

Eugene N Muratov

List of Publications by Year in descending order

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Version: 2024-02-01

126
papers

8,742
citations

71004

43
h-index

53065

89
g-index

149
all docs

149
docs citations

149
times ranked

9929
citing authors

#	ARTICLE	IF	CITATIONS
1	Four diterpenes identified <i>in silico</i> were isolated from Hyptidinae and demonstrated <i>in vitro</i> activity against <i>Mycobacterium tuberculosis</i> . <i>Natural Product Research</i> , 2023, 37, 903-911.	1.0	3
2	Dataset Modelability by QSAR: Continuous Response Variable. , 2022, , 233-253.		0
3	Knowledge-based approaches to drug discovery for rare diseases. <i>Drug Discovery Today</i> , 2022, 27, 490-502.	3.2	15
4	Computer-Assisted Discovery of Alkaloids with Schistosomicidal Activity. <i>Current Issues in Molecular Biology</i> , 2022, 44, 383-408.	1.0	7
5	Defining clinical outcome pathways. <i>Drug Discovery Today</i> , 2022, 27, 1671-1678.	3.2	5
6	STopTox: An <i>in Silico</i> Alternative to Animal Testing for Acute Systemic and Topical Toxicity. <i>Environmental Health Perspectives</i> , 2022, 130, 27012.	2.8	38
7	Allosteric Binders of ACE2 Are Promising Anti-SARS-CoV-2 Agents. <i>ACS Pharmacology and Translational Science</i> , 2022, 5, 468-478.	2.5	3
8	Conserved coronavirus proteins as targets of broad-spectrum antivirals. <i>Antiviral Research</i> , 2022, 204, 105360.	1.9	13
9	Natural Products from Annonaceae as Potential Antichagasic Agents. <i>ChemMedChem</i> , 2022, 17, .	1.6	0
10	QSAR Modeling of SARS-CoV M ^{pro} Inhibitors Identifies Sufugolix, Cenicriviroc, Proglumetacin, and other Drugs as Candidates for Repurposing against SARS-CoV-2. <i>Molecular Informatics</i> , 2021, 40, e2000113.	1.4	57
11	Pred-Skin: A Web Portal for Accurate Prediction of Human Skin Sensitizers. <i>Chemical Research in Toxicology</i> , 2021, 34, 258-267.	1.7	32
12	COVID-KOP: integrating emerging COVID-19 data with the ROBOKOP database. <i>Bioinformatics</i> , 2021, 37, 586-587.	1.8	15
13	Computer-assisted discovery of compounds with insecticidal activity against <i>Musca domestica</i> and <i>Mythimna separata</i> . <i>Food and Chemical Toxicology</i> , 2021, 147, 111899.	1.8	7
14	Synergistic and Antagonistic Drug Combinations against SARS-CoV-2. <i>Molecular Therapy</i> , 2021, 29, 873-885.	3.7	78
15	Discovery of Alternative Chemotherapy Options for Leishmaniasis through Computational Studies of Asteraceae. <i>ChemMedChem</i> , 2021, 16, 1234-1245.	1.6	5
16	Natural Bioactive Products with Antioxidant Properties Useful in Neurodegenerative Diseases 2020. <i>Oxidative Medicine and Cellular Longevity</i> , 2021, 2021, 1-2.	1.9	7
17	Large-Scale Modeling of Multispecies Acute Toxicity End Points Using Consensus of Multitask Deep Learning Methods. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 653-663.	2.5	35
18	ZINC Express: A Virtual Assistant for Purchasing Compounds Annotated in the ZINC Database. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 1033-1036.	2.5	5

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19	QSAR Modeling for Multi-Target Drug Discovery: Designing Simultaneous Inhibitors of Proteins in Diverse Pathogenic Parasites. <i>Frontiers in Chemistry</i> , 2021, 9, 634663.	1.8	16
20	CATMoS: Collaborative Acute Toxicity Modeling Suite. <i>Environmental Health Perspectives</i> , 2021, 129, 47013.	2.8	63
21	Curated Data In "Trustworthy <i>In Silico</i> Models Out: The Impact of Data Quality on the Reliability of Artificial Intelligence Models as Alternatives to Animal Testing. <i>ATLA Alternatives To Laboratory Animals</i> , 2021, 49, 73-82.	0.7	20
22	The Sistemax Web Portal of Natural Products: An Update. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2516-2522.	2.5	17
23	Simplex representation of molecular structure as universal QSAR/QSPR tool. <i>Structural Chemistry</i> , 2021, 32, 1365-1392.	1.0	17
24	Editorial: Cheminformatics Approaches in Drug Discovery for Neglected Tropical Diseases. <i>Frontiers in Chemistry</i> , 2021, 9, 719223.	1.8	0
25	Recent Studies on Neglected Drug Design. <i>Current Topics in Medicinal Chemistry</i> , 2021, 21, 1943-1974.	1.0	2
26	Natural Products as Potential Agents against SARS-CoV and SARSCoV- 2. <i>Current Medicinal Chemistry</i> , 2021, 28, 5498-5526.	1.2	4
27	Selenium and Computational Studies. <i>Mini-Reviews in Medicinal Chemistry</i> , 2021, 21, 1865-1887.	1.1	0
28	Chemical safety assessment of transformation products of landfill leachate formed during the Fenton process. <i>Journal of Hazardous Materials</i> , 2021, 419, 126438.	6.5	3
29	A critical overview of computational approaches employed for COVID-19 drug discovery. <i>Chemical Society Reviews</i> , 2021, 50, 9121-9151.	18.7	128
30	Virtual Screening of Natural Products Database. <i>Mini-Reviews in Medicinal Chemistry</i> , 2021, 21, 2657-2730.	1.1	17
31	COVID-19 Knowledge Extractor (COKE): A Curated Repository of Drug-Target Associations Extracted from the COVID-19 Corpus of Scientific Publications on COVID-19. <i>Journal of Chemical Information and Modeling</i> , 2021, , .	2.5	5
32	Novel computational models offer alternatives to animal testing for assessing eye irritation and corrosion potential of chemicals. <i>Artificial Intelligence in the Life Sciences</i> , 2021, 1, 100028.	1.6	7
33	BeeToxAI: An artificial intelligence-based web app to assess acute toxicity of chemicals to honey bees. <i>Artificial Intelligence in the Life Sciences</i> , 2021, 1, 100013.	1.6	8
34	Development and characterization of chitosan/polyvinyl alcohol polymer material with elastolytic and collagenolytic activities. <i>Enzyme and Microbial Technology</i> , 2020, 132, 109399.	1.6	7
35	Learning from history: do not flatten the curve of antiviral research!. <i>Drug Discovery Today</i> , 2020, 25, 1604-1613.	3.2	26
36	SCAM Detective: Accurate Predictor of Small, Colloidally Aggregating Molecules. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 4056-4063.	2.5	21

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37	Synthesis and Structure-Activity Relationships of DCLK1 Kinase Inhibitors Based on a 5,11-Dihydro-6H-benzopyrimido[5,4-b][1,4]diazepin-6-one Scaffold. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 7817-7826.	2.9	16
38	Computer-Aided Discovery of New Solubility-Enhancing Drug Delivery System. <i>Biomolecules</i> , 2020, 10, 913.	1.8	10
39	Deep Learning-driven research for drug discovery: Tackling Malaria. <i>PLoS Computational Biology</i> , 2020, 16, e1007025.	1.5	34
40	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. <i>Environmental Health Perspectives</i> , 2020, 128, 27002.	2.8	120
41	QSAR without borders. <i>Chemical Society Reviews</i> , 2020, 49, 3525-3564.	18.7	427
42	Quantitative Structure-Activity Relationship Modeling and Docking of Monoterpenes with Insecticidal Activity Against <i>Reticulitermes chinensis</i> Snyder and <i>Drosophila melanogaster</i> . <i>Journal of Agricultural and Food Chemistry</i> , 2020, 68, 4687-4698.	2.4	14
43	Mining Complex Biomedical Literature for Actionable Knowledge on Rare Diseases. <i>Human Perspectives in Health Sciences and Technology</i> , 2020, , 77-94.	0.2	4
44	Recent progress on cheminformatics approaches to epigenetic drug discovery. <i>Drug Discovery Today</i> , 2020, 25, 2268-2276.	3.2	33
45	New Experimental and Computational Tools for Drug Discovery - Part-VIII. <i>Current Topics in Medicinal Chemistry</i> , 2020, 20, 277-279.	1.0	0
46	Computer-Assisted Design of Thiophene-Indole Hybrids as Leishmanial Agents. <i>Current Topics in Medicinal Chemistry</i> , 2020, 20, 1704-1719.	1.0	4
47	New Experimental and Computational Tools for Drug Discovery. - Part-VII. <i>Current Topics in Medicinal Chemistry</i> , 2019, 19, 898-899.	1.0	0
48	Shortcuts to schistosomiasis drug discovery: The state-of-the-art. <i>Annual Reports in Medicinal Chemistry</i> , 2019, , 139-180.	0.5	3
49	Cheminformatics-driven discovery of polymeric micelle formulations for poorly soluble drugs. <i>Science Advances</i> , 2019, 5, eaav9784.	4.7	34
50	Unveiling the Kinomes of <i>Leishmania infantum</i> and <i>L. braziliensis</i> Empowers the Discovery of New Kinase Targets and Antileishmanial Compounds. <i>Computational and Structural Biotechnology Journal</i> , 2019, 17, 352-361.	1.9	16
51	Chalcones as a basis for computer-aided drug design: innovative approaches to tackle malaria. <i>Future Medicinal Chemistry</i> , 2019, 11, 2635-2646.	1.1	4
52	Discovery of new potent hits against intracellular <i>Trypanosoma cruzi</i> by QSAR-based virtual screening. <i>European Journal of Medicinal Chemistry</i> , 2019, 163, 649-659.	2.6	25
53	Oy Vey! A Comment on "Machine Learning of Toxicological Big Data Enables Read-Across Structure Activity Relationships Outperforming Animal Test Reproducibility". <i>Toxicological Sciences</i> , 2019, 167, 3-4.	1.4	24
54	Computer-Aided Discovery and Characterization of Novel Ebola Virus Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 3582-3594.	2.9	32

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55	A Perspective and a New Integrated Computational Strategy for Skin Sensitization Assessment. ACS Sustainable Chemistry and Engineering, 2018, 6, 2845-2859.	3.2	35
56	Chemotext: A Publicly Available Web Server for Mining Drug-Target-Disease Relationships in PubMed. Journal of Chemical Information and Modeling, 2018, 58, 212-218.	2.5	36
57	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.	1.8	57
58	Computational drug discovery for the Zika virus. Brazilian Journal of Pharmaceutical Sciences, 2018, 54, .	1.2	6
59	Conditional Toxicity Value (CTV) Predictor: An <i>In Silico</i> Approach for Generating Quantitative Risk Estimates for Chemicals. Environmental Health Perspectives, 2018, 126, 057008.	2.8	52
60	Computationally-guided drug repurposing enables the discovery of kinase targets and inhibitors as new schistosomicidal agents. PLoS Computational Biology, 2018, 14, e1006515.	1.5	29
61	QSAR-Based Virtual Screening: Advances and Applications in Drug Discovery. Frontiers in Pharmacology, 2018, 9, 1275.	1.6	291
62	Chemistry-Wide Association Studies (CWAS): A Novel Framework for Identifying and Interpreting Structure-Activity Relationships. Journal of Chemical Information and Modeling, 2018, 58, 2203-2213.	2.5	7
63	Multi-Descriptor Read Across (MuDRA): A Simple and Transparent Approach for Developing Accurate Quantitative Structure-Activity Relationship Models. Journal of Chemical Information and Modeling, 2018, 58, 1214-1223.	2.5	43
64	QSAR-Driven Design and Discovery of Novel Compounds With Antiplasmodial and Transmission Blocking Activities. Frontiers in Pharmacology, 2018, 9, 146.	1.6	22
65	Predicting Adverse Drug Effects from Literature- and Database-Mined Assertions. Drug Safety, 2018, 41, 1059-1072.	1.4	3
66	Quantitative high-throughput phenotypic screening of pediatric cancer cell lines identifies multiple opportunities for drug repurposing. Oncotarget, 2018, 9, 4758-4772.	0.8	10
67	Chembench: A Publicly Accessible, Integrated Cheminformatics Portal. Journal of Chemical Information and Modeling, 2017, 57, 105-108.	2.5	47
68	Phantom PAINS: Problems with the Utility of Alerts for <i>P</i> -an- <i>A</i> ssay <i>I</i> nterference Compound <i>S</i> . Journal of Chemical Information and Modeling, 2017, 57, 417-427.	2.5	188
69	QSAR-driven design, synthesis and discovery of potent chalcone derivatives with antitubercular activity. European Journal of Medicinal Chemistry, 2017, 137, 126-138.	2.6	96
70	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.	2.5	79
71	Computer-aided discovery of two novel chalcone-like compounds active and selective against <i>Leishmania infantum</i> . Bioorganic and Medicinal Chemistry Letters, 2017, 27, 2459-2464.	1.0	23
72	Computer-Assisted Decision Support for Student Admissions Based on Their Predicted Academic Performance. American Journal of Pharmaceutical Education, 2017, 81, 46.	0.7	16

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73	Modernization of Enoxaparin Molecular Weight Determination Using Homogeneous Standards. <i>Pharmaceuticals</i> , 2017, 10, 66.	1.7	5
74	Chalcone Derivatives: Promising Starting Points for Drug Design. <i>Molecules</i> , 2017, 22, 1210.	1.7	261
75	Progress towards a public chemogenomic set for protein kinases and a call for contributions. <i>PLoS ONE</i> , 2017, 12, e0181585.	1.1	131
76	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. <i>Environmental Health Perspectives</i> , 2016, 124, 1023-1033.	2.8	264
77	Open drug discovery for the Zika virus. <i>F1000Research</i> , 2016, 5, 150.	0.8	50
78	Discovery of New Anti-Schistosomal Hits by Integration of QSAR-Based Virtual Screening and High Content Screening. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 7075-7088.	2.9	67
79	Modelling of compound combination effects and applications to efficacy and toxicity: state-of-the-art, challenges and perspectives. <i>Drug Discovery Today</i> , 2016, 21, 225-238.	3.2	162
80	Gelatin/carboxymethyl cellulose mucoadhesive films with lysozyme: Development and characterization. <i>Carbohydrate Polymers</i> , 2016, 147, 208-215.	5.1	45
81	Modern approaches to accelerate discovery of new antischistosomal drugs. <i>Expert Opinion on Drug Discovery</i> , 2016, 11, 557-567.	2.5	19
82	QSAR models of human data can enrich or replace LLNA testing for human skin sensitization. <i>Green Chemistry</i> , 2016, 18, 6501-6515.	4.6	42
83	Activity prediction and identification of misannotated chemical compounds using extreme descriptors. <i>Journal of Chemometrics</i> , 2016, 30, 99-108.	0.7	2
84	Trust, but Verify II: A Practical Guide to Chemogenomics Data Curation. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1243-1252.	2.5	228
85	QSAR-Driven Discovery of Novel Chemical Scaffolds Active against <i>Schistosoma mansoni</i> . <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1357-1372.	2.5	47
86	Alarms about structural alerts. <i>Green Chemistry</i> , 2016, 18, 4348-4360.	4.6	103
87	Computational assessment of environmental hazards of nitroaromatic compounds: influence of the type and position of aromatic ring substituents on toxicity. <i>Structural Chemistry</i> , 2016, 27, 191-198.	1.0	11
88	QSAR Modeling and Prediction of Drug-Drug Interactions. <i>Molecular Pharmaceutics</i> , 2016, 13, 545-556.	2.3	65
89	Comprehensive characterization of the Published Kinase Inhibitor Set. <i>Nature Biotechnology</i> , 2016, 34, 95-103.	9.4	289
90	PredChERG: A Novel web-Accessible Computational Tool for Predicting Cardiac Toxicity. <i>Molecular Informatics</i> , 2015, 34, 698-701.	1.4	159

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91	Predicting chemically-induced skin reactions. Part II: QSAR models of skin permeability and the relationships between skin permeability and skin sensitization. <i>Toxicology and Applied Pharmacology</i> , 2015, 284, 273-280.	1.3	53
92	Predicting chemically-induced skin reactions. Part I: QSAR models of skin sensitization and their application to identify potentially hazardous compounds. <i>Toxicology and Applied Pharmacology</i> , 2015, 284, 262-272.	1.3	72
93	Curation of chemogenomics data. <i>Nature Chemical Biology</i> , 2015, 11, 535-535.	3.9	158
94	Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints. <i>Chemistry of Materials</i> , 2015, 27, 735-743.	3.2	209
95	Modelability Criteria: Statistical Characteristics Estimating Feasibility to Build Predictive QSAR Models for a Dataset. , 2014, , 187-230.		11
96	Short Communication: Cheminformatics Analysis to Identify Predictors of Antiviral Drug Penetration into the Female Genital Tract. <i>AIDS Research and Human Retroviruses</i> , 2014, 30, 1058-1064.	0.5	14
97	QSAR Modeling: Where Have You Been? Where Are You Going To?. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 4977-5010.	2.9	1,401
98	Data Set Modelability by QSAR. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1-4.	2.5	105
99	Expanding the scope of drug repurposing in pediatrics: The Children's Pharmacy Collaborative. <i>Drug Discovery Today</i> , 2014, 19, 1696-1698.	3.2	22
100	Tuning hERG Out: Antitarget QSAR Models for Drug Development. <i>Current Topics in Medicinal Chemistry</i> , 2014, 14, 1399-1415.	1.0	82
101	Predicting Binding Affinity of CSAR Ligands Using Both Structure-Based and Ligand-Based Approaches. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 1915-1922.	2.5	20
102	QSAR analysis of poliovirus inhibition by dual combinations of antivirals. <i>Structural Chemistry</i> , 2013, 24, 1665-1679.	1.0	19
103	Universal Approach for Structural Interpretation of QSAR/QSPR Models. <i>Molecular Informatics</i> , 2013, 32, 843-853.	1.4	57
104	Does Rational Selection of Training and Test Sets Improve the Outcome of QSAR Modeling?. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 2570-2578.	2.5	232
105	New Advances in QSPR/QSAR Analysis of Nitrocompounds: Solubility, Lipophilicity, and Toxicity. , 2012, , 279-334.		2
106	Existing and Developing Approaches for QSAR Analysis of Mixtures. <i>Molecular Informatics</i> , 2012, 31, 202-221.	1.4	105
107	Predicting Drug-Induced Hepatotoxicity Using QSAR and Toxicogenomics Approaches. <i>Chemical Research in Toxicology</i> , 2011, 24, 1251-1262.	1.7	190
108	QSAR analysis of [(biphenyloxy)propyl]isoxazoles: agents against coxsackievirus B3. <i>Future Medicinal Chemistry</i> , 2011, 3, 15-27.	1.1	17

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109	Applicability Domains for Classification Problems: Benchmarking of Distance to Models for Ames Mutagenicity Set. Journal of Chemical Information and Modeling, 2010, 50, 2094-2111.	2.5	202
110	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.	1.4	37
111	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.	2.5	611
112	<i>Per aspera ad astra</i>: application of Simplex QSAR approach in antiviral research. Future Medicinal Chemistry, 2010, 2, 1205-1226.	1.1	58
113	New QSPR equations for prediction of aqueous solubility for military compounds. Chemosphere, 2010, 79, 887-890.	4.2	17
114	Virtual Screening and Molecular Design Based on Hierarchical Qsar Technology. Challenges and Advances in Computational Chemistry and Physics, 2010, , 127-176.	0.6	23
115	HiT QSAR Study of Antiviralsâ€™ Bioavailability. Antiviral Research, 2009, 82, A56.	1.9	3
116	Application of Quantum Chemical Approximations to Environmental Problems: Prediction of Water Solubility for Nitro Compounds. Environmental Science & Technology, 2009, 43, 9208-9215.	4.6	30
117	Application of Random Forest Approach to QSAR Prediction of Aquatic Toxicity. Journal of Chemical Information and Modeling, 2009, 49, 2481-2488.	2.5	147
118	The effects of characteristics of substituents on toxicity of the nitroaromatics: HiT QSAR study. Journal of Computer-Aided Molecular Design, 2008, 22, 747-759.	1.3	41
119	Quantitative Structure~Activity Relationship Studies of [(Biphenyloxy)propyl]isoxazole Derivatives. Inhibitors of Human Rhinovirus 2 Replication. Journal of Medicinal Chemistry, 2007, 50, 4205-4213.	2.9	73
120	Hierarchic system of QSAR models (1D~4D) on the base of simplex representation of molecular structure. Journal of Molecular Modeling, 2005, 11, 457-467.	0.8	88
121	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 /@verlock	0.7	10
122	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@verlock 10 Tf 50 2	0.7	10
123	Development of Web and Mobile Applications for Chemical Toxicity Prediction. Journal of the Brazilian Chemical Society, 0, , .	0.6	18
124	Automated Framework for Developing Predictive Machine Learning Models for Data-Driven Drug Discovery. Journal of the Brazilian Chemical Society, 0, , .	0.6	1
125	Secondary Metabolites Extracted from Annonaceae and Chemotaxonomy Study of Terpenoids. Journal of the Brazilian Chemical Society, 0, , .	0.6	2
126	QUIMIOINFORMÁTICA: UMA INTRODUÇÃO. Quimica Nova, 0, , .	0.3	7