Ovanes G Mekenyan

List of Publications by Year in descending order

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56 papers	1,798 citations	279798 23 h-index	265206 42 g-index
57 all docs	57 docs citations	57 times ranked	1244 citing authors

#	Article	IF	Citations
1	Estimating the reliability of simulated metabolism using documented data and theoretical knowledge. QSAR application. Computational Toxicology, 2022, , 100218.	3.3	0
2	Assessment of uncertainty and credibility of predictions by the OECD QSAR Toolbox automated read-across workflow for predicting acute oral toxicity. Computational Toxicology, 2022, 22, 100219.	3.3	2
3	Assessing metabolic similarity for read-across predictions. Computational Toxicology, 2021, 18, 100160.	3.3	6
4	Criteria for quantitative assessment of metabolic similarity between chemicals. II. Application to human health endpoints. Computational Toxicology, 2021, 19, 100173.	3.3	6
5	Selection of Representative Constituents for Unknown, Variable, Complex, or Biological Origin Substance Assessment Based on Hierarchical Clustering. Environmental Toxicology and Chemistry, 2021, 40, 3205-3218.	4.3	3
6	Automated read-across workflow for predicting acute oral toxicity: I. The decision scheme in the QSAR toolbox. Regulatory Toxicology and Pharmacology, 2021, 125, 105015.	2.7	14
7	The QSAR Toolbox automated read-across workflow for predicting acute oral toxicity: II. Verification and validation. Computational Toxicology, 2021, 20, 100194.	3.3	11
8	Modeling hazard assessment of chemicals based on adducts formation. I. A basis for inclusion of kinetic factors in simulating skin sensitization. Computational Toxicology, 2020, 15, 100130.	3.3	3
9	Using metabolic information for categorization and read-across in the OECD QSAR Toolbox. Computational Toxicology, 2019, 12, 100102.	3.3	11
10	Automated and standardized workflows in the OECD QSAR Toolbox. Computational Toxicology, 2019, 10, 89-104.	3.3	25
11	UVCB substances II: Development of an endpointâ€nonspecific procedure for selection of computationally generated representative constituents. Environmental Toxicology and Chemistry, 2019, 38, 682-694.	4.3	9
12	Mechanistic relationship between biodegradation and bioaccumulation. Practical outcomes. Regulatory Toxicology and Pharmacology, 2019, 107, 104411.	2.7	4
13	Sabcho Dimitrov (1952â€“2018) â€“ A dedication. Computational Toxicology, 2019, 11, 90.	3.3	0
14	Category consistency in the OECD QSAR Toolbox: Assessment and reporting tool to justify read-across. Computational Toxicology, 2019, 11, 65-71.	3.3	9
15	The implementation of RAAF in the OECD QSAR Toolbox. Regulatory Toxicology and Pharmacology, 2019, 105, 51-61.	2.7	22
16	Validation of the performance of TIMES genotoxicity models with EFSA pesticide data. Mutagenesis, 2019, 34, 83-90.	2.6	0
17	Alert performance: A new functionality in the OECD QSAR Toolbox. Computational Toxicology, 2019, 10, 26-37.	3.3	10
18	Procedure for toxicological predictions based on mechanistic weight of evidences: Application to Ames mutagenicity. Computational Toxicology, 2019, 12, 100009.	3.3	2

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19	The OECD QSAR Toolbox Starts Its Second Decade. Methods in Molecular Biology, 2018, 1800, 55-77.	0.9	69
20	The Adverse Outcome Pathway for Skin Sensitisation: Moving Closer to Replacing Animal Testing. ATLA Alternatives To Laboratory Animals, 2016, 44, 453-460.	1.0	16
21	Integrated approach to testing and assessment for predicting rodent genotoxic carcinogenicity. Journal of Applied Toxicology, 2016, 36, 1536-1550.	2.8	13
22	UVCB substances: Methodology for structural description and application to fate and hazard assessment. Environmental Toxicology and Chemistry, 2015, 34, 2450-2462.	4.3	20
23	A feasibility study: Can information collected to classify for mutagenicity be informative in predicting carcinogenicity?. Regulatory Toxicology and Pharmacology, 2015, 72, 17-25.	2.7	18
24	Towards AOP application â€“ Implementation of an integrated approach to testing and assessment (IATA) into a pipeline tool for skin sensitization. Regulatory Toxicology and Pharmacology, 2014, 69, 529-545.	2.7	89
25	A Mechanistic Approach to Modeling Respiratory Sensitization. Chemical Research in Toxicology, 2014, 27, 219-239.	3.3	33
26	Accessing and Using Chemical Databases. Methods in Molecular Biology, 2013, 930, 29-52.	0.9	0
27	Investigating the Relationship between in Vitroâ€“in Vivo Genotoxicity: Derivation of Mechanistic QSAR Models for in Vivo Liver Genotoxicity and in Vivo Bone Marrow Micronucleus Formation Which Encompass Metabolism. Chemical Research in Toxicology, 2012, 25, 277-296.	3.3	23
28	MetaPath: An electronic knowledge base for collating, exchanging and analyzing case studies of xenobiotic metabolism. Regulatory Toxicology and Pharmacology, 2012, 63, 84-96.	2.7	25
29	Use of Genotoxicity Information in the Development of Integrated Testing Strategies (ITS) for Skin Sensitization. Chemical Research in Toxicology, 2010, 23, 1519-1540.	3.3	22
30	Conformational Coverage by a Genetic Algorithm:â€‰ Saturation of Conformational Space. Journal of Chemical Information and Modeling, 2007, 47, 851-863.	5.4	26
31	Identifying the Structural Requirements for Chromosomal Aberration by Incorporating Molecular Flexibility and Metabolic Activation of Chemicals. Chemical Research in Toxicology, 2007, 20, 1927-1941.	3.3	31
32	Representation of Chemical Information in OASIS Centralized 3D Database for Existing Chemicals. Journal of Chemical Information and Modeling, 2006, 46, 2537-2551.	5.4	15
33	A Stepwise Approach for Defining the Applicability Domain of SAR and QSAR Models. Journal of Chemical Information and Modeling, 2005, 45, 839-849.	5.4	243
34	Skin Sensitization: Modeling Based on Skin Metabolism Simulation and Formation of Protein Conjugates. International Journal of Toxicology, 2005, 24, 189-204.	1.2	79
35	2D-3D Migration of Large Chemical Inventories with Conformational Multiplication. Application of the Genetic Algorithm. Journal of Chemical Information and Modeling, 2005, 45, 283-292.	5.4	20
36	A Systematic Approach to Simulating Metabolism in Computational Toxicology. I. The TIMES Heuristic Modelling Framework. Current Pharmaceutical Design, 2004, 10, 1273-1293.	1.9	109

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37	COREPA-M: A Multi-Dimensional Formulation of COREPA. QSAR and Combinatorial Science, 2004, 23, 5-18.	1.4	24
38	Identification of the Structural Requirements for Mutagenicity by Incorporating Molecular Flexibility and Metabolic Activation of Chemicals I:Â TA100 Model. Chemical Research in Toxicology, 2004, 17, 753-766.	3.3	52
39	Rule interpreter: a chemical language for structure-based screening. Computational and Theoretical Chemistry, 2003, 622, 53-62.	1.5	7
40	Dynamic 3D QSAR techniques: applications in toxicology. Computational and Theoretical Chemistry, 2003, 622, 147-165.	1.5	29
41	Dynamic QSAR Techniques: Applications in Drug Design and Toxicology. Current Pharmaceutical Design, 2002, 8, 1605-1621.	1.9	22
42	ESTROGENICITY OF ALKYLPHENOLIC COMPOUNDS: A 3-D STRUCTUREâ€“ACTIVITY EVALUATION OF GENE ACTIVATION. Environmental Toxicology and Chemistry, 2000, 19, 1727.	4.3	23
43	New developments in a hazard identification algorithm for hormone receptor ligands. QSAR and Combinatorial Science, 1999, 18, 139-153.	1.2	40
44	Conformational Coverage by a Genetic Algorithm. Journal of Chemical Information and Computer Sciences, 1999, 39, 997-1016.	2.8	35
45	The role of ligand flexibility in predicting biological activity: Structureâ€“activity relationships for aryl hydrocarbon, estrogen, and androgen receptor binding affinity. Environmental Toxicology and Chemistry, 1998, 17, 15-25.	4.3	27
46	A Kinetic Analysis of the Conformational Flexibility of Steroid Hormones. QSAR and Combinatorial Science, 1998, 17, 437-449.	1.2	5
47	A Kinetic Analysis of the Conformational Flexibility of Steroid Hormones. QSAR and Combinatorial Science, 1998, 17, 437-449.	1.2	18
48	THE ROLE OF LIGAND FLEXIBILITY IN PREDICTING BIOLOGICAL ACTIVITY: STRUCTUREâ€“ACTIVITY RELATIONSHIPS FOR ARYL HYDROCARBON, ESTROGEN, AND ANDROGEN RECEPTOR BINDING AFFINITY. Environmental Toxicology and Chemistry, 1998, 17, 15.	4.3	14
49	A Computationally-Based Hazard Identification Algorithm That Incorporates Ligand Flexibility. 1. Identification of Potential Androgen Receptor Ligands. Environmental Science & Technology, 1997, 31, 3702-3711.	10.0	67
50	â€˜Dynamicâ€™ QSAR For Semicarbazide-induced Mortality in Frog Embryos. , 1996, 16, 355-363.		22
51	Quantum-chemical Descriptors for Estimating the Acute Toxicity of Electrophiles to the Fathed minnow (Pimephales promelas): An Analysis Based on Molecular Mechanisms. QSAR and Combinatorial Science, 1996, 15, 302-310.	1.2	77
52	Quantum-chemical Descriptors for Estimating the Acute Toxicity of Substituted Benzenes to the Guppy (Poecilia reticulata) and Fathead Minnow (Pimephales promelas). QSAR and Combinatorial Science, 1996, 15, 311-320.	1.2	52
53	QSAR Evaluation of .alpha.-Terthienyl Phototoxicity. Environmental Science & Technology, 1995, 29, 1267-1272.	10.0	33
54	A new development of the oasis computer system for modeling molecular properties. Computers & Chemistry, 1994, 18, 173-187.	1.2	48

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55	A QSAR Approach for Estimating the Aquatic Toxicity of Soft Electrophiles [QSAR for Soft Electrophiles]. QSAR and Combinatorial Science, 1993, 12, 349-356.	1.2	90
56	The microcomputer OASIS system for predicting the biological activity of chemical compounds. Computers & Chemistry, 1990, 14, 193-200.	1.2	49