Alexey A Lagunin

List of Publications by Year
in descending order

109	4,844	136950	102487
papers	citations	32 h-index	66 g-index

121	121	121	4389
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	PASS: prediction of activity spectra for biologically active substances. Bioinformatics, 2000, 16, 747-748.	4.1	737
2	Prediction of the Biological Activity Spectra of Organic Compounds Using the Pass Online Web Resource. Chemistry of Heterocyclic Compounds, 2014, 50, 444-457.	1.2	630
3	QSAR Modelling of Rat Acute Toxicity on the Basis of PASS Prediction. Molecular Informatics, 2011, 30, 241-250.	2.5	278
4	PASS Biological Activity Spectrum Predictions in the Enhanced Open NCI Database Browser. Journal of Chemical Information and Computer Sciences, 2003, 43, 228-236.	2.8	203
5	Computer-Aided Discovery of Anti-Inflammatory Thiazolidinones with Dual Cyclooxygenase/Lipoxygenase Inhibition. Journal of Medicinal Chemistry, 2008, 51, 1601-1609.	6.4	161
6	PASS-assisted exploration of new therapeutic potential of natural products. Medicinal Chemistry Research, 2011, 20, 1509-1514.	2.4	134
7	Multi-Targeted Natural Products Evaluation Based on Biological Activity Prediction with PASS. Current Pharmaceutical Design, 2010, 16, 1703-1717.	1.9	126
8	CLC-Pred: A freely available web-service for in silico prediction of human cell line cytotoxicity for drug-like compounds. PLoS ONE, 2018, 13, e0191838.	2.5	116
9	Design, synthesis, computational and biological evaluation of new anxiolytics. Bioorganic and Medicinal Chemistry, 2004, 12, 6559-6568.	3.0	114
10	Chemo- and bioinformatics resources for inÂsilico drug discovery from medicinal plants beyond their traditional use: a critical review. Natural Product Reports, 2014, 31, 1585-1611.	10.3	104
11	Computer-aided prediction of biological activity spectra for chemical compounds: opportunities and limitation. Biomedical Chemistry Research and Methods, 2018, 1, e00004.	0.4	99
12	PASS: identification of probable targets and mechanisms of toxicity. SAR and QSAR in Environmental Research, 2007, 18, 101-110.	2.2	95
13	Collaborative development of predictive toxicology applications. Journal of Cheminformatics, 2010, 2, 7.	6.1	91
14	DIGEP-Pred: web service for in silico prediction of drug-induced gene expression profiles based on structural formula. Bioinformatics, 2013, 29, 2062-2063.	4.1	87
15	QNA-based â€˜Star Trackâ€™ QSAR approach. SAR and QSAR in Environmental Research, 2009, 20, 679-709.	2.2	84
16	SOMP: web server for in silico prediction of sites of metabolism for drug-like compounds. Bioinformatics, 2015, 31, 2046-2048.	4.1	83
17	Design of New Cognition Enhancers:â€‰ From Computer Prediction to Synthesis and Biological Evaluation. Journal of Medicinal Chemistry, 2004, 47, 2870-2876.	6.4	75
18	Quantitative Prediction of Antitarget Interaction Profiles for Chemical Compounds. Chemical Research in Toxicology, 2012, 25, 2378-2385.	3.3	70

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19	QSAR Modeling and Prediction of Drugâ€“Drug Interactions. Molecular Pharmaceutics, 2016, 13, 545-556.	4.6	65
20	Computational platform Way2Drug: from the prediction of biological activity to drug repurposing. Russian Chemical Bulletin, 2017, 66, 1832-1841.	1.5	60
21	Prediction of Biological Activity Spectra via The Internet. SAR and QSAR in Environmental Research, 2003, 14, 339-347.	2.2	56
22	Computer-aided prediction of biological activity spectra for organic compounds: the possibilities and limitations. Russian Chemical Bulletin, 2019, 68, 2143-2154.	1.5	56
23	PASS Targets: Ligand-based multi-target computational system based on a public data and naÃ¯ve Bayes approach. SAR and QSAR in Environmental Research, 2015, 26, 783-793.	2.2	52
24	In silico assessment of adverse drug reactions and associated mechanisms. Drug Discovery Today, 2016, 21, 58-71.	6.4	51
25	Synthesis and in silico biological activity evaluation of new N-substituted pyrazolo-oxazin-2-one systems. Bioorganic and Medicinal Chemistry, 2008, 16, 3059-3066.	3.0	50
26	Metabolism Site Prediction Based on Xenobiotic Structural Formulas and PASS Prediction Algorithm. Journal of Chemical Information and Modeling, 2014, 54, 498-507.	5.4	50
27	MetaTox: Web Application for Predicting Structure and Toxicity of Xenobioticsâ€™ Metabolites. Journal of Chemical Information and Modeling, 2017, 57, 638-642.	5.4	50
28	ADVERPredâ€“Web Service for Prediction of Adverse Effects of Drugs. Journal of Chemical Information and Modeling, 2018, 58, 8-11.	5.4	50
29	A new approach to QSAR modelling of acute toxicityâ€. SAR and QSAR in Environmental Research, 2007, 18, 285-298.	2.2	49
30	Computerâ€Aided Prediction of Rodent Carcinogenicity by PASS and CISOCâ€PSCT. QSAR and Combinatorial Science, 2009, 28, 806-810.	1.4	43
31	Evaluation of the local anaesthetic activity of 3-aminobenzo[d]isothiazole derivatives using the rat sciatic nerve model. European Journal of Medicinal Chemistry, 2009, 44, 473-481.	5.5	43
32	Computer-Aided Selection of Potential Antihypertensive Compounds with Dual Mechanism of Action. Journal of Medicinal Chemistry, 2003, 46, 3326-3332.	6.4	40
33	Computer-aided prediction of QT-prolongation. SAR and QSAR in Environmental Research, 2008, 19, 81-90.	2.2	27
34	How to Achieve Better Results Using PASS-Based Virtual Screening: Case Study for Kinase Inhibitors. Frontiers in Chemistry, 2018, 6, 133.	3.6	27
35	Prediction of reacting atoms for the major biotransformation reactions of organic xenobiotics. Journal of Cheminformatics, 2016, 8, 68.	6.1	24
36	ROSC-Pred: web-service for rodent organ-specific carcinogenicity prediction. Bioinformatics, 2018, 34, 710-712.	4.1	24

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37	AntiBac-Pred: A Web Application for Predicting Antibacterial Activity of Chemical Compounds. Journal of Chemical Information and Modeling, 2019, 59, 4513-4518.	5.4	24
38	Computer-aided prediction of xenobiotic metabolism in the human body. Russian Chemical Reviews, 2016, 85, 854-879.	6.5	22
39	Online resources for the prediction of biological activity of organic compounds. Russian Chemical Bulletin, 2016, 65, 384-393.	1.5	22
40	Computer-aided rodent carcinogenicity prediction. Mutation Research - Genetic Toxicology and Environmental Mutagenesis, 2005, 586, 138-146.	1.7	21
41	OpenTox predictive toxicology framework: toxicological ontology and semantic media wiki-based OpenToxipedia. Journal of Biomedical Semantics, 2012, 3, S7.	1.6	21
42	Drug-drug interaction prediction using PASS. SAR and QSAR in Environmental Research, 2019, 30, 655-664.	2.2	19
43	Prediction of Proteinâ€“Ligand Interaction Based on the Positional Similarity Scores Derived from Amino Acid Sequences. International Journal of Molecular Sciences, 2020, 21, 24.	4.1	19
44	Revealing Medicinal Plants That Are Useful for the Comprehensive Management of Epilepsy and Associated Comorbidities through In Silico Mining of Their Phytochemical Diversity. Planta Medica, 2015, 81, 495-506.	1.3	18
45	Computer aided prediction of biological activity spectra: Evaluating versus known and predicting of new activities for thiazole derivatives. SAR and QSAR in Environmental Research, 2002, 13, 457-471.	2.2	17
46	Prediction of biological activity profiles of cyanobacterial secondary metabolites. SAR and QSAR in Environmental Research, 2007, 18, 629-643.	2.2	17
47	Design, Synthesis and Pharmacological Evaluation of Novel Vanadium-Containing Complexes as Antidiabetic Agents. PLoS ONE, 2014, 9, e100386.	2.5	17
48	Comparison of Quantitative and Qualitative (Q)SAR Models Created for the Prediction of Ki and IC50 Values of Antitarget Inhibitors. Frontiers in Pharmacology, 2018, 9, 1136.	3.5	17
49	Rational Use of Heterogeneous Data in Quantitative Structureâ€“Activity Relationship (QSAR) Modeling of Cyclooxygenase/Lipoxygenase Inhibitors. Journal of Chemical Information and Modeling, 2019, 59, 713-730.	5.4	17
50	CYCLONET--an integrated database on cell cycle regulation and carcinogenesis. Nucleic Acids Research, 2007, 35, D550-D556.	14.5	16
51	Pharmacological repositioning of Achyranthes aspera as an antidepressant using pharmacoinformatic tools PASS and PharmaExpert: a case study with wet lab validation. SAR and QSAR in Environmental Research, 2018, 29, 69-81.	2.2	16
52	Combined network pharmacology and virtual reverse pharmacology approaches for identification of potential targets to treat vascular dementia. Scientific Reports, 2020, 10, 257.	3.3	16
53	Prediction of Severity of Drug-Drug Interactions Caused by Enzyme Inhibition and Activation. Molecules, 2019, 24, 3955.	3.8	15
54	Antihypoxic Action of Panax Japonicus, Tribulus Terrestris and Dioscorea Deltoidea Cell Cultures: In Silico and Animal Studies. Molecular Informatics, 2020, 39, e2000093.	2.5	15

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55	Prediction of Drug-Drug Interactions Related to Inhibition or Induction of Drug-Metabolizing Enzymes. Current Topics in Medicinal Chemistry, 2019, 19, 319-336.	2.1	15
56	Functional classification of proteins based on projection of amino acid sequences: application for prediction of protein kinase substrates. BMC Bioinformatics, 2010, 11, 313.	2.6	14
57	Identification of Drug-Induced Myocardial Infarction-Related Protein Targets through the Prediction of Drugâ€“Target Interactions and Analysis of Biological Processes. Chemical Research in Toxicology, 2014, 27, 1263-1281.	3.3	14
58	Quantitative analysis of structure-activity relationships of tetrahydro-2H-isoindole cyclooxygenase-2 inhibitors. Biochemistry (Moscow), 2015, 80, 74-86.	1.5	14
59	Network-Based Analysis of OMICs Data to Understand the HIVâ€“Host Interaction. Frontiers in Microbiology, 2020, 11, 1314.	3.5	14
60	Metatox - Web application for generation of metabolic pathways and toxicity estimation. Journal of Bioinformatics and Computational Biology, 2019, 17, 1940001.	0.8	13
61	A Computational Approach for the Prediction of Treatment History and the Effectiveness or Failure of Antiretroviral Therapy. International Journal of Molecular Sciences, 2020, 21, 748.	4.1	13
62	In silicomethod for identification of promising anticancer drug targets. SAR and QSAR in Environmental Research, 2009, 20, 755-766.	2.2	12
63	Computer Evaluation of Drug Interactions with P-Glycoprotein. Bulletin of Experimental Biology and Medicine, 2013, 154, 521-524.	0.8	12
64	In Silico Identification of Proteins Associated with Drug-induced Liver Injury Based on the Prediction of Drug-target Interactions. Molecular Informatics, 2017, 36, 1600142.	2.5	12
65	Prediction of metabolites of epoxidation reaction in MetaTox. SAR and QSAR in Environmental Research, 2017, 28, 833-842.	2.2	12
66	Computerized Prediction, Synthesis, and Antimicrobial Activity of New Amino-Acid Derivatives of 2-Chloro-N-(9,10-Dioxo-9,10-Dihydroanthracen-1-Yl)Acetamide. Pharmaceutical Chemistry Journal, 2014, 48, 582-586.	0.8	11
67	Identification of Drug Targets Related to the Induction of Ventricular Tachyarrhythmia Through a Systems Chemical Biology Approach. Toxicological Sciences, 2015, 145, 321-336.	3.1	11
68	N,N-Bis-(dimethylfluorosilylmethyl)amides of N-organosulfonylproline and sarcosine: synthesis, structure, stereodynamic behaviour and in silico studies. RSC Advances, 2016, 6, 75315-75327.	3.6	11
69	Study of local anesthetic activity of some derivatives of 3-amino-BENZO-[d]-Isothiazole. SAR and QSAR in Environmental Research, 2003, 14, 485-495.	2.2	10
70	Nootropic action of some antihypertensive drugs: computer predicting and experimental testing. Pharmaceutical Chemistry Journal, 2012, 45, 605-611.	0.8	10
71	PASS-based prediction of metabolites detection in biological systems. SAR and QSAR in Environmental Research, 2019, 30, 751-758.	2.2	10
72	A Novel Phenylpyrrolidine Derivative: Synthesis and Effect on Cognitive Functions in Rats with Experimental Ischemic Stroke. Molecules, 2021, 26, 6124.	3.8	10

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73	Virtual screening of chemical compounds active against breast cancer cell lines based on cell cycle modelling, prediction of cytotoxicity and interaction with targets. SAR and QSAR in Environmental Research, 2015, 26, 595-604.	2.2	9
74	Attenuation of hyperhomocysteinemia induced vascular dementia by sodium orthovanadate perhaps via PTP1B: Pertinent downstream outcomes. Behavioural Brain Research, 2019, 364, 29-40.	2.2	9
75	In Silico Prediction of Drugâ€“Drug Interactions Mediated by Cytochrome P450 Isoforms. Pharmaceutics, 2021, 13, 538.	4.5	9
76	QNA-Based Prediction of Sites of Metabolism. Molecules, 2017, 22, 2123.	3.8	8
77	Glycogen synthase kinase-3 inhibition as a potential pharmacological target for vascular dementia: In silico and in vivo evidence. Computers in Biology and Medicine, 2019, 108, 305-316.	7.0	8
78	Computational Toxicology in Drug Discovery: Opportunities and Limitations. Challenges and Advances in Computational Chemistry and Physics, 2014, , 325-367.	0.6	8
79	Integral estimation of xenobioticsâ€™ toxicity with regard to their metabolism in human organism. Pure and Applied Chemistry, 2017, 89, 1449-1458.	1.9	8
80	Internet System Predicting the Spectrum of Biological Activity of Chemical Compounds. Pharmaceutical Chemistry Journal, 2002, 36, 538-543.	0.8	7
81	In Silico fragment-based drug design using a PASS approach. SAR and QSAR in Environmental Research, 2012, 23, 279-296.	2.2	7
82	Computer modeling of blood brain barrier permeability for physiologically active compounds. Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry, 2013, 7, 95-107.	0.4	7
83	QSAR Modelling of Thymidylate Synthase Inhibitors in a Series of Quinazoline Derivatives. Pharmaceutical Chemistry Journal, 2018, 51, 884-888.	0.8	7
84	Assessment of the cardiovascular adverse effects of drug-drug interactions through a combined analysis of spontaneous reports and predicted drug-target interactions. PLoS Computational Biology, 2019, 15, e1006851.	3.2	7
85	Synthesis and anti-inflammatory activity of ethynylthiazoles. Chemistry of Heterocyclic Compounds, 2006, 42, 675-680.	1.2	6
86	Prediction of Proteinâ€“ligand Interaction Based on Sequence Similarity and Ligand Structural Features. International Journal of Molecular Sciences, 2020, 21, 8152.	4.1	6
87	Recent Advances in the Development of Pharmaceutical Agents for Metabolic Disorders: A Computational Perspective. Current Medicinal Chemistry, 2019, 25, 5432-5463.	2.4	6
88	Lactamomethyl derivatives of diphenols: synthesis, structure, and potential biological activity. Russian Chemical Bulletin, 2018, 67, 1518-1529.	1.5	5
89	MetaPASS: A Web Application for Analyzing the Biological Activity Spectrum of Organic Compounds Taking into Account their Biotransformation. Molecular Informatics, 2021, 40, 2000231.	2.5	5
90	Computer search for molecular mechanisms of ulcerogenic action of non-steroidal anti-inflammatory drugs. Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry, 2013, 7, 40-45.	0.4	4

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91	Determination of Amino Acid Residues Responsible for Specific Interaction of Protein Kinases with Small Molecule Inhibitors. Molecular Biology, 2018, 52, 478-487.	1.3	4
92	Relationships between the Structure and Severe Drug-Induced Liver Injury for Low, Medium, and High Doses of Drugs. Chemical Research in Toxicology, 2022, 35, 402-411.	3.3	4
93	The method predicting interaction between protein targets and small-molecular ligands with the wide applicability domain. Computational Biology and Chemistry, 2022, 98, 107674.	2.3	4
94	Virtual Screening for Potential Substances for the Prophylaxis of HIV Infection in Libraries of Commercially Available Organic Compounds. Pharmaceutical Chemistry Journal, 2013, 47, 343-360.	0.8	3
95	Computer Prediction of Adverse Drug Effects on the Cardiovascular System. Pharmaceutical Chemistry Journal, 2018, 52, 758-762.	0.8	3
96	Computer-Aided Xenobiotic Toxicity Prediction Taking into Account their Metabolism in the Human Body. Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry, 2019, 13, 228-236.	0.4	3
97	New lactam-containing benzenesulfonamides: design, synthesis, and in silico and in vitro studies. Russian Chemical Bulletin, 2021, 70, 479-486.	1.5	3
98	In silico assessment of acute toxicity in rodents. Toxicology Letters, 2009, 189, S264.	0.8	2
99	Prediction of the action of ligands of steroid hormone receptors. Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry, 2014, 8, 53-58.	0.4	2
100	Capacities of computer evaluation of hidden potential of phytochemicals of medicinal plants of the traditional Indian Ayurvedic medicine. Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry, 2016, 10, 43-54.	0.4	2
101	Synthesis and structure of the first representative of pentacoordinate C,O-chelates with a dipeptide fragment, the fluorosilane Tsâ€”Glyâ€”(S)-Proâ€”N(Me)CH2SiMe2F. Russian Chemical Bulletin, 2017, 66, 571-573.	1.5	2
102	Improving (Q)SAR predictions by examining bias in the selection of compounds for experimental testing. SAR and QSAR in Environmental Research, 2019, 30, 759-773.	2.2	2
103	Bioinformatics guided rotenone adjuvant kindling in mice as a new animal model of drug-resistant epilepsy. Computers in Biology and Medicine, 2022, 147, 105754.	7.0	2
104	Computer-Aided Search for Potential Drugs Exhibiting a Combined Antihypertensive Effect. Pharmaceutical Chemistry Journal, 2001, 35, 375-381.	0.8	1
105	Quantitative structure-activity relationships of cyclin-dependent kinase 1 inhibitors. Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry, 2007, 1, 17-28.	0.4	1
106	Human embryo genome editing: an interdisciplinary approach. Vestnik Rossiiskoi Akademii Meditsinskikh Nauk, 2021, 76, 86-92.	0.6	1
107	Prospective pharmacological effects of psoralen photoxidation products and their cycloadducts with aminothiols: chemoinformatic analysis. Bulletin of Russian State Medical University, 2020, , .	0.2	1
108	Tools for prediction of xenobiotics interaction with human cytochrome P450. Chemistry Central Journal, 2009, 3, .	2.6	0

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109	Computer Assessment of the Xenobiotic Metabolites Formationâ€™s Probability in the Human Body. Biophysics (Russian Federation), 2020, 65, 1023-1029.	0.7	0