Eugene V Radchenko

List of Publications by Year
in descending order

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52 papers	2,647 citations	430442 18 h-index	197535 49 g-index
54 all docs	54 docs citations	54 times ranked	3901 citing authors

#	Article	IF	Citations
1	Virtual Computational Chemistry Laboratory â€“ Design and Description. Journal of Computer-Aided Molecular Design, 2005, 19, 453-463.	1.3	1,250
2	Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. Journal of Computer-Aided Molecular Design, 2011, 25, 533-554.	1.3	453
3	Prediction of human intestinal absorption of drug compounds. Russian Chemical Bulletin, 2016, 65, 576-580.	0.4	74
4	Progress in visual representations of chemical space. Expert Opinion on Drug Discovery, 2015, 10, 959-973.	2.5	68
5	Organophosphorus compound esterase profiles as predictors of therapeutic and toxic effects. Chemico-Biological Interactions, 2013, 203, 231-237.	1.7	66
6	Nonpeptide Inhibitors of Measles Virus Entry. Journal of Medicinal Chemistry, 2006, 49, 5080-5092.	2.9	65
7	Molecular Field Topology Analysis Method in QSAR Studies of Organic Compounds. Journal of Chemical Information and Computer Sciences, 2000, 40, 659-667.	2.8	61
8	Computer-aided estimation of the hERG-mediated cardiotoxicity risk of potential drug components. Doklady Biochemistry and Biophysics, 2017, 473, 128-131.	0.3	47
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	Prediction of blood-brain barrier permeability of organic compounds. Doklady Biochemistry and Biophysics, 2016, 470, 371-374.	0.3	43
11	Combined QSAR studies of inhibitor properties ofO-phosphorylated oximes toward serine esterases involved in neurotoxicity, drug metabolism and Alzheimer's disease. SAR and QSAR in Environmental Research, 2012, 23, 627-647.	1.0	37
12	Molecular design, synthesis and biological evaluation of cage compound-based inhibitors of hepatitis C virus p7 ion channels. European Journal of Medicinal Chemistry, 2018, 158, 214-235.	2.6	32
13	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
14	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
15	Machine Learning Classification Models to Improve the Dockingâ€based Screening: A Case of PI3Kâ€Tankyrase Inhibitors. Molecular Informatics, 2018, 37, e1800030.	1.4	24
16	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
17	Time-Domain Analysis of Molecular Dynamics Trajectories Using Deep Neural Networks: Application to Activity Ranking of Tankyrase Inhibitors. Journal of Chemical Information and Modeling, 2019, 59, 3519-3532.	2.5	23
18	Towards Deep Neural Network Models for the Prediction of the Bloodâ€“Brain Barrier Permeability for Diverse Organic Compounds. Molecules, 2020, 25, 5901.	1.7	22

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19	Amiridine-piperazine hybrids as cholinesterase inhibitors and potential multitarget agents for Alzheimer's disease treatment. Bioorganic Chemistry, 2021, 112, 104974.	2.0	22
20	Synthesis and biological evaluation of novel 5-hydroxylaminoisoxazole derivatives as lipoxygenase inhibitors and metabolism enhancing agents. Bioorganic and Medicinal Chemistry, 2016, 24, 712-720.	1.4	19
21	Modeling of the relationships between the structure of O-phosphorylated oximes and their anticholinesterase activity and selectivity using molecular field topology analysis (MFTA). Doklady Biochemistry and Biophysics, 2008, 418, 47-51.	0.3	18
22	Discovery of Novel Tankyrase Inhibitors through Molecular Docking-Based Virtual Screening and Molecular Dynamics Simulation Studies. Molecules, 2020, 25, 3171.	1.7	18
23	Structural requirements for molecular design of positive allosteric modulators of AMPA receptor. Mendeleev Communications, 2017, 27, 623-625.	0.6	16
24	Complex formation of albumin with tricarbocyanine dyes containing phosphonate groups. Photochemical and Photobiological Sciences, 2016, 15, 1377-1384.	1.6	13
25	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
26	Molecular Field Topology Analysis in Drug Design and Virtual Screening. , 2008, , 150-181.		12
27	A Facile Approach to Bis(isoxazoles), Promising Ligands of the AMPA Receptor. Molecules, 2021, 26, 6411.	1.7	11
28	Molecular design of O-phosphorylated oximesâ€"Selective inhibitors of butyrylcholinesterase. Doklady Biochemistry and Biophysics, 2012, 443, 91-95.	0.3	10
29	Bis-Amiridines as Acetylcholinesterase and Butyrylcholinesterase Inhibitors: N-Functionalization Determines the Multitarget Anti-Alzheimerâ€™s Activity Profile. Molecules, 2022, 27, 1060.	1.7	10
30	Study of the structural determinants of acute and delayed neurotoxicity of O-phosphorylated oximes by molecular field topology analysis (MFTA). Doklady Biochemistry and Biophysics, 2009, 429, 309-314.	0.3	9
31	Ab Initio Kinetic Modeling of Living Anionic and Zwitterionic Chain Polymerization Mechanisms. Macromolecules, 2010, 43, 9674-9681.	2.2	9
32	Ramified derivatives of 5-(perylen-3-ylethynyl)uracil-1-acetic acid and their antiviral properties. RSC Advances, 2019, 9, 26014-26023.	1.7	8
33	Generation of chemical structures on the basis of QSAR models of molecular field topology analysis. Doklady Chemistry, 2007, 415, 196-199.	0.2	7
34	Computer-aided design of selective ligands of the benzodiazepine-binding site of the GABAA receptor. Doklady Chemistry, 2008, 422, 227-230.	0.2	7
35	Design of Broad-Spectrum Inhibitors of Influenza A Virus M2 Proton Channels: A Molecular Modeling Approach. Current Computer-Aided Drug Design, 2016, 12, 154-164.	0.8	6
36	Molecular design of N,N-disubstituted 2-aminothiazolines as selective carboxylesterase inhibitors. Russian Chemical Bulletin, 2016, 65, 570-575.	0.4	6

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37	Bis-Î³-carbolines as new potential multitarget agents for Alzheimerâ€™s disease. Pure and Applied Chemistry, 2020, 92, 1057-1080.	0.9	6
38	Novel substituted 5â€methylâ€4â€acylaminoisoxazoles as antimitotic agents: Evaluation of selectivity to LNCaP cancer cells. Archiv Der Pharmazie, 2022, 355, e2100425.	2.1	6
39	Positive and negative AMPA receptor modulators based on tricyclic bispidine derivative: Minor structural change inverts the type of activity. Mendeleev Communications, 2022, 32, 360-363.	0.6	6
40	On mechanism of allosteric modulation of NMDA receptor via amino-terminal domains. Biochemical and Biophysical Research Communications, 2012, 424, 687-690.	1.0	5
41	Influence of Descriptor Implementation on Compound Ranking Based on Multiparameter Assessment. Journal of Chemical Information and Modeling, 2018, 58, 1083-1093.	2.5	4
42	Computer-aided design of arylphthalazines as potential smoothened receptor antagonists. Doklady Chemistry, 2012, 443, 97-100.	0.2	3
43	Computer-aided modeling of activity and selectivity of quinazolinones as noncompetitive NMDA receptor antagonists. Doklady Biochemistry and Biophysics, 2012, 443, 118-122.	0.3	3
44	New phosphonate-substituted tricarbocyanines and their interaction with bovine serum albumin. Doklady Chemistry, 2016, 470, 264-267.	0.2	3
45	Computer-aided design of negative allosteric modulators of NMDA receptor. Doklady Biochemistry and Biophysics, 2013, 448, 22-26.	0.3	2
46	Molecular design of selective ligands of chemokine receptors. Doklady Biochemistry and Biophysics, 2015, 461, 131-134.	0.3	2
47	Molecular design of proneurogenic and neuroprotective compoundsâ€”allosteric NMDA receptor modulators. Doklady Biochemistry and Biophysics, 2017, 473, 132-136.	0.3	2
48	Analysis of Chemical Spaces: Implications for Drug Repurposing. , 2019, , 359-395.		2
49	Molecular modeling of the transmembrane domain of mGluR2 metabotropic glutamate receptor and the binding site of its positive allosteric modulators. Doklady Biochemistry and Biophysics, 2014, 454, 13-16.	0.3	1
50	Generalized fragmental approach in QSAR/QSPR studies. Doklady Chemistry, 2015, 463, 185-188.	0.2	1
51	Molecular Field Topology Analysis (MFTA) in the Design of Neuroprotective Compounds. Neuromethods, 2018, , 139-159.	0.2	0
52	Molecular Field Topology Analysis (MFTA) as the Basis for Molecular Design. , 2000, , 460-461.		0