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	CurveP Method for Rendering High-Throughput Screening Doseâ€“Response Data into Digital Fingerprints. Methods in Molecular Biology, 2022, 2474, 147-154.	0.9	0
2	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
3	Construction of a web-based nanomaterial database by big data curation and modeling friendly nanostructure annotations. Nature Communications, 2020, 11, 2519.	12.8	77
4	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
5	Universal nanohydrophobicity predictions using virtual nanoparticle library. Journal of Cheminformatics, 2019, 11, 6.	6.1	14
6	Identifying Compounds with Genotoxicity Potential Using Tox21 High-Throughput Screening Assays. Chemical Research in Toxicology, 2019, 32, 1384-1401.	3.3	27
7	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
8	In silico profiling nanoparticles: predictive nanomodeling using universal nanodescriptors and various machine learning approaches. Nanoscale, 2019, 11, 8352-8362.	5.6	64
9	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
10	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
11	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
12	Predicting Adverse Drug Effects from Literature- and Database-Mined Assertions. Drug Safety, 2018, 41, 1059-1072.	3.2	3
13	Experimental Errors in QSAR Modeling Sets: What We Can Do and What We Cannot Do. ACS Omega, 2017, 2, 2805-2812.	3.5	47
14	Predicting Nanoâ€“Bio Interactions by Integrating Nanoparticle Libraries and Quantitative Nanostructure Activity Relationship Modeling. ACS Nano, 2017, 11, 12641-12649.	14.6	80
15	Real-time cell toxicity profiling of Tox21 10K compounds reveals cytotoxicity dependent toxicity pathway linkage. PLoS ONE, 2017, 12, e0177902.	2.5	40
16	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
17	CurveP Method for Rendering High-Throughput Screening Dose-Response Data into Digital Fingerprints. Methods in Molecular Biology, 2016, 1473, 135-141.	0.9	5
18	Alarms about structural alerts. Green Chemistry, 2016, 18, 4348-4360.	9.0	103

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19	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
20	Toxicokinetic Triage for Environmental Chemicals. Toxicological Sciences, 2015, 147, 55-67.	3.1	117
21	Developing Enhanced Bloodâ€“Brain Barrier Permeability Models: Integrating External Bio-Assay Data in QSAR Modeling. Pharmaceutical Research, 2015, 32, 3055-3065.	3.5	70
22	Modelability Criteria: Statistical Characteristics Estimating Feasibility to Build Predictive QSAR Models for a Dataset. , 2014, , 187-230.		11
23	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
24	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
25	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
26	Critical Evaluation of Human Oral Bioavailability for Pharmaceutical Drugs by Using Various Cheminformatics Approaches. Pharmaceutical Research, 2014, 31, 1002-1014.	3.5	76
27	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
28	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
29	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
30	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
31	Human Intestinal Transporter Database: QSAR Modeling and Virtual Profiling of Drug Uptake, Efflux and Interactions. Pharmaceutical Research, 2013, 30, 996-1007.	3.5	76
32	Integrative Chemicalâ€“Biological Read-Across Approach for Chemical Hazard Classification. Chemical Research in Toxicology, 2013, 26, 1199-1208.	3.3	107
33	Discovery of Novel Antimalarial Compounds Enabled by QSAR-Based Virtual Screening. Journal of Chemical Information and Modeling, 2013, 53, 475-492.	5.4	77
34	The Use of Pseudo-Equilibrium Constant Affords Improved QSAR Models of Human Plasma Protein Binding. Pharmaceutical Research, 2013, 30, 1790-1798.	3.5	43
35	Quantitative High-Throughput Screening for Chemical Toxicity in a Population-Based In Vitro Model. Toxicological Sciences, 2012, 126, 578-588.	3.1	47
36	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

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37	Predicting Chemical Ocular Toxicity Using a Combinatorial QSAR Approach. Chemical Research in Toxicology, 2012, 25, 2763-2769.	3.3	42
38	Predicting Drug-Induced Hepatotoxicity Using QSAR and Toxicogenomics Approaches. Chemical Research in Toxicology, 2011, 24, 1251-1262.	3.3	190
39	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
40	Quantitative Structureâ^'Activity Relationship Modeling of Rat Acute Toxicity by Oral Exposure. Chemical Research in Toxicology, 2009, 22, 1913-1921.	3.3	210