Eugene N Muratov

List of Publications by Year
in descending order

126 papers	8,742 citations	61984 43 h-index	46799 89 g-index
149 all docs	149 docs citations	149 times ranked	8955 citing authors

#	Article	IF	Citations
1	QSAR Modeling: Where Have You Been? Where Are You Going To?. Journal of Medicinal Chemistry, 2014, 57, 4977-5010.	6.4	1,401
2	Trust, But Verify: On the Importance of Chemical Structure Curation in Cheminformatics and QSAR Modeling Research. Journal of Chemical Information and Modeling, 2010, 50, 1189-1204.	5.4	611
3	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	38.1	427
4	QSAR-Based Virtual Screening: Advances and Applications in Drug Discovery. Frontiers in Pharmacology, 2018, 9, 1275.	3.5	291
5	Comprehensive characterization of the Published Kinase Inhibitor Set. Nature Biotechnology, 2016, 34, 95-103.	17.5	289
6	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	6.0	264
7	Chalcone Derivatives: Promising Starting Points for Drug Design. Molecules, 2017, 22, 1210.	3.8	261
8	Does Rational Selection of Training and Test Sets Improve the Outcome of QSAR Modeling?. Journal of Chemical Information and Modeling, 2012, 52, 2570-2578.	5.4	232
9	Trust, but Verify II: A Practical Guide to Chemogenomics Data Curation. Journal of Chemical Information and Modeling, 2016, 56, 1243-1252.	5.4	228
10	Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints. Chemistry of Materials, 2015, 27, 735-743.	6.7	209
11	Applicability Domains for Classification Problems: Benchmarking of Distance to Models for Ames Mutagenicity Set. Journal of Chemical Information and Modeling, 2010, 50, 2094-2111.	5.4	202
12	Predicting Drug-Induced Hepatotoxicity Using QSAR and Toxicogenomics Approaches. Chemical Research in Toxicology, 2011, 24, 1251-1262.	3.3	190
13	Phantom PAINS: Problems with the Utility of Alerts for <u>P</u>an-<u>A</u>ssay <u>IN</u>terference Compound<u>S</u>. Journal of Chemical Information and Modeling, 2017, 57, 417-427.	5.4	188
14	Modelling of compound combination effects and applications to efficacy and toxicity: state-of-the-art, challenges and perspectives. Drug Discovery Today, 2016, 21, 225-238.	6.4	162
15	Predâ€hERG: A Novel webâ€Accessible Computational Tool for Predicting Cardiac Toxicity. Molecular Informatics, 2015, 34, 698-701.	2.5	159
16	Curation of chemogenomics data. Nature Chemical Biology, 2015, 11, 535-535.	8.0	158
17	Application of Random Forest Approach to QSAR Prediction of Aquatic Toxicity. Journal of Chemical Information and Modeling, 2009, 49, 2481-2488.	5.4	147
18	Progress towards a public chemogenomic set for protein kinases and a call for contributions. PLoS ONE, 2017, 12, e0181585.	2.5	131

#	Article	IF	Citations
19	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	38.1	128
20	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	6.0	120
21	Existing and Developing Approaches for QSAR Analysis of Mixtures. Molecular Informatics, 2012, 31, 202-221.	2.5	105
22	Data Set Modelability by QSAR. Journal of Chemical Information and Modeling, 2014, 54, 1-4.	5.4	105
23	Alarms about structural alerts. Green Chemistry, 2016, 18, 4348-4360.	9.0	103
24	QSAR-driven design, synthesis and discovery of potent chalcone derivatives with antitubercular activity. European Journal of Medicinal Chemistry, 2017, 137, 126-138.	5.5	96
25	Hierarchic system of QSAR models (1Dâ€“4D) on the base of simplex representation of molecular structure. Journal of Molecular Modeling, 2005, 11, 457-467.	1.8	88
26	Tuning hERG Out: Antitarget QSAR Models for Drug Development. Current Topics in Medicinal Chemistry, 2014, 14, 1399-1415.	2.1	82
27	Pred-Skin: A Fast and Reliable Web Application to Assess Skin Sensitization Effect of Chemicals. Journal of Chemical Information and Modeling, 2017, 57, 1013-1017.	5.4	79
28	Synergistic and Antagonistic Drug Combinations against SARS-CoV-2. Molecular Therapy, 2021, 29, 873-885.	8.2	78
29	Quantitative Structureâ^'Activity Relationship Studies of [(Biphenyloxy)propyl]isoxazole Derivatives. Inhibitors of Human Rhinovirus 2 Replication. Journal of Medicinal Chemistry, 2007, 50, 4205-4213.	6.4	73
30	Predicting chemically-induced skin reactions. Part I: QSAR models of skin sensitization and their application to identify potentially hazardous compounds. Toxicology and Applied Pharmacology, 2015, 284, 262-272.	2.8	72
31	Discovery of New Anti-Schistosomal Hits by Integration of QSAR-Based Virtual Screening and High Content Screening. Journal of Medicinal Chemistry, 2016, 59, 7075-7088.	6.4	67
32	QSAR Modeling and Prediction of Drugâ€“Drug Interactions. Molecular Pharmaceutics, 2016, 13, 545-556.	4.6	65
33	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	6.0	63
34	Per aspera ad astra: application of Simplex QSAR approach in antiviral research. Future Medicinal Chemistry, 2010, 2, 1205-1226.	2.3	58
35	Universal Approach for Structural Interpretation of QSAR/QSPR Models. Molecular Informatics, 2013, 32, 843-853.	2.5	57
36	Chemical toxicity prediction for major classes of industrial chemicals: Is it possible to develop universal models covering cosmetics, drugs, and pesticides?. Food and Chemical Toxicology, 2018, 112, 526-534.	3.6	57

#	Article	IF	Citations
37	QSAR Modeling of SARSâ€CoV M^{pro} Inhibitors Identifies Sufugolix, Cenicriviroc, Proglumetacin, and other Drugs as Candidates for Repurposing against SARSâ€CoVâ€2. Molecular Informatics, 2021, 40, e2000113.	2.5	57
38	Predicting chemically-induced skin reactions. Part II: QSAR models of skin permeability and the relationships between skin permeability and skin sensitization. Toxicology and Applied Pharmacology, 2015, 284, 273-280.	2.8	53
39	Conditional Toxicity Value (CTV) Predictor: An In Silico Approach for Generating Quantitative Risk Estimates for Chemicals. Environmental Health Perspectives, 2018, 126, 057008.	6.0	52
40	Open drug discovery for the Zika virus. F1000Research, 2016, 5, 150.	1.6	50
41	QSAR-Driven Discovery of Novel Chemical Scaffolds Active against Schistosoma mansoni. Journal of Chemical Information and Modeling, 2016, 56, 1357-1372.	5.4	47
42	Chembench: A Publicly Accessible, Integrated Cheminformatics Portal. Journal of Chemical Information and Modeling, 2017, 57, 105-108.	5.4	47
43	Gelatin/carboxymethyl cellulose mucoadhesive films with lysozyme: Development and characterization. Carbohydrate Polymers, 2016, 147, 208-215.	10.2	45
44	Multi-Descriptor Read Across (MuDRA): A Simple and Transparent Approach for Developing Accurate Quantitative Structureâ€“Activity Relationship Models. Journal of Chemical Information and Modeling, 2018, 58, 1214-1223.	5.4	43
45	QSAR models of human data can enrich or replace LLNA testing for human skin sensitization. Green Chemistry, 2016, 18, 6501-6515.	9.0	42
46	The effects of characteristics of substituents on toxicity of the nitroaromatics: HiT QSAR study. Journal of Computer-Aided Molecular Design, 2008, 22, 747-759.	2.9	41
47	STopTox: An in Silico Alternative to Animal Testing for Acute Systemic and Topical Toxicity. Environmental Health Perspectives, 2022, 130, 27012.	6.0	38
48	Application of Random Forest and Multiple Linear Regression Techniques to QSPR Prediction of an Aqueous Solubility for Military Compounds. Molecular Informatics, 2010, 29, 394-406.	2.5	37
49	Chemotext: A Publicly Available Web Server for Mining Drugâ€“Targetâ€“Disease Relationships in PubMed. Journal of Chemical Information and Modeling, 2018, 58, 212-218.	5.4	36
50	A Perspective and a New Integrated Computational Strategy for Skin Sensitization Assessment. ACS Sustainable Chemistry and Engineering, 2018, 6, 2845-2859.	6.7	35
51	Large-Scale Modeling of Multispecies Acute Toxicity End Points Using Consensus of Multitask Deep Learning Methods. Journal of Chemical Information and Modeling, 2021, 61, 653-663.	5.4	35
52	Cheminformatics-driven discovery of polymeric micelle formulations for poorly soluble drugs. Science Advances, 2019, 5, eaav9784.	10.3	34
53	Deep Learning-driven research for drug discovery: Tackling Malaria. PLoS Computational Biology, 2020, 16, e1007025.	3.2	34
54	The analysis of structure-anticancer and antiviral activity relationships for macrocyclic pyridinophanes and their analogues on the basis of 4D QSAR models (simplex representation of) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 5		34

#	Article	IF	Citations
55	Recent progress on cheminformatics approaches to epigenetic drug discovery. Drug Discovery Today, 2020, 25, 2268-2276.	6.4	33
56	Computer-Aided Discovery and Characterization of Novel Ebola Virus Inhibitors. Journal of Medicinal Chemistry, 2018, 61, 3582-3594.	6.4	32
57	Pred-Skin: A Web Portal for Accurate Prediction of Human Skin Sensitizers. Chemical Research in Toxicology, 2021, 34, 258-267.	3.3	32
58	Application of Quantum Chemical Approximations to Environmental Problems: Prediction of Water Solubility for Nitro Compounds. Environmental Science & Technology, 2009, 43, 9208-9215.	10.0	30
59	Computationally-guided drug repurposing enables the discovery of kinase targets and inhibitors as new schistosomicidal agents. PLoS Computational Biology, 2018, 14, e1006515.	3.2	29
60	Learning from history: do not flatten the curve of antiviral research!. Drug Discovery Today, 2020, 25, 1604-1613.	6.4	26
61	Discovery of new potent hits against intracellular Trypanosoma cruzi by QSAR-based virtual screening. European Journal of Medicinal Chemistry, 2019, 163, 649-659.	5.5	25
62	Oy Vey! A Comment on â€œMachine Learning of Toxicological Big Data Enables Read-Across Structure Activity Relationships Outperforming Animal Test Reproducibilityâ€• Toxicological Sciences, 2019, 167, 3-4.	3.1	24
63	Computer-aided discovery of two novel chalcone-like compounds active and selective against Leishmania infantum. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 2459-2464.	2.2	23
64	Virtual Screening and Molecular Design Based on Hierarchical Qsar Technology. Challenges and Advances in Computational Chemistry and Physics, 2010, , 127-176.	0.6	23
65	Expanding the scope of drug repurposing in pediatrics: The Children's Pharmacy Collaborativeâ„¢. Drug Discovery Today, 2014, 19, 1696-1698.	6.4	22
66	QSAR-Driven Design and Discovery of Novel Compounds With Antiplasmodial and Transmission Blocking Activities. Frontiers in Pharmacology, 2018, 9, 146.	3.5	22
67	SCAM Detective: Accurate Predictor of Small, Colloidally Aggregating Molecules. Journal of Chemical Information and Modeling, 2020, 60, 4056-4063.	5.4	21
68	Predicting Binding Affinity of CSAR Ligands Using Both Structure-Based and Ligand-Based Approaches. Journal of Chemical Information and Modeling, 2013, 53, 1915-1922.	5.4	20
69	Curated Data In â€" Trustworthy In Silico Models Out: The Impact of Data Quality on the Reliability of Artificial Intelligence Models as Alternatives to Animal Testing. ATLA Alternatives To Laboratory Animals, 2021, 49, 73-82.	1.0	20
70	QSAR analysis of poliovirus inhibition by dual combinations of antivirals. Structural Chemistry, 2013, 24, 1665-1679.	2.0	19
71	Modern approaches to accelerate discovery of new antischistosomal drugs. Expert Opinion on Drug Discovery, 2016, 11, 557-567.	5.0	19
72	Development of Web and Mobile Applications for Chemical Toxicity Prediction. Journal of the Brazilian Chemical Society, 0, , .	0.6	18

#	Article	IF	Citations
73	New QSPR equations for prediction of aqueous solubility for military compounds. Chemosphere, 2010, 79, 887-890.	8.2	17
74	QSAR analysis of [(biphenyloxy)propyl]isoxazoles: agents against coxsackievirus B3. Future Medicinal Chemistry, 2011, 3, 15-27.	2.3	17
75	The SistematX Web Portal of Natural Products: An Update. Journal of Chemical Information and Modeling, 2021, 61, 2516-2522.	5.4	17
76	Simplex representation of molecular structure as universal QSAR/QSPR tool. Structural Chemistry, 2021, 32, 1365-1392.	2.0	17
77	Virtual Screening of Natural Products Database. Mini-Reviews in Medicinal Chemistry, 2021, 21, 2657-2730.	2.4	17
78	Computer-Assisted Decision Support for Student Admissions Based on Their Predicted Academic Performance. American Journal of Pharmaceutical Education, 2017, 81, 46.	2.1	16
79	Unveiling the Kinomes of Leishmania infantum and L. braziliensis Empowers the Discovery of New Kinase Targets and Antileishmanial Compounds. Computational and Structural Biotechnology Journal, 2019, 17, 352-361.	4.1	16
80	Synthesis and Structureâ€“Activity Relationships of DCLK1 Kinase Inhibitors Based on a 5,11-Dihydro-6H-benzo[e]pyrimido[5,4-b][1,4]diazepin-6-one Scaffold. Journal of Medicinal Chemistry, 2020, 63, 7817-7826.	6.4	16
81	QSAR Modeling for Multi-Target Drug Discovery: Designing Simultaneous Inhibitors of Proteins in Diverse Pathogenic Parasites. Frontiers in Chemistry, 2021, 9, 634663.	3.6	16
82	COVID-KOP: integrating emerging COVID-19 data with the ROBOKOP database. Bioinformatics, 2021, 37, 586-587.	4.1	15
83	Knowledge-based approaches to drug discovery for rare diseases. Drug Discovery Today, 2022, 27, 490-502.	6.4	15
84	Short Communication: Cheminformatics Analysis to Identify Predictors of Antiviral Drug Penetration into the Female Genital Tract. AIDS Research and Human Retroviruses, 2014, 30, 1058-1064.	1.1	14
85	Quantitative Structureâ€“Activity Relationship Modeling and Docking of Monoterpenes with Insecticidal Activity Against Reticulitermes chinensis Snyder and Drosophila melanogaster. Journal of Agricultural and Food Chemistry, 2020, 68, 4687-4698.	5.2	14
86	Conserved coronavirus proteins as targets of broad-spectrum antivirals. Antiviral Research, 2022, 204, 105360.	4.1	13
87	Modelability Criteria: Statistical Characteristics Estimating Feasibility to Build Predictive QSAR Models for a Dataset. , 2014, , 187-230.		11
88	Computational assessment of environmental hazards of nitroaromatic compounds: influence of the type and position of aromatic ring substituents on toxicity. Structural Chemistry, 2016, 27, 191-198.	2.0	11
89	Computer-Aided Discovery of New Solubility-Enhancing Drug Delivery System. Biomolecules, 2020, 10, 913.	4.0	10
90	Quantitative high-throughput phenotypic screening of pediatric cancer cell lines identifies multiple opportunities for drug repurposing. Oncotarget, 2018, 9, 4758-4772.	1.8	10

#	Article	IF	Citations
91	The analysis of structure-anticancer and antiviral activity relationships for macrocyclic pyridinophanes and their analogues on the basis of 4D QSAR models (simplex representation of) Tj ETQq1 1 0.784314 rgBT /Overlock	3.4	10
92	BeeToxAI: An artificial intelligence-based web app to assess acute toxicity of chemicals to honey bees. Artificial Intelligence in the Life Sciences, 2021, 1, 100013.	2.2	8
93	Chemistry-Wide Association Studies (CWAS): A Novel Framework for Identifying and Interpreting Structureâ€“Activity Relationships. Journal of Chemical Information and Modeling, 2018, 58, 2203-2213.	5.4	7
94	Development and characterization of chitosan/polyvinyl alcohol polymer material with elastolytic and collagenolytic activities. Enzyme and Microbial Technology, 2020, 132, 109399.	3.2	7
95	Computer-assisted discovery of compounds with insecticidal activity against Musca domestica and Mythimna separata. Food and Chemical Toxicology, 2021, 147, 111899.	3.6	7
96	Natural Bioactive Products with Antioxidant Properties Useful in Neurodegenerative Diseases 2020. Oxidative Medicine and Cellular Longevity, 2021, 2021, 1-2.	4.0	7
97	QUIMIOINFORMÃ‡TICA: UMA INTRODUÃ‡Ãƒ O. Quimica Nova, 0, , .	0.3	7
98	Computer-Assisted Discovery of Alkaloids with Schistosomicidal Activity. Current Issues in Molecular Biology, 2022, 44, 383-408.	2.4	7
99	Novel computational models offer alternatives to animal testing for assessing eye irritation and corrosion potential of chemicals. Artificial Intelligence in the Life Sciences, 2021, 1, 100028.	2.2	7
100	Computational drug discovery for the Zika virus. Brazilian Journal of Pharmaceutical Sciences, 2018, 54, .	1.2	6
101	Modernization of Enoxaparin Molecular Weight Determination Using Homogeneous Standards. Pharmaceuticals, 2017, 10, 66.	3.8	5
102	Discovery of Alternative Chemotherapy Options for Leishmaniasis through Computational Studies of Asteraceae. ChemMedChem, 2021, 16, 1234-1245.	3.2	5
103	ZINC Express: A Virtual Assistant for Purchasing Compounds Annotated in the ZINC Database. Journal of Chemical Information and Modeling, 2021, 61, 1033-1036.	5.4	5
104	COVID-19 Knowledge Extractor (COKE): A Curated Repository of Drugâ€“Target Associations Extracted from the CORD-19 Corpus of Scientific Publications on COVID-19. Journal of Chemical Information and Modeling, 2021, , .	5.4	5
105	Defining clinical outcome pathways. Drug Discovery Today, 2022, 27, 1671-1678.	6.4	5
106	Chalcones as a basis for computer-aided drug design: innovative approaches to tackle malaria. Future Medicinal Chemistry, 2019, 11, 2635-2646.	2.3	4
107	Mining Complex Biomedical Literature for Actionable Knowledge on Rare Diseases. Human Perspectives in Health Sciences and Technology, 2020, , 77-94.	0.4	4
108	Natural Products as Potential Agents against SARS-CoV and SARSCoV- 2. Current Medicinal Chemistry, 2021, 28, 5498-5526.	2.4	4

#	Article	IF	Citations
109	Computer-Assisted Design of Thiophene-Indole Hybrids as Leishmanial Agents. Current Topics in Medicinal Chemistry, 2020, 20, 1704-1719.	2.1	4
110	HiT QSAR Study of Antiviralsâ€™ Bioavailability. Antiviral Research, 2009, 82, A56.	4.1	3
111	Predicting Adverse Drug Effects from Literature- and Database-Mined Assertions. Drug Safety, 2018, 41, 1059-1072.	3.2	3
112	Shortcuts to schistosomiasis drug discovery: The state-of-the-art. Annual Reports in Medicinal Chemistry, 2019, , 139-180.	0.9	3
113	Chemical safety assessment of transformation products of landfill leachate formed during the Fenton process. Journal of Hazardous Materials, 2021, 419, 126438.	12.4	3
114	Allosteric Binders of ACE2 Are Promising Anti-SARS-CoV-2 Agents. ACS Pharmacology and Translational Science, 2022, 5, 468-478.	4.9	3
115	Four diterpenes identified in silico were isolated from Hyptidinae and demonstrated in vitro activity against Mycobacterium tuberculosis. Natural Product Research, 2023, 37, 903-911.	1.8	3
116	New Advances in QSPR/QSAR Analysis of Nitrocompounds: Solubility, Lipophilicity, and Toxicity. , 2012, , 279-334.		2
117	Activity prediction and identification of misâ€annotated chemical compounds using extreme descriptors. Journal of Chemometrics, 2016, 30, 99-108.	1.3	2
118	Secondary Metabolites Extracted from Annonaceae and Chemotaxonomy Study of Terpenoids. Journal of the Brazilian Chemical Society, 0, , .	0.6	2
119	Recent Studies on Neglected Drug Design. Current Topics in Medicinal Chemistry, 2021, 21, 1943-1974.	2.1	2
120	Automated Framework for Developing Predictive Machine Learning Models for Data-Driven Drug Discovery. Journal of the Brazilian Chemical Society, 0, , .	0.6	1
121	New Experimental and Computational Tools for Drug Discovery. - Part-VII. Current Topics in Medicinal Chemistry, 2019, 19, 898-899.	2.1	0
122	Editorial: Cheminformatics Approaches in Drug Discovery for Neglected Tropical Diseases. Frontiers in Chemistry, 2021, 9, 719223.	3.6	0
123	Selenium and Computational Studies. Mini-Reviews in Medicinal Chemistry, 2021, 21, 1865-1887.	2.4	0
124	Dataset Modelability by QSAR: Continuous Response Variable. , 2022, , 233-253.		0
125	New Experimental and Computational Tools for Drug Discovery - Part-VIII. Current Topics in Medicinal Chemistry, 2020, 20, 277-279.	2.1	0
126	Natural Products from Annonaceae as Potential Antichagasic Agents. ChemMedChem, 2022, 17, .	3.2	0