	1.1	34
17	6â€Methyluracil Derivatives as Bifunctional Acetylcholinesterase Inhibitors for the Treatment of Alzheimer's Disease. ChemMedChem, 2015, 10, 1863-1874.	1.6	33
18	Computer-designed active human butyrylcholinesterase double mutant with a new catalytic triad. Chemico-Biological Interactions, 2019, 306, 138-146.	1.7	31

#	Article	IF	Citations
19	Quantum chemical modelling in the research of molecular mechanisms of enzymatic catalysis. Russian Chemical Reviews, 2012, 81, 1011-1025.	2.5	28
20	New Multifunctional Agents Based on Conjugates of 4-Amino-2,3-polymethylenequinoline and Butylated Hydroxytoluene for Alzheimerâ€™s Disease Treatment. Molecules, 2020, 25, 5891.	1.7	28
21	Characterization of a novel butyrylcholinesterase point mutation (p.Ala34Val), â€œsilentâ€•with mivacurium. Biochemical Pharmacology, 2014, 92, 476-483.	2.0	27
22	Slow-binding inhibition of cholinesterases, pharmacological and toxicological relevance. Archives of Biochemistry and Biophysics, 2016, 593, 60-68.	1.4	27
23	3D structure of the natural tetrameric form of human butyrylcholinesterase as revealed by cryoEM, SAXS and MD. Biochimie, 2019, 156, 196-205.	1.3	26
24	New Hybrids of 4-Amino-2,3-polymethylene-quinoline and p-Tolylsulfonamide as Dual Inhibitors of Acetyl- and Butyrylcholinesterase and Potential Multifunctional Agents for Alzheimerâ€™s Disease Treatment. Molecules, 2020, 25, 3915.	1.7	26
25	Modeling the Complete Catalytic Cycle of Aspartoacylase. Journal of Physical Chemistry B, 2016, 120, 4221-4231.	1.2	25
26	Conjugates of methylene blue with Î^3-carboline derivatives as new multifunctional agents for the treatment of neurodegenerative diseases. Scientific Reports, 2019, 9, 4873.	1.6	25
27	Focused design of polypharmacophoric neuroprotective compounds: Conjugates of Î^3-carbolines with carbazole derivatives and tetrahydrocarbazole. Pure and Applied Chemistry, 2017, 89, 1167-1184.	0.9	24
28	Role of Acetylcholinesterase in Î^2-Amyloid Aggregation Studied by Accelerated Molecular Dynamics. BioNanoScience, 2017, 7, 396-402.	1.5	23
29	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.	1.4	23
30	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.	2.0	23
31	Amiridine-piperazine hybrids as cholinesterase inhibitors and potential multitarget agents for Alzheimer's disease treatment. Bioorganic Chemistry, 2021, 112, 104974.	2.0	22
32	Characterization of butyrylcholinesterase in bovine serum. Chemico-Biological Interactions, 2017, 266, 17-27.	1.7	19
33	Slow-binding inhibitors of acetylcholinesterase of medical interest. Neuropharmacology, 2020, 177, 108236.	2.0	19
34	Bi-functional sterically hindered phenol lipid-based delivery systems as potential multi-target agents against Alzheimer's disease <i>via</i> an intranasal route. Nanoscale, 2020, 12, 13757-13770.	2.8	19
35	Arachidonoylcholine and Other Unsaturated Long-Chain Acylcholines Are Endogenous Modulators of the Acetylcholine Signaling System. Biomolecules, 2020, 10, 283.	1.8	19
36	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.	2.5	18

#	Article	IF	Citations
37	Computation of hydration free energies of organic solutes with an implicit water model. Journal of Computational Chemistry, 2006, 27, 552-570.	1.5	17
38	Molecular modeling of butyrylcholinesterase inhibition by cresyl saligenin phosphate. Russian Chemical Bulletin, 2013, 62, 2527-2537.	0.4	17
39	New Infestin-4 Mutants with Increased Selectivity against Factor XIIa. PLoS ONE, 2015, 10, e0144940.	1.1	17
40	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.	1.4	17
41	Structural basis of diversity and homodimerization specificity of zinc-finger-associated domains in Drosophila. Nucleic Acids Research, 2021, 49, 2375-2389.	6.5	17
42	On quantum mechanical â€“ molecular mechanical (QM/MM) approaches to model hydrolysis of acetylcholine by acetylcholinesterase. Chemico-Biological Interactions, 2013, 203, 51-56.	1.7	16
43	Alkyl 2-arylhydrazinylidene-3-oxo-3-polyfluoroalkylpropionates as new effective and selective inhibitors of carboxylesterase. Doklady Biochemistry and Biophysics, 2015, 465, 381-385.	0.3	16
44	Molecular Modeling Evidence for His438 Flip in the Mechanism of Butyrylcholinesterase Hysteretic Behavior. Journal of Molecular Neuroscience, 2014, 52, 434-445.	1.1	14
45	Modeling reactivation of the phosphorylated human butyrylcholinesterase by QM(DFTB)/MM calculations. Journal of Theoretical and Computational Chemistry, 2015, 14, 1550051.	1.8	14
46	Conjugation of Aminoadamantane and Î³-Carboline Pharmacophores Gives Rise to Unexpected Properties of Multifunctional Ligands. Molecules, 2021, 26, 5527.	1.7	14
47	Three Faces of N-Acetylaspartate: Activator, Substrate, and Inhibitor of Human Aspartoacylase. Journal of Physical Chemistry B, 2017, 121, 9389-9397.	1.2	13
48	Novel potent bifunctional carboxylesterase inhibitors based on a polyfluoroalkyl-2-imino-1,3-dione scaffold. European Journal of Medicinal Chemistry, 2021, 218, 113385.	2.6	13
49	Catalytic bioscavengers against organophosphorus agents: mechanistic issues of self-reactivating cholinesterases. Toxicology, 2018, 409, 91-102.	2.0	12
50	Novel Acetylcholinesterase Inhibitors Based on Uracil Moiety for Possible Treatment of Alzheimer Disease. Molecules, 2020, 25, 4191.	1.7	12
51	Macrocyclic derivatives of 6-methyluracil as ligands of the peripheral anionic site of acetylcholinesterase. MedChemComm, 2014, 5, 1729-1735.	3.5	11
52	C-547, a 6-methyluracil derivative with long-lasting binding and rebinding on acetylcholinesterase: Pharmacokinetic and pharmacodynamic studies. Neuropharmacology, 2018, 131, 304-315.	2.0	11
53	Conjugates of Tacrine with Salicylamide as Promising Multitarget Agents for Alzheimer's Disease. ChemMedChem, 2022, 17, e202200080.	1.6	11
54	Research on cholinesterases in the Soviet Union and Russia: A historical perspective. Chemico-Biological Interactions, 2013, 203, 3-9.	1.7	10

#	Article	IF	Citations
55	Prebiotic synthesis and selection of macromolecules: Thermal cycling as a condition for synthesis and combinatorial selection. Geochemistry International, 2014, 52, 1197-1206.	0.2	10
56	Time-course of human cholinesterases-catalyzed competing substrate kinetics. Chemico-Biological Interactions, 2019, 310, 108702.	1.7	10
57	Water-soluble betaines and amines based on thiacalix[4]arene scaffold as new cholinesterase inhibitors. Bioorganic Chemistry, 2020, 94, 103455.	2.0	10
58	Impact of Sucrose as Osmolyte on Molecular Dynamics of Mouse Acetylcholinesterase. Biomolecules, 2020, 10, 1664.	1.8	10
59	ORGANOPHOSPHORUS NEUROTOXINS. , 2020, , .		10
60	Bis-Amiridines as Acetylcholinesterase and Butyrylcholinesterase Inhibitors: N-Functionalization Determines the Multitarget Anti-Alzheimerâ€™s Activity Profile. Molecules, 2022, 27, 1060.	1.7	10
61	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, 14109-14120.	1.6	9
62	A new sensitive spectrofluorimetric method for measurement of activity and kinetic study of cholinesterases. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2020, 1868, 140270.	1.1	9
63	6-Methyluracil derivatives as peripheral site ligand-hydroxamic acid conjugates: Reactivation for paraoxon-inhibited acetylcholinesterase. European Journal of Medicinal Chemistry, 2020, 185, 111787.	2.6	9
64	Modeling chemical transformations at the active sites of cholinesterases by quantum-based simulations. Moscow University Chemistry Bulletin, 2015, 70, 274-277.	0.2	8
65	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.	0.4	8
66	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.	1.7	8
67	Conjugates of Tacrine and Its Cyclic Homologues with p-Toluenesulfonamide as Novel Acetylcholinesterase and Butyrylcholinesterase Inhibitors. Doklady Biochemistry and Biophysics, 2018, 483, 369-373.	0.3	8
68	1-(3-Tert-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, 1608.	1.8	8
69	Steady-State Kinetics of Enzyme-Catalyzed Hydrolysis of Echothiophate, a Pâ€"S Bonded Organophosphorus as Monitored by Spectrofluorimetry. Molecules, 2020, 25, 1371.	1.7	7
70	6-Methyluracil derivatives as acetylcholinesterase inhibitors for treatment of Alzheimerâ€™s disease. International Journal of Risk and Safety in Medicine, 2015, 27, S69-S71.	0.3	6
71	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
72	Water structure changes in oxime-mediated reactivation process of phosphorylated human acetylcholinesterase. Bioscience Reports, 2018, 38, .	1.1	6

#	Article	IF	Citations
73	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.	1.0	6
74	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.	0.4	6
75	Bis-Î³-carbolines as new potential multitarget agents for Alzheimerâ€™s disease. Pure and Applied Chemistry, 2020, 92, 1057-1080.	0.9	6
76	Computation of entropy contribution to protein-ligand binding free energy. Biochemistry (Moscow), 2007, 72, 785-792.	0.7	5
77	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.	0.4	5
78	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.	1.7	5
79	Supercomputer simulation of the covalent inhibition of the main protease of SARS-CoV-2. Russian Chemical Bulletin, 2021, 70, 2084-2089.	0.4	5
80	Human butyrylcholinesterase polymorphism: Molecular modeling. International Journal of Risk and Safety in Medicine, 2015, 27, S80-S81.	0.3	4
81	Influence of the Î³-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.	0.4	4
82	The four-helix bundle in cholinesterase dimers: Structural and energetic determinants of stability. Chemico-Biological Interactions, 2019, 309, 108699.	1.7	4
83	Î±-tocopherol, a slow-binding inhibitor of acetylcholinesterase. Chemico-Biological Interactions, 2021, 348, 109646.	1.7	4
84	Steady-state kinetic analysis of human cholinesterases over wide concentration ranges of competing substrates. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2022, 1870, 140733.	1.1	4
85	Quantum mechanical/molecular mechanical analysis of mechanisms of enzyme action. Human acetylcholinesterase. Russian Chemical Bulletin, 2011, 60, 2196-2204.	0.4	3
86	Computational Exploration of Reactivity of 6-Methyluracil/Imidazole-2-Carbaldehyde Oxime Conjugate. BioNanoScience, 2017, 7, 229-232.	1.5	3
87	Kinetics and mechanism of inhibition of serine esterases by fluorinated carbethoxy 1-aminophosphonates. Doklady Biochemistry and Biophysics, 2013, 451, 203-206.	0.3	2
88	Computer simulation in molecular medicine and drug design. Herald of the Russian Academy of Sciences, 2016, 86, 185-192.	0.2	2
89	Supercomputer Modeling of Dual-Site Acetylcholinesterase (AChE) Inhibition. Supercomputing Frontiers and Innovations, 2018, 5, .	0.5	2
90	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.	0.2	1

#	Article	IF	Citations
91	Human cholinesterases. , 2020, , 69-126.		1
92	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, S74-S75.	0.3	0
93	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.	0.4	0
94	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.	1.5	0
95	Mechanisms of the Aspartoacylase Catalytic Activity Regulation According to the Computer Modeling Results. Moscow University Chemistry Bulletin, 2018, 73, 152-154.	0.2	0
96	Catalytic bioscavengers: the second generation of bioscavenger-based medical countermeasures. , 2020, , 1199-1229.		0
97	Abstract OR-21: 3D Structure of the Natural Tetrameric Form of Human Butyryl-cholinesterase as Revealed by Cryo-EM, MD and SAXS. International Journal of Biomedicine, 2019, 9, S14-S15.	0.1	0
98	Human cholinesterases. , 2020, , 63-120.		0
99	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.		0
100	Research on cholinesterases in the Soviet Union and Russia. , 2020, , 35-43.		0
101	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.		0
102	Research on cholinesterases in the Soviet Union and Russia. , 2020, , 29-37.		0