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	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
2	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
3	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
4	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
5	Skin Sensitization: Modeling Based on Skin Metabolism Simulation and Formation of Protein Conjugates. International Journal of Toxicology, 2005, 24, 189-204.	1.2	79
6	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
7	The OECD QSAR Toolbox Starts Its Second Decade. Methods in Molecular Biology, 2018, 1800, 55-77.	0.9	69
8	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
9	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
10	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
11	The microcomputer OASIS system for predicting the biological activity of chemical compounds. Computers & Chemistry, 1990, 14, 193-200.	1.2	49
12	A new development of the oasis computer system for modeling molecular properties. Computers & Chemistry, 1994, 18, 173-187.	1.2	48
13	New developments in a hazard identification algorithm for hormone receptor ligands. QSAR and Combinatorial Science, 1999, 18, 139-153.	1.2	40
14	Conformational Coverage by a Genetic Algorithm. Journal of Chemical Information and Computer Sciences, 1999, 39, 997-1016.	2.8	35
15	QSAR Evaluation of .alpha.-Terthienyl Phototoxicity. Environmental Science & Technology, 1995, 29, 1267-1272.	10.0	33
16	A Mechanistic Approach to Modeling Respiratory Sensitization. Chemical Research in Toxicology, 2014, 27, 219-239.	3.3	33
17	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
18	Dynamic 3D QSAR techniques: applications in toxicology. Computational and Theoretical Chemistry, 2003, 622, 147-165.	1.5	29

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19	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
20	Conformational Coverage by a Genetic Algorithm:â€‰ Saturation of Conformational Space. Journal of Chemical Information and Modeling, 2007, 47, 851-863.	5.4	26
21	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
22	Automated and standardized workflows in the OECD QSAR Toolbox. Computational Toxicology, 2019, 10, 89-104.	3.3	25
23	COREPA-M: A Multi-Dimensional Formulation of COREPA. QSAR and Combinatorial Science, 2004, 23, 5-18.	1.4	24
24	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
25	ESTROGENICITY OF ALKYLPHENOLIC COMPOUNDS: A 3-D STRUCTUREâ€“ACTIVITY EVALUATION OF GENE ACTIVATION. Environmental Toxicology and Chemistry, 2000, 19, 1727.	4.3	23
26	â€˜Dynamicâ€™ QSAR For Semicarbazide-induced Mortality in Frog Embryos. , 1996, 16, 355-363.		22
27	Dynamic QSAR Techniques: Applications in Drug Design and Toxicology. Current Pharmaceutical Design, 2002, 8, 1605-1621.	1.9	22
28	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
29	The implementation of RAAF in the OECD QSAR Toolbox. Regulatory Toxicology and Pharmacology, 2019, 105, 51-61.	2.7	22
30	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
31	UVCB substances: Methodology for structural description and application to fate and hazard assessment. Environmental Toxicology and Chemistry, 2015, 34, 2450-2462.	4.3	20
32	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
33	A Kinetic Analysis of the Conformational Flexibility of Steroid Hormones. QSAR and Combinatorial Science, 1998, 17, 437-449.	1.2	18
34	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
35	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
36	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

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37	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
38	Integrated approach to testing and assessment for predicting rodent genotoxic carcinogenicity. Journal of Applied Toxicology, 2016, 36, 1536-1550.	2.8	13
39	Using metabolic information for categorization and read-across in the OECD QSAR Toolbox. Computational Toxicology, 2019, 12, 100102.	3.3	11
40	The QSAR Toolbox automated read-across workflow for predicting acute oral toxicity: II. Verification and validation. Computational Toxicology, 2021, 20, 100194.	3.3	11
41	Alert performance: A new functionality in the OECD QSAR Toolbox. Computational Toxicology, 2019, 10, 26-37.	3.3	10
42	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
43	Category consistency in the OECD QSAR Toolbox: Assessment and reporting tool to justify read-across. Computational Toxicology, 2019, 11, 65-71.	3.3	9
44	Rule interpreter: a chemical language for structure-based screening. Computational and Theoretical Chemistry, 2003, 622, 53-62.	1.5	7
45	Assessing metabolic similarity for read-across predictions. Computational Toxicology, 2021, 18, 100160.	3.3	6
46	Criteria for quantitative assessment of metabolic similarity between chemicals. II. Application to human health endpoints. Computational Toxicology, 2021, 19, 100173.	3.3	6
47	A Kinetic Analysis of the Conformational Flexibility of Steroid Hormones. QSAR and Combinatorial Science, 1998, 17, 437-449.	1.2	5
48	Mechanistic relationship between biodegradation and bioaccumulation. Practical outcomes. Regulatory Toxicology and Pharmacology, 2019, 107, 104411.	2.7	4
49	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
50	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
51	Procedure for toxicological predictions based on mechanistic weight of evidences: Application to Ames mutagenicity. Computational Toxicology, 2019, 12, 100009.	3.3	2
52	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
53	Accessing and Using Chemical Databases. Methods in Molecular Biology, 2013, 930, 29-52.	0.9	0
54	Sabcho Dimitrov (1952â€“2018) â€“ A dedication. Computational Toxicology, 2019, 11, 90.	3.3	0

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55	Validation of the performance of TIMES genotoxicity models with EFSA pesticide data. Mutagenesis, 2019, 34, 83-90.	2.6	0
56	Estimating the reliability of simulated metabolism using documented data and theoretical knowledge. QSAR application. Computational Toxicology, 2022, , 100218.	3.3	0