Alexander Sedykh

List of Publications by Year
in descending order

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40 papers	2,332 citations	218677 26 h-index	315739 38 g-index
40 all docs	40 docs citations	40 times ranked	2752 citing authors

#	Article	IF	Citations
1	Quantitative Structureâ˜Activity Relationship Modeling of Rat Acute Toxicity by Oral Exposure. Chemical Research in Toxicology, 2009, 22, 1913-1921.	3.3	210
2	Predicting Drug-Induced Hepatotoxicity Using QSAR and Toxicogenomics Approaches. Chemical Research in Toxicology, 2011, 24, 1251-1262.	3.3	190
3	Big Data in Chemical Toxicity Research: The Use of High-Throughput Screening Assays To Identify Potential Toxicants. Chemical Research in Toxicology, 2014, 27, 1643-1651.	3.3	119
4	Toxicokinetic Triage for Environmental Chemicals. Toxicological Sciences, 2015, 147, 55-67.	3.1	117
5	Integrative Chemicalâ€“Biological Read-Across Approach for Chemical Hazard Classification. Chemical Research in Toxicology, 2013, 26, 1199-1208.	3.3	107
6	Use of in Vitro HTS-Derived Concentrationâ€“Response Data as Biological Descriptors Improves the Accuracy of QSAR Models of in Vivo Toxicity. Environmental Health Perspectives, 2011, 119, 364-370.	6.0	103
7	Alarms about structural alerts. Green Chemistry, 2016, 18, 4348-4360.	9.0	103
8	An updated review on drug-induced cholestasis: Mechanisms and investigation of physicochemical properties and pharmacokinetic parameters. Journal of Pharmaceutical Sciences, 2013, 102, 3037-3057.	3.3	95
9	Predicting Nanoâ€“Bio Interactions by Integrating Nanoparticle Libraries and Quantitative Nanostructure Activity Relationship Modeling. ACS Nano, 2017, 11, 12641-12649.	14.6	80
10	Identification of putative estrogen receptor-mediated endocrine disrupting chemicals using QSAR- and structure-based virtual screening approaches. Toxicology and Applied Pharmacology, 2013, 272, 67-76.	2.8	78
11	Discovery of Novel Antimalarial Compounds Enabled by QSAR-Based Virtual Screening. Journal of Chemical Information and Modeling, 2013, 53, 475-492.	5.4	77
12	Construction of a web-based nanomaterial database by big data curation and modeling friendly nanostructure annotations. Nature Communications, 2020, 11, 2519.	12.8	77
13	Human Intestinal Transporter Database: QSAR Modeling and Virtual Profiling of Drug Uptake, Efflux and Interactions. Pharmaceutical Research, 2013, 30, 996-1007.	3.5	76
14	Critical Evaluation of Human Oral Bioavailability for Pharmaceutical Drugs by Using Various Cheminformatics Approaches. Pharmaceutical Research, 2014, 31, 1002-1014.	3.5	76
15	A Data Analysis Pipeline Accounting for Artifacts in Tox21 Quantitative High-Throughput Screening Assays. Journal of Biomolecular Screening, 2015, 20, 887-897.	2.6	75
16	Developing Enhanced Bloodâ€“Brain Barrier Permeability Models: Integrating External Bio-Assay Data in QSAR Modeling. Pharmaceutical Research, 2015, 32, 3055-3065.	3.5	70
17	Predictive Modeling of Chemical Hazard by Integrating Numerical Descriptors of Chemical Structures and Short-term Toxicity Assay Data. Toxicological Sciences, 2012, 127, 1-9.	3.1	64
18	In silico profiling nanoparticles: predictive nanomodeling using universal nanodescriptors and various machine learning approaches. Nanoscale, 2019, 11, 8352-8362.	5.6	64

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19	Mechanism Profiling of Hepatotoxicity Caused by Oxidative Stress Using Antioxidant Response Element Reporter Gene Assay Models and Big Data. Environmental Health Perspectives, 2016, 124, 634-641.	6.0	56
20	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
21	Quantitative High-Throughput Screening for Chemical Toxicity in a Population-Based In Vitro Model. Toxicological Sciences, 2012, 126, 578-588.	3.1	47
22	Experimental Errors in QSAR Modeling Sets: What We Can Do and What We Cannot Do. ACS Omega, 2017, 2, 2805-2812.	3.5	47
23	The Use of Pseudo-Equilibrium Constant Affords Improved QSAR Models of Human Plasma Protein Binding. Pharmaceutical Research, 2013, 30, 1790-1798.	3.5	43
24	Predicting Chemical Ocular Toxicity Using a Combinatorial QSAR Approach. Chemical Research in Toxicology, 2012, 25, 2763-2769.	3.3	42
25	Hybrid in silico models for drugâ€induced liver injury using chemical descriptors and in vitro cellâ€imaging information. Journal of Applied Toxicology, 2014, 34, 281-288.	2.8	41
26	Real-time cell toxicity profiling of Tox21 10K compounds reveals cytotoxicity dependent toxicity pathway linkage. PLoS ONE, 2017, 12, e0177902.	2.5	40
27	Identifying Compounds with Genotoxicity Potential Using Tox21 High-Throughput Screening Assays. Chemical Research in Toxicology, 2019, 32, 1384-1401.	3.3	27
28	Design, synthesis and experimental validation of novel potential chemopreventive agents using random forest and support vector machine binary classifiers. Journal of Computer-Aided Molecular Design, 2014, 28, 631-646.	2.9	25
29	Analysis of model PM2.5-induced inflammation and cytotoxicity by the combination of a virtual carbon nanoparticle library and computational modeling. Ecotoxicology and Environmental Safety, 2020, 191, 110216.	6.0	20
30	Application of Benchmark Concentration (BMC) Analysis on Zebrafish Data: A New Perspective for Quantifying Toxicity in Alternative Animal Models. Toxicological Sciences, 2019, 167, 92-104.	3.1	19
31	Using Tox21 High-Throughput Screening Assays for the Evaluation of Botanical and Dietary Supplements. Applied in Vitro Toxicology, 2019, 5, 10-25.	1.1	15
32	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
33	Universal nanohydrophobicity predictions using virtual nanoparticle library. Journal of Cheminformatics, 2019, 11, 6.	6.1	14
34	Integrative Approaches for Predicting In Vivo Effects of Chemicals from their Structural Descriptors and the Results of Short-Term Biological Assays. Current Topics in Medicinal Chemistry, 2014, 14, 1356-1364.	2.1	14
35	Modelability Criteria: Statistical Characteristics Estimating Feasibility to Build Predictive QSAR Models for a Dataset. , 2014, , 187-230.		11
36	Harnessing In Silico, In Vitro, and In Vivo Data to Understand the Toxicity Landscape of Polycyclic Aromatic Compounds (PACs). Chemical Research in Toxicology, 2021, 34, 268-285.	3.3	9

#	Article	IF	Citations
37	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
38	CurveP Method for Rendering High-Throughput Screening Dose-Response Data into Digital Fingerprints. Methods in Molecular Biology, 2016, 1473, 135-141.	0.9	5
39	Predicting Adverse Drug Effects from Literature- and Database-Mined Assertions. Drug Safety, 2018, 41, 1059-1072.	3.2	3
40	CurveP Method for Rendering High-Throughput Screening Doseâ€“Response Data into Digital Fingerprints. Methods in Molecular Biology, 2022, 2474, 147-154.	0.9	0